



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:11 PM GMT

PDB ID : 3SDI  
Title : Structure of yeast 20S open-gate proteasome with Compound 20  
Authors : Sintchak, M.D.  
Deposited on : 2011-06-09  
Resolution : 2.65 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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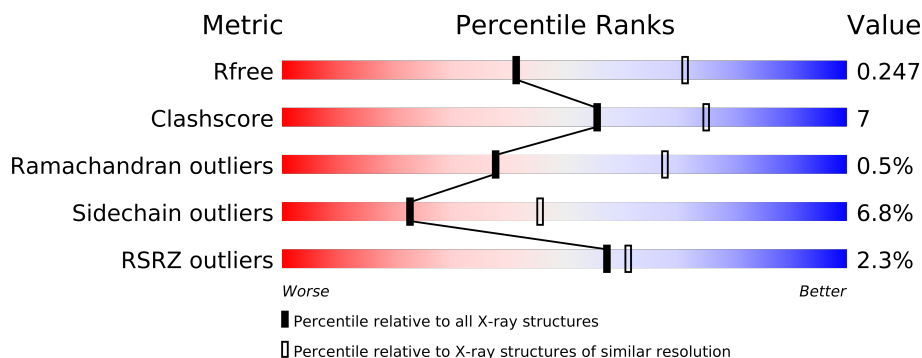
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.65 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.












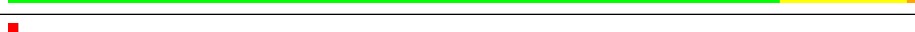

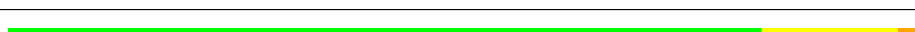

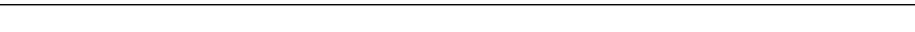
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 2232 (2.70-2.62)                                      |
| Clashscore            | 79885                       | 2700 (2.70-2.62)                                      |
| Ramachandran outliers | 78287                       | 2657 (2.70-2.62)                                      |
| Sidechain outliers    | 78261                       | 2657 (2.70-2.62)                                      |
| RSRZ outliers         | 66119                       | 2234 (2.70-2.62)                                      |

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 250    |                  |
| 1   | O     | 250    |                  |
| 2   | B     | 235    |                  |
| 2   | P     | 235    |                  |
| 3   | C     | 241    |                  |
| 3   | Q     | 241    |                  |
| 4   | D     | 260    |                  |
| 4   | R     | 260    |                  |
| 5   | E     | 233    |                  |
| 5   | S     | 233    |                  |
| 6   | F     | 242    |                  |
| 6   | T     | 242    |                  |
| 7   | G     | 243    |                  |
| 7   | U     | 243    |                  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | H     | 222    |  |
| 8   | V     | 222    |  |
| 9   | I     | 204    |  |
| 9   | W     | 204    |  |
| 10  | J     | 198    |  |
| 10  | X     | 198    |  |
| 11  | K     | 212    |  |
| 11  | Y     | 212    |  |
| 12  | L     | 222    |  |
| 12  | Z     | 222    |  |
| 13  | 1     | 233    |  |
| 13  | M     | 233    |  |
| 14  | 2     | 196    |  |
| 14  | N     | 196    |  |

## 2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49012 atoms, of which 0 are hydrogen and 0 are deuterium.

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 component Y7.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | A     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1881  | 1200 | 308 | 370 | 3 |         |         |       |
| 1   | O     | 246      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1881  | 1200 | 308 | 370 | 3 |         |         |       |

- Molecule 2 is a protein called Proteasome component Y13.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | B     | 235      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1827  | 1157 | 303 | 364 | 3 |         |         |       |
| 2   | P     | 235      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1827  | 1157 | 303 | 364 | 3 |         |         |       |

- Molecule 3 is a protein called Proteasome component PRE6.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | C     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1861  | 1163 | 325 | 369 | 4 |         |         |       |
| 3   | Q     | 238      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1861  | 1163 | 325 | 369 | 4 |         |         |       |

- Molecule 4 is a protein called Proteasome component PUP2.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4   | D     | 228      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1747  | 1094 | 291 | 355 | 7 |         |         |       |
| 4   | R     | 229      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1752  | 1097 | 292 | 356 | 7 |         |         |       |

- Molecule 5 is a protein called Proteasome component PRE5.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | E     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1103 | 304 | 344 | 4 |         |         |       |
| 5   | S     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1755  | 1103 | 304 | 344 | 4 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| E     | 127     | ALA      | TYR    | CONFLICT | UNP P40302 |
| S     | 127     | ALA      | TYR    | CONFLICT | UNP P40302 |

- Molecule 6 is a protein called Proteasome component C1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6   | F     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1886  | 1199 | 328 | 355 | 4 |         |         |       |
| 6   | T     | 242      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1886  | 1199 | 328 | 355 | 4 |         |         |       |

- Molecule 7 is a protein called Proteasome component C7-alpha.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7   | G     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1897  | 1206 | 319 | 364 | 8 |         |         |       |
| 7   | U     | 240      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1897  | 1206 | 319 | 364 | 8 |         |         |       |

- Molecule 8 is a protein called Proteasome component PUP1.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8   | H     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1685  | 1061 | 293 | 324 | 7 |         |         |       |
| 8   | V     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1685  | 1061 | 293 | 324 | 7 |         |         |       |

- Molecule 9 is a protein called Proteasome component PUP3.

| 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 component C11.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10  | J     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1582  | 1003 | 269 | 305 | 5 |         |         |       |
| 10  | X     | 198      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1582  | 1003 | 269 | 305 | 5 |         |         |       |

- Molecule 11 is a protein called Proteasome component PRE2.

| 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 component C5.

| 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 component PRE4.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13  | M     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |
| 13  | 1     | 233      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1824  | 1154 | 312 | 351 | 7 |         |         |       |

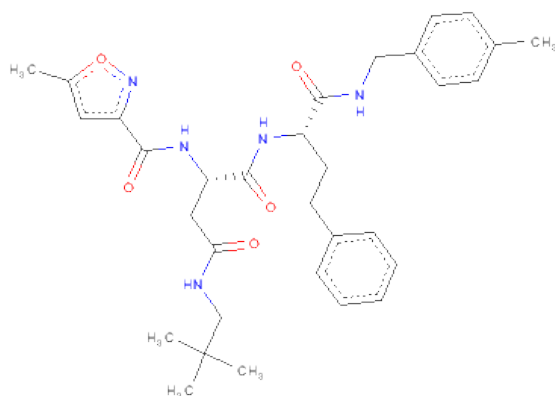
- Molecule 14 is a protein called Proteasome component PRE3.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14  | N     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |         |       |
| 14  | 2     | 196      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1512  | 955 | 250 | 300 | 7 |         |         |       |

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

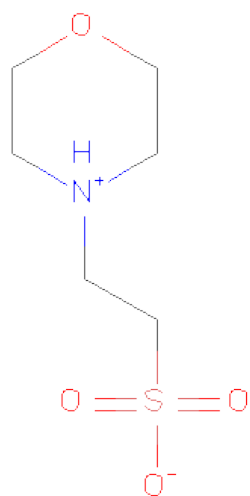
| Mol | Chain | Residues | Atoms        | ZeroOcc | AltConf |
|-----|-------|----------|--------------|---------|---------|
| 15  | G     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | K     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | H     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | I     | 2        | Total 2 Mg 2 | 0       | 0       |
| 15  | V     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | W     | 2        | Total 2 Mg 2 | 0       | 0       |
| 15  | Z     | 2        | Total 2 Mg 2 | 0       | 0       |
| 15  | T     | 2        | Total 2 Mg 2 | 0       | 0       |
| 15  | N     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | U     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | 2     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | Y     | 1        | Total 1 Mg 1 | 0       | 0       |
| 15  | L     | 2        | Total 2 Mg 2 | 0       | 0       |
| 15  | F     | 2        | Total 2 Mg 2 | 0       | 0       |

- Molecule 16 is N 4 -(2,2-DIMETHYLPROPYL)-N 1 -{(2S)-1-[(4-METHYLBENZYL)AMINO]-1-OXO-4-PHENYLBUTAN-2-YL}-N 2 -[(5-METHYL-1,2-OXAZOL-3-YL)CARBONYL]-L-ASPARTAMIDE (three-letter code: 3SD) (formula: C<sub>32</sub>H<sub>41</sub>N<sub>5</sub>O<sub>5</sub>).



| Mol | Chain | Residues | Atoms |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 16  | K     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 32 | 5 | 5 |         |         |
| 16  | Y     | 1        | Total | C  | N | O | 0       | 0       |
|     |       |          | 42    | 32 | 5 | 5 |         |         |

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 17  | K     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 17  | Y     | 1        | Total | C | N | O | S | 0       | 0       |
|     |       |          | 12    | 6 | 1 | 4 | 1 |         |         |

- Molecule 18 is water.

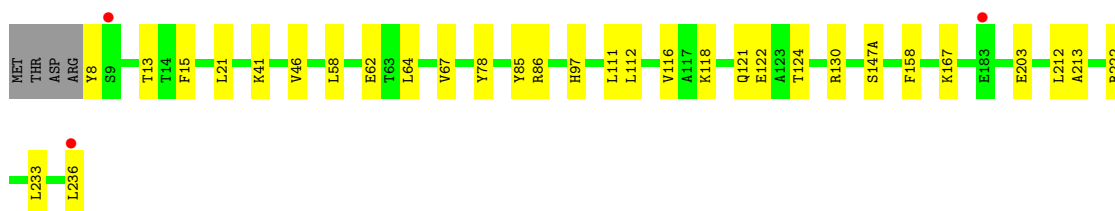
| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 18  | L     | 1        | Total | O | 0       | 0       |
|     |       |          | 1     | 1 |         |         |

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 component Y7

Chain A: 



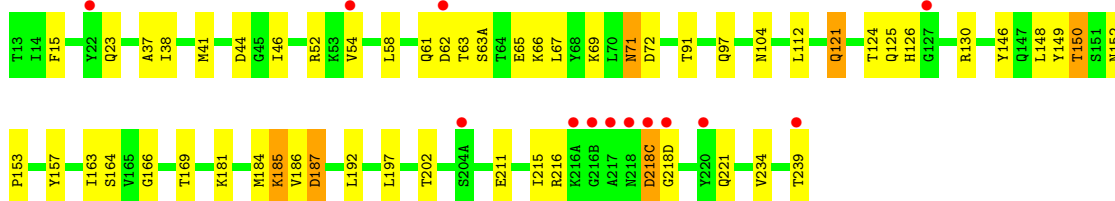
- Molecule 1: Proteasome component Y7

Chain O: 



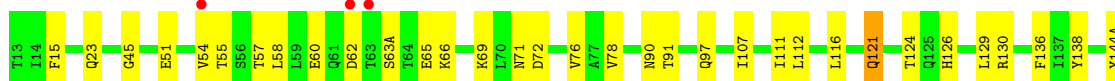
- Molecule 2: Proteasome component Y13

Chain B: 



- Molecule 2: Proteasome component Y13

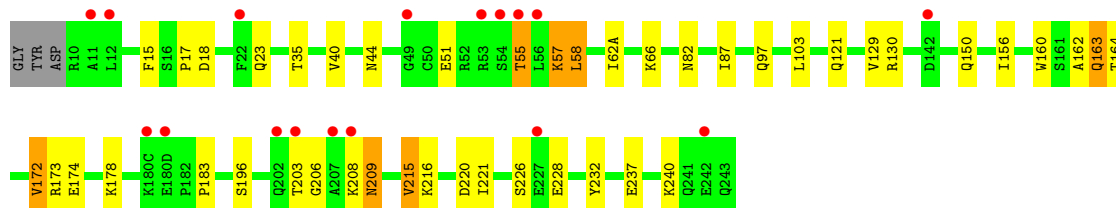
Chain P: 





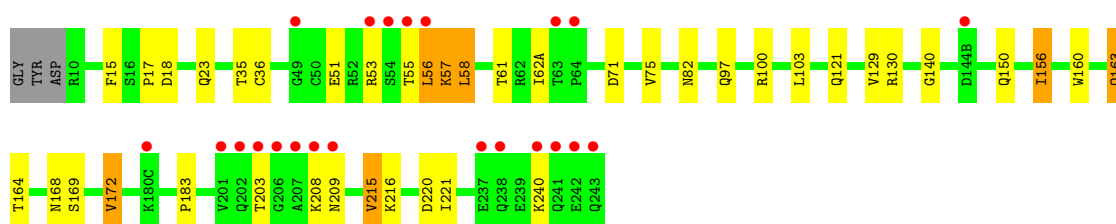
• Molecule 3: Proteasome component PRE6

Chain C:



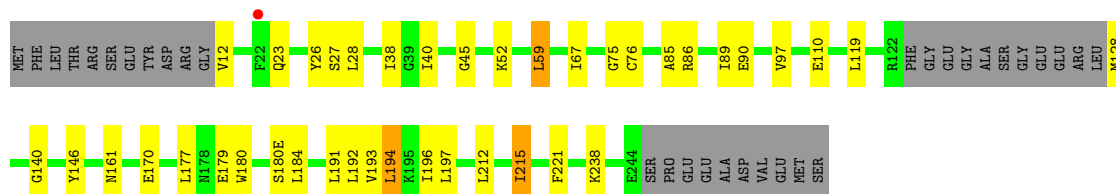
• Molecule 3: Proteasome component PRE6

Chain Q:



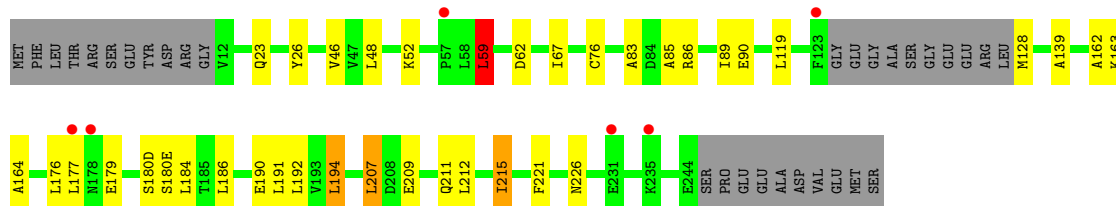
• Molecule 4: Proteasome component PUP2

Chain D:



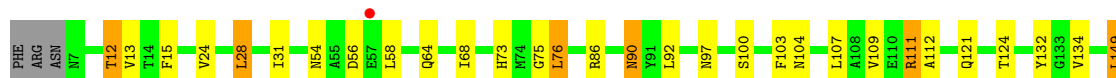
• Molecule 4: Proteasome component PUP2

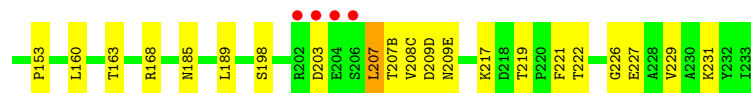
Chain R:



• Molecule 5: Proteasome component PRE5

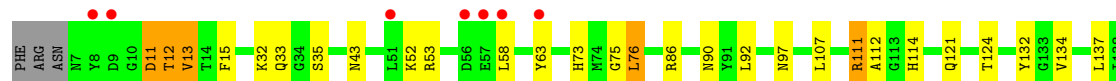
Chain E:





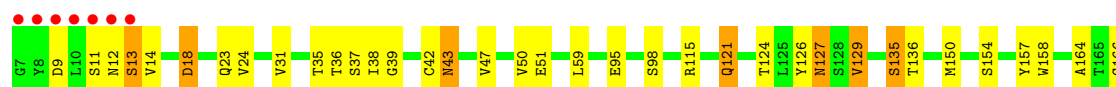
• Molecule 5: Proteasome component PRE5

Chain S:



• Molecule 6: Proteasome component C1

Chain F:



• Molecule 6: Proteasome component C1

Chain T:



• Molecule 7: Proteasome component C7-alpha

Chain G:



• Molecule 7: Proteasome component C7-alpha

Chain U:





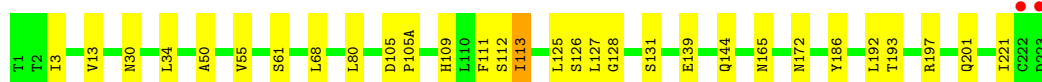
- Molecule 8: Proteasome component PUP1

Chain H:



- Molecule 8: Proteasome component PUP1

Chain V:



- Molecule 9: Proteasome component PUP3

Chain I:



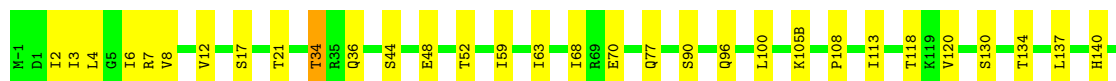
- Molecule 9: Proteasome component PUP3

Chain W:



- Molecule 10: Proteasome component C11

Chain J:



- Molecule 10: Proteasome component C11

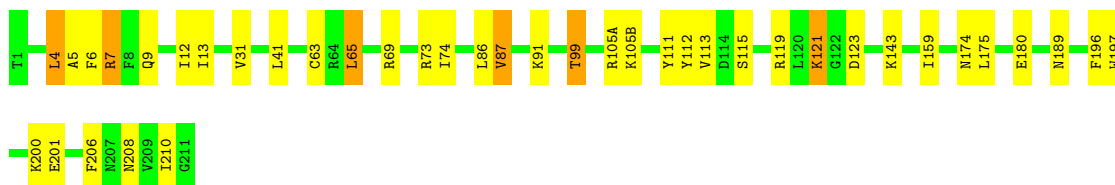
Chain X:



- Molecule 11: Proteasome component PRE2



Chain K: 



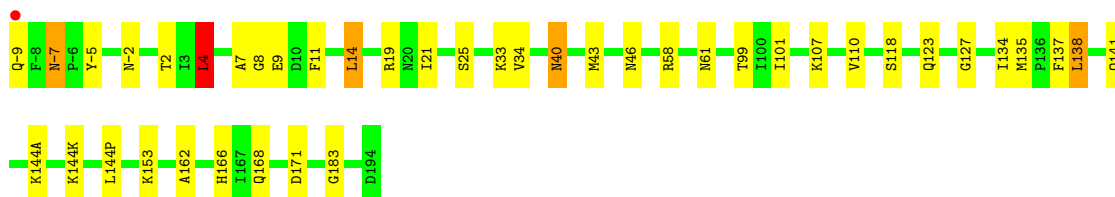
- Molecule 11: Proteasome component PRE2

Chain Y: 



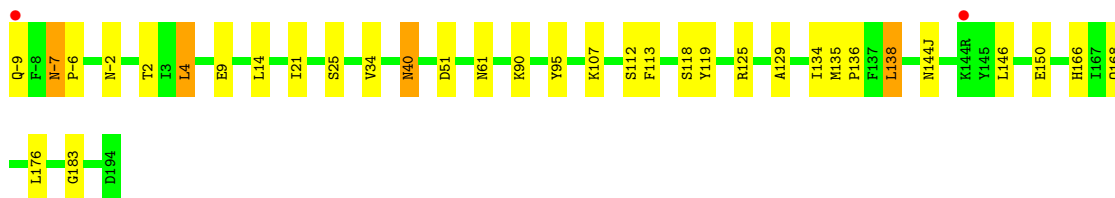
- Molecule 12: Proteasome component C5

Chain L: 



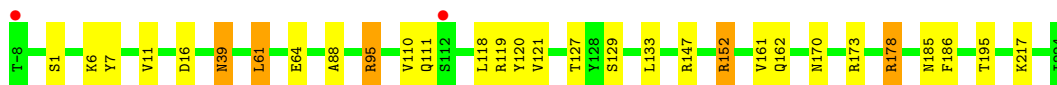
- Molecule 12: Proteasome component C5

Chain Z: 



- Molecule 13: Proteasome component PRE4

Chain M: 



- Molecule 13: Proteasome component PRE4

Chain 1: 





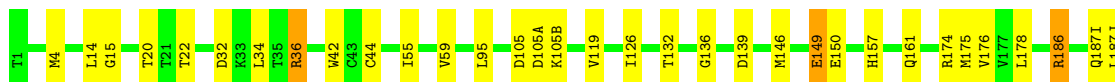
- Molecule 14: Proteasome component PRE3

Chain N:



- Molecule 14: Proteasome component PRE3

Chain 2:



## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 136.60Å 299.45Å 145.48Å<br>90.00° 113.17° 90.00°            | Depositor        |
| Resolution (Å)  | 30.00 – 2.65<br>29.95 – 2.65                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.4 (30.00-2.65)<br>95.5 (29.95-2.65)                      | Depositor<br>EDS |
| $R_{merge}$   | 0.10  | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.44 (at 2.64Å)   | Xtriage          |
| Refinement program  | REFMAC 5.5.0110   | Depositor        |
| R, $R_{free}$   | 0.219 , 0.253<br>0.215 , 0.247                              | Depositor<br>DCC |
| $R_{free}$ test set   | 5996 reflections (2.06%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 49.8  | Xtriage          |
| Anisotropy  | 0.120   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.32 , 14.7   | EDS              |
| Estimated twinning fraction   | No twinning to report.                                      | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$ | Xtriage          |
| Outliers  | 0 of 296914 reflections                                     | Xtriage          |
| $F_o, F_c$ correlation  | 0.93  | EDS              |
| Total number of atoms   | 49012   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 47.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3SD, MG, MES

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

| Mol | Chain | Bond lengths |                | Bond angles |                 |
|-----|-------|--------------|----------------|-------------|-----------------|
|     |       | RMSZ         | # Z  >5        | RMSZ        | # Z  >5         |
| 1   | A     | 0.50         | 0/1918         | 0.60        | 0/2597          |
| 1   | O     | 0.49         | 0/1918         | 0.59        | 0/2597          |
| 2   | B     | 0.46         | 0/1856         | 0.61        | 0/2513          |
| 2   | P     | 0.48         | 0/1856         | 0.61        | 0/2513          |
| 3   | C     | 0.46         | 0/1889         | 0.59        | 1/2557 (0.0%)   |
| 3   | Q     | 0.47         | 0/1889         | 0.61        | 2/2557 (0.1%)   |
| 4   | D     | 0.51         | 0/1770         | 0.66        | 1/2387 (0.0%)   |
| 4   | R     | 0.47         | 0/1775         | 0.63        | 2/2394 (0.1%)   |
| 5   | E     | 0.49         | 0/1781         | 0.61        | 0/2407          |
| 5   | S     | 0.47         | 0/1781         | 0.60        | 0/2407          |
| 6   | F     | 0.50         | 0/1926         | 0.59        | 0/2599          |
| 6   | T     | 0.54         | 1/1926 (0.1%)  | 0.63        | 0/2599          |
| 7   | G     | 0.52         | 0/1934         | 0.60        | 0/2618          |
| 7   | U     | 0.52         | 0/1934         | 0.62        | 0/2618          |
| 8   | H     | 0.51         | 0/1716         | 0.64        | 0/2326          |
| 8   | V     | 0.49         | 0/1716         | 0.61        | 0/2326          |
| 9   | I     | 0.58         | 0/1611         | 0.63        | 0/2174          |
| 9   | W     | 0.64         | 1/1611 (0.1%)  | 0.63        | 0/2174          |
| 10  | J     | 0.52         | 0/1610         | 0.66        | 0/2170          |
| 10  | X     | 0.54         | 0/1610         | 0.68        | 2/2170 (0.1%)   |
| 11  | K     | 0.51         | 0/1681         | 0.65        | 0/2274          |
| 11  | Y     | 0.49         | 0/1681         | 0.63        | 0/2274          |
| 12  | L     | 0.56         | 0/1795         | 0.63        | 1/2420 (0.0%)   |
| 12  | Z     | 0.56         | 0/1795         | 0.62        | 1/2420 (0.0%)   |
| 13  | 1     | 0.60         | 0/1855         | 0.76        | 1/2514 (0.0%)   |
| 13  | M     | 0.63         | 0/1855         | 0.70        | 1/2514 (0.0%)   |
| 14  | 2     | 0.59         | 0/1541         | 0.63        | 0/2087          |
| 14  | N     | 0.62         | 0/1541         | 0.61        | 0/2087          |
| All | All   | 0.53         | 2/49771 (0.0%) | 0.63        | 12/67293 (0.0%) |

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

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 13  | 1     | 0                   | 1                   |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 9   | W     | 38  | TYR  | CD1-CE1 | -5.17 | 1.31        | 1.39     |
| 6   | T     | 7   | GLY  | N-CA    | 5.01  | 1.53        | 1.46     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 13  | 1     | 74  | ALA  | O-C-N     | -16.84 | 95.75       | 122.70   |
| 4   | D     | 128 | MET  | N-CA-C    | -7.50  | 90.76       | 111.00   |
| 10  | X     | -1  | MET  | O-C-N     | -6.45  | 112.38      | 122.70   |
| 10  | X     | -1  | MET  | C-N-CA    | 6.29   | 137.43      | 121.70   |
| 4   | R     | 59  | LEU  | CA-CB-CG  | 6.21   | 129.59      | 115.30   |
| 3   | Q     | 56  | LEU  | CA-CB-CG  | 5.68   | 128.37      | 115.30   |
| 3   | Q     | 103 | LEU  | CA-CB-CG  | 5.57   | 128.12      | 115.30   |
| 12  | Z     | 4   | LEU  | CA-CB-CG  | 5.53   | 128.01      | 115.30   |
| 4   | R     | 128 | MET  | N-CA-C    | -5.25  | 96.82       | 111.00   |
| 12  | L     | 4   | LEU  | CA-CB-CG  | 5.16   | 127.17      | 115.30   |
| 13  | M     | 95  | ARG  | NE-CZ-NH1 | 5.16   | 122.88      | 120.30   |
| 3   | C     | 103 | LEU  | CA-CB-CG  | 5.12   | 127.09      | 115.30   |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group     |
|-----|-------|-----|------|-----------|
| 13  | 1     | 74  | ALA  | Mainchain |

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1881  | 0        | 1893     | 24      | 0            |
| 1   | O     | 1881  | 0        | 1893     | 26      | 0            |
| 2   | B     | 1827  | 0        | 1824     | 36      | 0            |
| 2   | P     | 1827  | 0        | 1824     | 39      | 0            |
| 3   | C     | 1861  | 0        | 1873     | 31      | 0            |
| 3   | Q     | 1861  | 0        | 1873     | 25      | 0            |
| 4   | D     | 1747  | 0        | 1718     | 22      | 0            |
| 4   | R     | 1752  | 0        | 1720     | 18      | 0            |
| 5   | E     | 1755  | 0        | 1761     | 27      | 0            |
| 5   | S     | 1755  | 0        | 1761     | 34      | 0            |
| 6   | F     | 1886  | 0        | 1876     | 36      | 0            |
| 6   | T     | 1886  | 0        | 1875     | 50      | 0            |
| 7   | G     | 1897  | 0        | 1891     | 44      | 0            |
| 7   | U     | 1897  | 0        | 1891     | 42      | 0            |
| 8   | H     | 1685  | 0        | 1688     | 15      | 0            |
| 8   | V     | 1685  | 0        | 1688     | 22      | 0            |
| 9   | I     | 1581  | 0        | 1574     | 15      | 0            |
| 9   | W     | 1581  | 0        | 1574     | 24      | 0            |
| 10  | J     | 1582  | 0        | 1583     | 17      | 0            |
| 10  | X     | 1582  | 0        | 1582     | 24      | 0            |
| 11  | K     | 1644  | 0        | 1595     | 24      | 0            |
| 11  | Y     | 1644  | 0        | 1595     | 21      | 0            |
| 12  | L     | 1757  | 0        | 1711     | 23      | 0            |
| 12  | Z     | 1757  | 0        | 1711     | 24      | 0            |
| 13  | 1     | 1824  | 0        | 1832     | 35      | 0            |
| 13  | M     | 1824  | 0        | 1832     | 20      | 0            |
| 14  | 2     | 1512  | 0        | 1481     | 21      | 0            |
| 14  | N     | 1512  | 0        | 1481     | 17      | 0            |
| 15  | 2     | 1     | 0        | 0        | 0       | 0            |
| 15  | F     | 2     | 0        | 0        | 0       | 0            |
| 15  | G     | 1     | 0        | 0        | 0       | 0            |
| 15  | H     | 1     | 0        | 0        | 0       | 0            |
| 15  | I     | 2     | 0        | 0        | 0       | 0            |
| 15  | K     | 1     | 0        | 0        | 0       | 0            |
| 15  | L     | 2     | 0        | 0        | 0       | 0            |
| 15  | N     | 1     | 0        | 0        | 0       | 0            |
| 15  | T     | 2     | 0        | 0        | 0       | 0            |
| 15  | U     | 1     | 0        | 0        | 0       | 0            |
| 15  | V     | 1     | 0        | 0        | 0       | 0            |
| 15  | W     | 2     | 0        | 0        | 0       | 0            |
| 15  | Y     | 1     | 0        | 0        | 0       | 0            |
| 15  | Z     | 2     | 0        | 0        | 0       | 0            |
| 16  | K     | 42    | 0        | 41       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 16  | Y     | 42    | 0        | 41       | 2       | 0            |
| 17  | K     | 12    | 0        | 13       | 1       | 0            |
| 17  | Y     | 12    | 0        | 13       | 0       | 0            |
| 18  | L     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 49012 | 0        | 48708    | 641     | 0            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (641) close contacts within the same asymmetric unit are listed below.

| Atom-1             | Atom-2              | Distance(Å) | Clash(Å) |
|--------------------|---------------------|-------------|----------|
| 14:N:161:GLN:HE21  | 14:2:136:GLY:HA2    | 1.17        | 1.09     |
| 7:G:96:ALA:HA      | 7:G:107:MET:HE2     | 1.31        | 1.06     |
| 7:U:96:ALA:HA      | 7:U:107:MET:HE2     | 1.36        | 1.04     |
| 3:C:163:GLN:NE2    | 3:C:164:THR:H       | 1.59        | 1.00     |
| 1:A:130:ARG:HH21   | 7:G:124:THR:CG2     | 1.76        | 0.97     |
| 3:C:163:GLN:HE21   | 3:C:164:THR:N       | 1.60        | 0.97     |
| 5:S:207:LEU:HA     | 5:S:209(E):ASN:HD22 | 1.27        | 0.96     |
| 1:A:130:ARG:HH21   | 7:G:124:THR:HG22    | 1.31        | 0.96     |
| 3:C:57:LYS:HD2     | 3:C:58:LEU:H        | 1.31        | 0.95     |
| 11:Y:174:ASN:HD21  | 11:Y:189:ASN:HD22   | 1.14        | 0.95     |
| 13:1:152:ARG:HH11  | 13:1:152:ARG:HG3    | 1.34        | 0.92     |
| 1:O:130:ARG:HH21   | 7:U:124:THR:HG22    | 1.35        | 0.91     |
| 5:S:52:LYS:HB2     | 5:S:63:TYR:HB3      | 1.54        | 0.89     |
| 3:C:15:PHE:H       | 4:D:23:GLN:HE22     | 1.15        | 0.89     |
| 1:O:130:ARG:HH21   | 7:U:124:THR:CG2     | 1.87        | 0.87     |
| 12:L:4:LEU:HD13    | 12:L:138:LEU:HD21   | 1.55        | 0.87     |
| 14:N:136:GLY:HA2   | 14:2:161:GLN:HE21   | 1.40        | 0.86     |
| 1:O:86:ARG:HE      | 7:U:118:ASN:HD21    | 1.24        | 0.85     |
| 6:T:170:GLN:CD     | 6:T:170:GLN:H       | 1.80        | 0.84     |
| 6:F:35:THR:HG21    | 6:F:51:GLU:O        | 1.77        | 0.84     |
| 13:1:69:ASN:ND2    | 13:1:72:ALA:HA      | 1.91        | 0.84     |
| 1:A:86:ARG:HE      | 7:G:118:ASN:HD21    | 1.22        | 0.84     |
| 6:F:95:GLU:HG2     | 6:F:115:ARG:HB3     | 1.60        | 0.83     |
| 11:Y:174:ASN:ND2   | 11:Y:189:ASN:HD22   | 1.76        | 0.83     |
| 8:V:80:LEU:HD12    | 8:V:113:ILE:HD11    | 1.61        | 0.82     |
| 7:G:184(G):GLU:HG2 | 7:G:188:LYS:HB3     | 1.61        | 0.82     |
| 12:Z:166:HIS:HD2   | 12:Z:168:GLN:H      | 1.27        | 0.81     |
| 14:N:161:GLN:NE2   | 14:2:136:GLY:HA2    | 1.94        | 0.81     |
| 11:K:174:ASN:HD21  | 11:K:189:ASN:HD22   | 1.29        | 0.81     |
| 3:C:163:GLN:HE21   | 3:C:164:THR:H       | 0.83        | 0.81     |
| 5:S:97:ASN:HD21    | 12:Z:61:ASN:HD21    | 1.26        | 0.80     |

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| Atom-1             | Atom-2               | Distance(Å) | Clash(Å) |
|--------------------|----------------------|-------------|----------|
| 5:E:97:ASN:HD21    | 12:L:61:ASN:HD21     | 1.29        | 0.80     |
| 3:Q:163:GLN:HE21   | 3:Q:164:THR:H        | 1.27        | 0.79     |
| 2:B:181:LYS:O      | 2:B:184:MET:HG3      | 1.83        | 0.79     |
| 14:2:157:HIS:HD2   | 14:2:187(J):LEU:HD13 | 1.47        | 0.79     |
| 5:E:15:PHE:H       | 6:F:23:GLN:HE22      | 1.32        | 0.77     |
| 7:G:184(G):GLU:HG2 | 7:G:188:LYS:CB       | 2.14        | 0.77     |
| 7:U:121:GLN:O      | 7:U:124:THR:HB       | 1.86        | 0.76     |
| 2:P:124:THR:HG22   | 3:Q:130:ARG:HH21     | 1.50        | 0.75     |
| 6:T:187:ARG:CG     | 6:T:187:ARG:HH11     | 1.99        | 0.75     |
| 7:U:96:ALA:HA      | 7:U:107:MET:CE       | 2.16        | 0.75     |
| 2:B:97:GLN:HE22    | 9:I:64:ASN:HD22      | 1.34        | 0.75     |
| 11:Y:143:LYS:HB2   | 11:Y:146:LEU:HD13    | 1.68        | 0.75     |
| 1:O:15:PHE:H       | 2:P:23:GLN:HE22      | 1.33        | 0.74     |
| 1:A:86:ARG:HE      | 7:G:118:ASN:ND2      | 1.85        | 0.74     |
| 12:L:40:ASN:HD21   | 12:L:183:GLY:HA2     | 1.51        | 0.73     |
| 1:O:124:THR:CG2    | 2:P:130:ARG:HH21     | 2.01        | 0.73     |
| 1:A:124:THR:HG22   | 2:B:130:ARG:HH21     | 1.53        | 0.73     |
| 6:T:95:GLU:HG2     | 6:T:115:ARG:HB3      | 1.69        | 0.72     |
| 3:C:57:LYS:HD2     | 3:C:58:LEU:N         | 2.03        | 0.72     |
| 12:L:33:LYS:HE3    | 12:L:46:ASN:ND2      | 2.04        | 0.72     |
| 4:D:97:VAL:HG21    | 11:K:65:LEU:HD13     | 1.70        | 0.72     |
| 3:Q:15:PHE:H       | 4:R:23:GLN:HE22      | 1.36        | 0.72     |
| 2:B:126:HIS:HB3    | 3:C:129:VAL:HG12     | 1.71        | 0.72     |
| 2:B:124:THR:HG22   | 3:C:130:ARG:HH21     | 1.52        | 0.72     |
| 14:2:157:HIS:CD2   | 14:2:187(J):LEU:HD13 | 2.25        | 0.72     |
| 2:P:121:GLN:O      | 2:P:124:THR:HB       | 1.90        | 0.72     |
| 1:A:15:PHE:H       | 2:B:23:GLN:HE22      | 1.35        | 0.72     |
| 11:K:4:LEU:CD1     | 11:K:159:ILE:HD11    | 2.20        | 0.72     |
| 7:G:170:GLN:HE21   | 7:G:174:THR:HG23     | 1.54        | 0.71     |
| 13:M:170:ASN:HD22  | 13:M:173:ARG:HH11    | 1.36        | 0.71     |
| 3:C:57:LYS:O       | 3:C:58:LEU:HB2       | 1.91        | 0.71     |
| 6:F:36:THR:HG22    | 6:F:51:GLU:OE2       | 1.90        | 0.71     |
| 1:O:124:THR:HG22   | 2:P:130:ARG:HH21     | 1.54        | 0.71     |
| 4:D:179:GLU:HB3    | 4:D:192:LEU:HD21     | 1.70        | 0.71     |
| 4:D:215:ILE:HG22   | 4:D:221:PHE:HD2      | 1.54        | 0.71     |
| 1:O:86:ARG:HH21    | 7:U:118:ASN:HD22     | 1.39        | 0.71     |
| 7:U:184(G):GLU:HG2 | 7:U:188:LYS:HB2      | 1.72        | 0.70     |
| 12:L:14:LEU:HD13   | 12:L:34:VAL:HG13     | 1.73        | 0.70     |
| 5:E:207:LEU:HA     | 5:E:209(E):ASN:HD22  | 1.56        | 0.70     |
| 3:C:163:GLN:HE22   | 3:C:173:ARG:HE       | 1.39        | 0.70     |
| 8:H:128:GLY:O      | 8:H:131:SER:HB2      | 1.91        | 0.70     |
| 7:G:96:ALA:HA      | 7:G:107:MET:CE       | 2.14        | 0.69     |

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| Atom-1            | Atom-2               | Distance(Å) | Clash(Å) |
|-------------------|----------------------|-------------|----------|
| 2:P:97:GLN:HE22   | 9:W:64:ASN:HD22      | 1.38        | 0.69     |
| 12:Z:4:LEU:HD13   | 12:Z:138:LEU:HD21    | 1.74        | 0.69     |
| 2:B:71:ASN:HD22   | 2:B:72:ASP:H         | 1.41        | 0.69     |
| 2:B:38:ILE:HD12   | 2:B:197:LEU:HG       | 1.75        | 0.69     |
| 14:N:136:GLY:HA2  | 14:2:161:GLN:NE2     | 2.08        | 0.68     |
| 2:B:121:GLN:O     | 2:B:124:THR:HB       | 1.93        | 0.68     |
| 13:M:152:ARG:HH11 | 13:M:152:ARG:HG3     | 1.57        | 0.68     |
| 2:P:124:THR:CG2   | 3:Q:130:ARG:HH21     | 2.07        | 0.68     |
| 2:P:51:GLU:OE2    | 2:P:202:THR:HG23     | 1.94        | 0.68     |
| 2:B:71:ASN:ND2    | 2:B:72:ASP:H         | 1.90        | 0.68     |
| 13:M:170:ASN:HD22 | 13:M:173:ARG:NH1     | 1.91        | 0.67     |
| 6:T:192:GLN:HE21  | 6:T:195:LYS:CE       | 2.06        | 0.67     |
| 6:F:12:ASN:HD21   | 6:F:124:THR:HA       | 1.58        | 0.67     |
| 5:S:15:PHE:H      | 6:T:23:GLN:HE22      | 1.40        | 0.67     |
| 2:B:71:ASN:ND2    | 2:B:72:ASP:N         | 2.41        | 0.67     |
| 11:K:208:ASN:O    | 9:W:29:ASN:ND2       | 2.27        | 0.67     |
| 6:F:95:GLU:HG3    | 6:F:115:ARG:HH11     | 1.59        | 0.67     |
| 13:1:0:THR:HG23   | 13:1:1:SER:N         | 2.11        | 0.66     |
| 2:B:65:GLU:HG3    | 2:B:66:LYS:HG3       | 1.78        | 0.65     |
| 1:A:130:ARG:NH2   | 7:G:124:THR:HG22     | 2.07        | 0.65     |
| 1:O:130:ARG:NH2   | 7:U:124:THR:HG22     | 2.11        | 0.65     |
| 14:N:157:HIS:HD2  | 14:N:187(J):LEU:HD13 | 1.61        | 0.65     |
| 14:N:55:ILE:HD11  | 14:N:95:LEU:HD13     | 1.77        | 0.65     |
| 11:K:4:LEU:HD13   | 11:K:159:ILE:HD11    | 1.77        | 0.65     |
| 2:B:67:LEU:HD22   | 2:B:211:GLU:HB3      | 1.77        | 0.65     |
| 12:L:4:LEU:CD1    | 12:L:138:LEU:HD21    | 2.26        | 0.64     |
| 5:S:35:SER:HB2    | 5:S:53:ARG:HB2       | 1.78        | 0.64     |
| 13:1:152:ARG:HH11 | 13:1:152:ARG:CG      | 2.10        | 0.64     |
| 2:B:124:THR:CG2   | 3:C:130:ARG:HH21     | 2.11        | 0.64     |
| 6:T:35:THR:HG21   | 6:T:51:GLU:O         | 1.98        | 0.64     |
| 13:M:147:ARG:HH11 | 8:V:165:ASN:HD22     | 1.46        | 0.64     |
| 6:T:31:VAL:HG11   | 6:T:135:SER:HB2      | 1.78        | 0.63     |
| 3:Q:163:GLN:NE2   | 3:Q:164:THR:H        | 1.95        | 0.63     |
| 7:G:49:ILE:CD1    | 7:G:193:ALA:HB1      | 2.28        | 0.63     |
| 5:S:97:ASN:HD21   | 12:Z:61:ASN:ND2      | 1.94        | 0.63     |
| 1:O:121:GLN:O     | 1:O:124:THR:HB       | 1.98        | 0.63     |
| 7:G:49:ILE:CD1    | 7:G:193:ALA:CB       | 2.77        | 0.63     |
| 10:X:32:ASP:OD2   | 10:X:34:THR:HG22     | 1.98        | 0.63     |
| 8:V:197:ARG:HH21  | 9:W:139:GLU:HG3      | 1.63        | 0.63     |
| 1:O:86:ARG:HH21   | 7:U:118:ASN:ND2      | 1.95        | 0.62     |
| 6:F:169:ARG:HG3   | 6:F:173:LYS:HE3      | 1.81        | 0.62     |
| 4:D:40:ILE:HD12   | 4:D:193:VAL:HG23     | 1.80        | 0.62     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 12:L:134:ILE:HD11  | 12:L:162:ALA:HB2   | 1.82        | 0.62     |
| 12:Z:34:VAL:HG12   | 12:Z:176:LEU:HD22  | 1.81        | 0.62     |
| 2:P:69:LYS:HG3     | 2:P:221:GLN:OE1    | 2.00        | 0.62     |
| 1:O:86:ARG:HE      | 7:U:118:ASN:ND2    | 1.96        | 0.61     |
| 7:U:67:ILE:HD12    | 7:U:211:GLU:HG2    | 1.81        | 0.61     |
| 6:T:192:GLN:HE21   | 6:T:195:LYS:HE2    | 1.65        | 0.61     |
| 6:T:166:GLY:O      | 6:T:169:ARG:HB3    | 2.01        | 0.61     |
| 7:U:184(G):GLU:HG2 | 7:U:188:LYS:CB     | 2.30        | 0.61     |
| 10:J:143:ARG:O     | 10:J:146:MET:HG3   | 2.00        | 0.61     |
| 5:S:73:HIS:HE1     | 5:S:107:LEU:O      | 1.83        | 0.61     |
| 12:L:43:MET:HG3    | 12:L:101:ILE:HG22  | 1.82        | 0.61     |
| 2:P:97:GLN:HE21    | 9:W:61:TYR:HA      | 1.66        | 0.61     |
| 14:2:176:VAL:HG12  | 14:2:178:LEU:HD13  | 1.82        | 0.61     |
| 9:I:29:ASN:ND2     | 11:Y:208:ASN:O     | 2.34        | 0.60     |
| 7:G:77:VAL:CG1     | 7:G:137:THR:HB     | 2.30        | 0.60     |
| 5:E:24:VAL:O       | 5:E:28:LEU:HD12    | 2.01        | 0.60     |
| 2:P:65:GLU:HG3     | 2:P:66:LYS:HG3     | 1.84        | 0.60     |
| 14:2:55:ILE:HD11   | 14:2:95:LEU:HD13   | 1.82        | 0.60     |
| 6:T:187:ARG:HG2    | 6:T:187:ARG:HH11   | 1.66        | 0.60     |
| 4:D:140:GLY:HA2    | 4:D:215:ILE:HG12   | 1.81        | 0.60     |
| 7:G:77:VAL:HG12    | 7:G:137:THR:HB     | 1.84        | 0.60     |
| 1:A:97:HIS:HD2     | 8:H:61:SER:OG      | 1.84        | 0.60     |
| 6:T:169:ARG:HG3    | 6:T:173:LYS:HE3    | 1.84        | 0.60     |
| 5:S:207:LEU:HA     | 5:S:209(E):ASN:ND2 | 2.09        | 0.59     |
| 3:C:216:LYS:HB2    | 3:C:220:ASP:HB3    | 1.84        | 0.59     |
| 14:N:14:LEU:HD11   | 14:N:102:ALA:HB3   | 1.84        | 0.59     |
| 7:G:121:GLN:O      | 7:G:124:THR:HB     | 2.02        | 0.59     |
| 7:G:79:ASN:OD1     | 7:G:165:THR:HB     | 2.02        | 0.59     |
| 13:1:170:ASN:HD22  | 13:1:173:ARG:HH11  | 1.49        | 0.59     |
| 6:T:42:CYS:HB2     | 6:T:184:LEU:O      | 2.03        | 0.59     |
| 10:J:21:THR:HG21   | 10:X:167:PRO:HB3   | 1.85        | 0.59     |
| 11:K:111:TYR:CZ    | 11:K:121:LYS:HG3   | 2.37        | 0.59     |
| 5:E:227:GLU:CD     | 5:E:227:GLU:H      | 2.06        | 0.59     |
| 2:P:202:THR:HG22   | 2:P:204:SER:H      | 1.68        | 0.59     |
| 9:I:165:ARG:NH2    | 12:Z:135:MET:CE    | 2.66        | 0.59     |
| 3:Q:55:THR:HG22    | 3:Q:56:LEU:HD22    | 1.84        | 0.58     |
| 2:P:169:THR:O      | 2:P:173:GLN:HB2    | 2.03        | 0.58     |
| 5:E:132:TYR:O      | 5:E:153:PRO:HB3    | 2.04        | 0.58     |
| 10:X:6:ILE:HD11    | 10:X:142:TYR:CE1   | 2.39        | 0.58     |
| 5:S:114:HIS:HB3    | 6:T:86:ARG:NH2     | 2.18        | 0.58     |
| 13:1:69:ASN:HB3    | 13:1:72:ALA:HB2    | 1.84        | 0.58     |
| 6:T:95:GLU:HG3     | 6:T:115:ARG:HH11   | 1.67        | 0.58     |

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| Atom-1           | Atom-2               | Distance(Å) | Clash(Å) |
|------------------|----------------------|-------------|----------|
| 6:F:37:SER:HB3   | 6:F:50:VAL:HG23      | 1.86        | 0.58     |
| 6:F:13:SER:HB2   | 7:G:130:ARG:HB3      | 1.86        | 0.58     |
| 5:S:132:TYR:O    | 5:S:153:PRO:HB3      | 2.04        | 0.57     |
| 6:F:36:THR:HB    | 6:F:168:GLY:H        | 1.69        | 0.57     |
| 2:B:97:GLN:NE2   | 9:I:64:ASN:HD22      | 2.01        | 0.57     |
| 7:G:87:ASN:C     | 7:G:87:ASN:HD22      | 2.08        | 0.57     |
| 13:1:69:ASN:ND2  | 13:1:72:ALA:CA       | 2.66        | 0.57     |
| 3:C:206:GLY:HA3  | 3:C:209:ASN:CB       | 2.34        | 0.57     |
| 5:E:73:HIS:HE1   | 5:E:107:LEU:O        | 1.87        | 0.57     |
| 4:D:12:VAL:HA    | 4:D:23:GLN:HG3       | 1.87        | 0.57     |
| 6:F:95:GLU:CG    | 6:F:115:ARG:HD2      | 2.34        | 0.57     |
| 4:R:162:ALA:HB1  | 4:R:176:LEU:HD22     | 1.87        | 0.57     |
| 6:T:13:SER:HB2   | 7:U:130:ARG:HB3      | 1.86        | 0.57     |
| 12:L:135:MET:CE  | 9:W:165:ARG:NH2      | 2.67        | 0.57     |
| 5:E:12:THR:HG21  | 5:E:124:THR:HA       | 1.85        | 0.57     |
| 1:A:130:ARG:NH2  | 7:G:124:THR:CG2      | 2.59        | 0.57     |
| 5:E:109:VAL:HG12 | 5:E:149:LEU:HD22     | 1.87        | 0.56     |
| 3:C:160:TRP:CZ2  | 4:D:59:LEU:HD23      | 2.39        | 0.56     |
| 3:C:206:GLY:HA3  | 3:C:209:ASN:HB3      | 1.86        | 0.56     |
| 6:T:9:ASP:HB2    | 6:T:26:TYR:HE2       | 1.70        | 0.56     |
| 2:B:185:LYS:HD3  | 2:B:186:VAL:N        | 2.19        | 0.56     |
| 10:X:48:GLU:HB3  | 10:X:96:GLN:HB2      | 1.87        | 0.56     |
| 5:S:143:LYS:HE3  | 13:1:82:TYR:OH       | 2.06        | 0.56     |
| 1:A:124:THR:CG2  | 2:B:130:ARG:HH21     | 2.18        | 0.56     |
| 6:T:35:THR:CG2   | 6:T:51:GLU:O         | 2.53        | 0.56     |
| 2:B:15:PHE:H     | 3:C:23:GLN:HE22      | 1.51        | 0.56     |
| 5:E:86:ARG:O     | 5:E:90:ASN:HB2       | 2.06        | 0.56     |
| 6:T:192:GLN:HE21 | 6:T:195:LYS:HE3      | 1.70        | 0.56     |
| 13:M:170:ASN:ND2 | 13:M:173:ARG:HH11    | 2.04        | 0.56     |
| 4:D:215:ILE:HG22 | 4:D:221:PHE:CD2      | 2.40        | 0.56     |
| 12:Z:-2:ASN:HA   | 12:Z:21:ILE:O        | 2.05        | 0.56     |
| 7:U:87:ASN:C     | 7:U:87:ASN:HD22      | 2.08        | 0.56     |
| 3:Q:160:TRP:CZ2  | 4:R:59:LEU:HD23      | 2.41        | 0.56     |
| 14:N:157:HIS:CD2 | 14:N:187(J):LEU:HD13 | 2.41        | 0.56     |
| 5:S:209(B):THR:H | 5:S:209(E):ASN:HB2   | 1.71        | 0.55     |
| 8:H:172:ASN:HD22 | 8:H:193:THR:HA       | 1.71        | 0.55     |
| 6:T:170:GLN:N    | 6:T:170:GLN:CD       | 2.54        | 0.55     |
| 6:T:12:ASN:O     | 6:T:14:VAL:N         | 2.40        | 0.55     |
| 10:X:24:ILE:O    | 10:X:24:ILE:HG12     | 2.06        | 0.55     |
| 3:C:57:LYS:O     | 3:C:58:LEU:CB        | 2.55        | 0.55     |
| 2:P:71:ASN:ND2   | 2:P:72:ASP:H         | 2.04        | 0.55     |
| 9:W:110:ILE:HD12 | 9:W:125:ILE:HG12     | 1.87        | 0.55     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 10:X:161:GLU:HA    | 10:X:161:GLU:OE2   | 2.06        | 0.55     |
| 10:J:34:THR:HG21   | 10:J:176:LYS:NZ    | 2.21        | 0.55     |
| 11:K:4:LEU:CD1     | 11:K:159:ILE:CD1   | 2.85        | 0.55     |
| 13:1:130:SER:HB3   | 13:1:132:THR:O     | 2.07        | 0.54     |
| 14:N:176:VAL:HG12  | 14:N:178:LEU:HD13  | 1.88        | 0.54     |
| 2:P:181:LYS:O      | 2:P:184:MET:HG3    | 2.08        | 0.54     |
| 10:X:7:ARG:HG3     | 10:X:7:ARG:O       | 2.06        | 0.54     |
| 9:I:2:ILE:HG21     | 9:I:130:ALA:HB3    | 1.88        | 0.54     |
| 14:N:36:ARG:HG3    | 14:N:42:TRP:CE2    | 2.43        | 0.54     |
| 12:L:166:HIS:HD2   | 12:L:168:GLN:H     | 1.56        | 0.54     |
| 5:S:97:ASN:ND2     | 12:Z:61:ASN:HD21   | 2.00        | 0.54     |
| 1:A:121:GLN:O      | 1:A:124:THR:HB     | 2.08        | 0.54     |
| 5:E:207:LEU:HD23   | 5:E:207:LEU:H      | 1.73        | 0.54     |
| 6:T:120:VAL:HG21   | 6:T:151:LEU:HD21   | 1.89        | 0.54     |
| 9:I:165:ARG:NH2    | 12:Z:135:MET:HE3   | 2.23        | 0.53     |
| 12:L:-2:ASN:HA     | 12:L:21:ILE:O      | 2.07        | 0.53     |
| 7:G:184(G):GLU:HG2 | 7:G:188:LYS:HB2    | 1.91        | 0.53     |
| 8:H:80:LEU:HD12    | 8:H:113:ILE:HD11   | 1.91        | 0.53     |
| 12:Z:-6:PRO:O      | 13:1:95:ARG:NH1    | 2.39        | 0.53     |
| 7:G:49:ILE:HD11    | 7:G:193:ALA:HB3    | 1.91        | 0.53     |
| 10:J:4:LEU:HD21    | 10:J:134:THR:HG21  | 1.91        | 0.53     |
| 12:Z:40:ASN:HD21   | 12:Z:183:GLY:HA2   | 1.73        | 0.53     |
| 4:R:67:ILE:HG22    | 4:R:221:PHE:HZ     | 1.74        | 0.53     |
| 12:L:40:ASN:ND2    | 12:L:183:GLY:HA2   | 2.22        | 0.53     |
| 6:T:186:ALA:O      | 6:T:190:VAL:HG23   | 2.09        | 0.53     |
| 1:A:8:TYR:HE2      | 6:F:127:ASN:OD1    | 1.92        | 0.53     |
| 14:N:161:GLN:HE21  | 14:2:136:GLY:CA    | 2.06        | 0.53     |
| 5:E:54:ASN:ND2     | 5:E:56:ASP:O       | 2.42        | 0.53     |
| 8:V:105:ASP:HB2    | 8:V:105(A):PRO:HD2 | 1.91        | 0.53     |
| 2:B:112:LEU:HD23   | 2:B:112:LEU:C      | 2.29        | 0.53     |
| 6:F:43:ASN:HD22    | 6:F:43:ASN:N       | 2.07        | 0.53     |
| 14:N:67:THR:HA     | 14:N:72:GLY:O      | 2.08        | 0.53     |
| 6:T:192:GLN:NE2    | 6:T:195:LYS:HE2    | 2.24        | 0.52     |
| 10:X:6:ILE:HD11    | 10:X:142:TYR:CD1   | 2.44        | 0.52     |
| 11:Y:196:PHE:HZ    | 11:Y:209:VAL:HG21  | 1.74        | 0.52     |
| 13:1:73:ASP:HA     | 13:1:77:ALA:HB2    | 1.91        | 0.52     |
| 8:V:172:ASN:HB3    | 8:V:192:LEU:O      | 2.08        | 0.52     |
| 12:Z:134:ILE:HG22  | 12:Z:138:LEU:HD22  | 1.91        | 0.52     |
| 4:R:215:ILE:HG22   | 4:R:221:PHE:HD2    | 1.75        | 0.52     |
| 4:R:186:LEU:O      | 4:R:190:GLU:HG3    | 2.09        | 0.52     |
| 9:W:113:PHE:HA     | 9:W:118:CYS:O      | 2.10        | 0.52     |
| 13:M:118:LEU:HG    | 13:M:133:LEU:HD12  | 1.92        | 0.52     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 1:A:203:GLU:CD    | 1:A:203:GLU:H     | 2.13        | 0.52     |
| 7:G:224:LEU:HB3   | 7:G:228:ASN:HB2   | 1.91        | 0.52     |
| 6:F:158:TRP:CZ3   | 7:G:64:VAL:HA     | 2.45        | 0.52     |
| 1:A:86:ARG:HH21   | 7:G:118:ASN:HD22  | 1.58        | 0.52     |
| 10:X:24:ILE:HD13  | 11:Y:132:THR:HG21 | 1.91        | 0.52     |
| 9:W:166:ASP:OD2   | 9:W:168:LEU:N     | 2.41        | 0.52     |
| 8:H:197:ARG:HH21  | 9:I:139:GLU:HG3   | 1.75        | 0.52     |
| 7:U:152:ASP:HB2   | 7:U:153:PRO:CD    | 2.40        | 0.52     |
| 5:S:134:VAL:O     | 5:S:153:PRO:HG3   | 2.11        | 0.51     |
| 14:2:4:MET:HB3    | 14:2:126:ILE:HG22 | 1.92        | 0.51     |
| 11:K:174:ASN:HD21 | 11:K:189:ASN:ND2  | 2.03        | 0.51     |
| 5:E:107:LEU:HD11  | 5:E:111:ARG:HG2   | 1.92        | 0.51     |
| 12:L:9:GLU:O      | 12:L:107:LYS:HA   | 2.11        | 0.51     |
| 3:C:40:VAL:HG12   | 3:C:162:ALA:HB1   | 1.93        | 0.51     |
| 5:E:31:ILE:HD11   | 5:E:153:PRO:HD3   | 1.91        | 0.51     |
| 2:P:107:ILE:HD11  | 2:P:111:ILE:HG22  | 1.92        | 0.51     |
| 11:K:200:LYS:HG3  | 11:K:206:PHE:HB2  | 1.93        | 0.51     |
| 16:K:302:3SD:H28  | 17:K:303:MES:H81  | 1.91        | 0.51     |
| 13:1:170:ASN:HD22 | 13:1:173:ARG:NH1  | 2.08        | 0.51     |
| 12:L:19:ARG:NE    | 12:L:171:ASP:OD2  | 2.39        | 0.51     |
| 7:U:79:ASN:OD1    | 7:U:165:THR:HB    | 2.10        | 0.51     |
| 6:T:52:LYS:HG2    | 6:T:66:LYS:HD3    | 1.92        | 0.51     |
| 6:T:126:TYR:HB2   | 6:T:129:VAL:HG22  | 1.92        | 0.51     |
| 6:T:187:ARG:HG3   | 6:T:187:ARG:HH11  | 1.72        | 0.51     |
| 8:V:50:ALA:HB2    | 9:W:118:CYS:HB2   | 1.93        | 0.51     |
| 2:B:163:ILE:HG13  | 2:B:164:SER:N     | 2.26        | 0.51     |
| 6:T:12:ASN:C      | 6:T:14:VAL:H      | 2.13        | 0.51     |
| 5:E:207:LEU:CD2   | 5:E:207:LEU:H     | 2.24        | 0.51     |
| 7:G:151:THR:HG22  | 7:G:157:TYR:CB    | 2.40        | 0.51     |
| 1:A:112:LEU:O     | 1:A:116:VAL:HG23  | 2.11        | 0.51     |
| 9:I:182:ASP:N     | 9:I:182:ASP:OD1   | 2.40        | 0.51     |
| 12:L:135:MET:HE2  | 9:W:165:ARG:NH2   | 2.26        | 0.50     |
| 14:N:14:LEU:O     | 14:N:175:MET:HA   | 2.11        | 0.50     |
| 2:B:41:MET:HB2    | 2:B:148:LEU:HD22  | 1.93        | 0.50     |
| 6:F:31:VAL:HG11   | 6:F:135:SER:HB2   | 1.93        | 0.50     |
| 7:G:49:ILE:HD13   | 7:G:193:ALA:HB1   | 1.94        | 0.50     |
| 5:E:111:ARG:HG2   | 5:E:111:ARG:HH11  | 1.74        | 0.50     |
| 2:P:78:VAL:HG22   | 2:P:136:PHE:CE2   | 2.47        | 0.50     |
| 14:2:14:LEU:HD23  | 14:2:44:CYS:SG    | 2.52        | 0.50     |
| 2:B:69:LYS:HG3    | 2:B:221:GLN:OE1   | 2.11        | 0.50     |
| 1:A:233:LEU:O     | 1:A:236:LEU:HB2   | 2.11        | 0.50     |
| 12:Z:9:GLU:O      | 12:Z:107:LYS:HA   | 2.12        | 0.50     |

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| Atom-1            | Atom-2            | Distance(Å) | Clash(Å) |
|-------------------|-------------------|-------------|----------|
| 8:V:105:ASP:HB2   | 8:V:105(A):PRO:CD | 2.41        | 0.50     |
| 3:Q:156:ILE:HD12  | 4:R:83:ALA:HB2    | 1.94        | 0.50     |
| 2:P:97:GLN:NE2    | 9:W:64:ASN:HD22   | 2.07        | 0.50     |
| 6:F:203:GLU:HA    | 6:F:206:LYS:HB3   | 1.94        | 0.49     |
| 6:T:176:LEU:HB3   | 7:U:58:LEU:HD21   | 1.93        | 0.49     |
| 12:L:135:MET:HE3  | 9:W:165:ARG:NH2   | 2.28        | 0.49     |
| 6:F:187:ARG:HG2   | 6:F:187:ARG:HH11  | 1.76        | 0.49     |
| 7:G:233:LEU:O     | 7:G:236:ILE:HG13  | 2.12        | 0.49     |
| 6:F:38:ILE:HG22   | 6:F:164:ALA:HB2   | 1.94        | 0.49     |
| 12:L:7:ALA:HB2    | 12:L:110:VAL:HG23 | 1.94        | 0.49     |
| 2:B:52:ARG:HH22   | 2:B:63(A):SER:HB3 | 1.77        | 0.49     |
| 6:T:12:ASN:C      | 6:T:12:ASN:OD1    | 2.50        | 0.49     |
| 13:1:71:LEU:C     | 13:1:73:ASP:H     | 2.16        | 0.49     |
| 2:P:126:HIS:HB3   | 3:Q:129:VAL:HG12  | 1.95        | 0.49     |
| 5:S:226:GLY:O     | 5:S:229:VAL:HG22  | 2.13        | 0.49     |
| 2:B:215:ILE:HG12  | 2:B:221:GLN:HG2   | 1.95        | 0.49     |
| 7:G:49:ILE:CD1    | 7:G:193:ALA:HB3   | 2.42        | 0.49     |
| 3:Q:168:ASN:O     | 3:Q:172:VAL:HG12  | 2.13        | 0.49     |
| 3:Q:71:ASP:HA     | 10:X:68:ILE:HD13  | 1.94        | 0.48     |
| 1:O:39:GLY:HA2    | 1:O:47:VAL:O      | 2.12        | 0.48     |
| 3:Q:163:GLN:HE21  | 3:Q:164:THR:N     | 2.03        | 0.48     |
| 2:P:152:ASN:HB2   | 2:P:153:PRO:HD2   | 1.95        | 0.48     |
| 7:G:105:TYR:OH    | 8:H:66:HIS:HE1    | 1.95        | 0.48     |
| 2:P:15:PHE:H      | 3:Q:23:GLN:HE22   | 1.60        | 0.48     |
| 4:R:179:GLU:HB3   | 4:R:192:LEU:HD21  | 1.95        | 0.48     |
| 7:G:59:LEU:O      | 7:G:61:PRO:HD3    | 2.13        | 0.48     |
| 7:U:96:ALA:CA     | 7:U:107:MET:HE2   | 2.25        | 0.48     |
| 11:Y:114:ASP:OD1  | 11:Y:116:ASP:HB2  | 2.14        | 0.48     |
| 6:T:95:GLU:HG2    | 6:T:115:ARG:CB    | 2.41        | 0.48     |
| 6:T:9:ASP:HB2     | 6:T:26:TYR:CE2    | 2.49        | 0.48     |
| 11:K:87:VAL:CG1   | 11:K:115:SER:HA   | 2.43        | 0.48     |
| 7:U:77:VAL:HG12   | 7:U:137:THR:HB    | 1.95        | 0.48     |
| 5:S:12:THR:HG21   | 5:S:124:THR:HA    | 1.94        | 0.48     |
| 13:1:150:VAL:HG23 | 13:1:150:VAL:O    | 2.13        | 0.48     |
| 13:M:147:ARG:HH11 | 8:V:165:ASN:ND2   | 2.09        | 0.48     |
| 8:H:124:TYR:HB2   | 8:H:138:LEU:HD13  | 1.94        | 0.48     |
| 5:E:100:SER:O     | 5:E:104:ASN:HA    | 2.14        | 0.48     |
| 5:S:139:ILE:HD12  | 5:S:215:VAL:HG12  | 1.95        | 0.48     |
| 8:V:172:ASN:HD22  | 8:V:193:THR:HA    | 1.79        | 0.48     |
| 5:S:52:LYS:HD2    | 5:S:63:TYR:O      | 2.14        | 0.47     |
| 6:F:35:THR:CG2    | 6:F:51:GLU:O      | 2.56        | 0.47     |
| 13:1:118:LEU:HG   | 13:1:133:LEU:HD12 | 1.96        | 0.47     |

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| Atom-1           | Atom-2             | Distance(Å) | Clash(Å) |
|------------------|--------------------|-------------|----------|
| 14:2:36:ARG:HG3  | 14:2:42:TRP:CE2    | 2.49        | 0.47     |
| 7:U:39:ALA:HB2   | 7:U:48:VAL:HG12    | 1.97        | 0.47     |
| 13:M:88:ALA:HA   | 13:M:121:VAL:HG21  | 1.96        | 0.47     |
| 13:M:120:TYR:O   | 13:M:127:THR:HA    | 2.13        | 0.47     |
| 9:W:2:ILE:HG21   | 9:W:130:ALA:HB3    | 1.97        | 0.47     |
| 2:P:146:TYR:OH   | 2:P:216(A):LYS:HB2 | 2.14        | 0.47     |
| 13:1:6:LYS:HB3   | 13:1:11:VAL:HG12   | 1.96        | 0.47     |
| 12:L:-7:ASN:ND2  | 12:L:-5:TYR:H      | 2.12        | 0.47     |
| 5:S:227:GLU:H    | 5:S:227:GLU:CD     | 2.16        | 0.47     |
| 8:V:197:ARG:NH2  | 9:W:139:GLU:HG3    | 2.28        | 0.47     |
| 14:2:55:ILE:O    | 14:2:59:VAL:HG23   | 2.15        | 0.47     |
| 6:T:7:GLY:C      | 6:T:9:ASP:H        | 2.18        | 0.47     |
| 5:S:160:LEU:HD13 | 5:S:163:THR:HB     | 1.96        | 0.47     |
| 11:Y:18:SER:OG   | 11:Y:29:GLN:O      | 2.32        | 0.47     |
| 5:S:86:ARG:O     | 5:S:90:ASN:HB2     | 2.14        | 0.47     |
| 1:O:118:LYS:O    | 1:O:122:GLU:HG3    | 2.14        | 0.47     |
| 2:P:76:VAL:HG12  | 2:P:138:TYR:CD2    | 2.50        | 0.47     |
| 13:1:84:PHE:CZ   | 13:1:119:ARG:HG2   | 2.48        | 0.47     |
| 13:1:66:ALA:HA   | 13:1:72:ALA:CB     | 2.44        | 0.47     |
| 9:W:29:ASN:HB3   | 9:W:171:TRP:CE3    | 2.50        | 0.47     |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:HD2    | 1.79        | 0.47     |
| 2:P:78:VAL:HG22  | 2:P:136:PHE:HE2    | 1.78        | 0.47     |
| 11:K:197:TRP:CD1 | 9:W:190:LYS:HE3    | 2.50        | 0.47     |
| 6:F:18:ASP:OD2   | 6:F:18:ASP:N       | 2.47        | 0.47     |
| 6:T:237:GLN:HA   | 6:T:237:GLN:NE2    | 2.30        | 0.47     |
| 13:1:152:ARG:HG3 | 13:1:152:ARG:NH1   | 2.14        | 0.47     |
| 4:R:194:LEU:HD12 | 4:R:207:LEU:HD11   | 1.95        | 0.47     |
| 11:Y:156:LYS:HD3 | 11:Y:195:LEU:HD11  | 1.96        | 0.47     |
| 12:Z:112:SER:HB3 | 12:Z:125:ARG:HG2   | 1.97        | 0.47     |
| 11:Y:4:LEU:HD13  | 11:Y:159:ILE:HD11  | 1.96        | 0.47     |
| 10:J:113:ILE:HA  | 10:J:118:THR:O     | 2.15        | 0.47     |
| 6:F:42:CYS:HB2   | 6:F:184:LEU:O      | 2.14        | 0.47     |
| 7:G:87:ASN:ND2   | 7:G:87:ASN:C       | 2.69        | 0.46     |
| 7:U:87:ASN:C     | 7:U:87:ASN:ND2     | 2.68        | 0.46     |
| 2:B:185:LYS:HD3  | 2:B:187:ASP:H      | 1.81        | 0.46     |
| 8:H:144:GLN:O    | 8:H:145:ASP:HB2    | 2.15        | 0.46     |
| 6:F:210:LEU:HD21 | 6:F:212:ILE:HD11   | 1.96        | 0.46     |
| 2:P:112:LEU:HD23 | 2:P:112:LEU:C      | 2.35        | 0.46     |
| 8:V:126:SER:O    | 8:V:127:LEU:HD23   | 2.16        | 0.46     |
| 13:1:120:TYR:O   | 13:1:127:THR:HA    | 2.16        | 0.46     |
| 10:X:113:ILE:HA  | 10:X:118:THR:O     | 2.16        | 0.46     |
| 4:R:52:LYS:HE3   | 4:R:211:GLN:HB2    | 1.97        | 0.46     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 14:2:149:GLU:H    | 14:2:149:GLU:HG3   | 1.56        | 0.46     |
| 10:X:12:VAL:HG23  | 10:X:108:PRO:HB2   | 1.97        | 0.46     |
| 7:U:49:ILE:HD13   | 7:U:193:ALA:HB1    | 1.98        | 0.46     |
| 6:T:169:ARG:HE    | 6:T:169:ARG:HB3    | 1.68        | 0.46     |
| 12:Z:113:PHE:CD2  | 12:Z:119:TYR:HB3   | 2.50        | 0.46     |
| 5:S:188:GLU:OE1   | 5:S:191:LYS:HD2    | 2.16        | 0.46     |
| 10:X:2:ILE:HG13   | 10:X:130:SER:OG    | 2.14        | 0.46     |
| 6:F:150:MET:O     | 6:F:157:TYR:HA     | 2.15        | 0.46     |
| 13:1:71:LEU:C     | 13:1:73:ASP:N      | 2.69        | 0.46     |
| 2:P:138:TYR:HB2   | 2:P:149:TYR:HB2    | 1.97        | 0.46     |
| 4:R:215:ILE:O     | 4:R:215:ILE:HG13   | 2.16        | 0.46     |
| 11:Y:87:VAL:CG1   | 11:Y:115:SER:HA    | 2.46        | 0.46     |
| 2:P:152:ASN:HB2   | 2:P:153:PRO:CD     | 2.46        | 0.46     |
| 1:A:13:THR:HG22   | 1:A:21:LEU:HD22    | 1.98        | 0.46     |
| 2:B:166:GLY:O     | 2:B:169:THR:HG23   | 2.15        | 0.46     |
| 11:K:6:PHE:HA     | 11:K:123:ASP:O     | 2.15        | 0.46     |
| 3:Q:216:LYS:HB2   | 3:Q:220:ASP:HB3    | 1.97        | 0.46     |
| 11:K:210:ILE:HB   | 9:W:30:LYS:HE3     | 1.96        | 0.46     |
| 7:U:233:LEU:O     | 7:U:236:ILE:HG13   | 2.16        | 0.46     |
| 7:U:168:LYS:HD2   | 7:U:201:LEU:HD22   | 1.98        | 0.46     |
| 7:G:39:ALA:HB2    | 7:G:48:VAL:HG12    | 1.97        | 0.46     |
| 4:D:161:ASN:HB3   | 4:D:180:TRP:CE2    | 2.51        | 0.46     |
| 6:F:126:TYR:HE1   | 7:G:129:MET:SD     | 2.40        | 0.45     |
| 3:Q:169:SER:HA    | 3:Q:172:VAL:HG13   | 1.97        | 0.45     |
| 2:P:147:GLN:HG2   | 3:Q:62(A):ILE:HG21 | 1.98        | 0.45     |
| 1:O:97:HIS:HD2    | 8:V:61:SER:OG      | 1.98        | 0.45     |
| 10:X:120:VAL:HG13 | 10:X:122:LEU:HG    | 1.97        | 0.45     |
| 4:R:85:ALA:O      | 4:R:89:ILE:HG12    | 2.17        | 0.45     |
| 8:H:3:ILE:HG13    | 8:H:100:ILE:HD12   | 1.98        | 0.45     |
| 7:G:215:ALA:HB2   | 7:G:221:PHE:HD2    | 1.81        | 0.45     |
| 6:T:126:TYR:HE1   | 7:U:129:MET:SD     | 2.39        | 0.45     |
| 1:O:78:TYR:HB3    | 1:O:85:TYR:CD1     | 2.52        | 0.45     |
| 4:R:209:GLU:HG3   | 4:R:226:ASN:HB3    | 1.98        | 0.45     |
| 14:N:32:ASP:OD1   | 14:N:186:ARG:NH2   | 2.50        | 0.45     |
| 10:J:2:ILE:HB     | 10:J:17:SER:HB3    | 1.98        | 0.45     |
| 2:B:150:THR:O     | 2:B:157:TYR:HA     | 2.16        | 0.45     |
| 7:G:78:VAL:HG11   | 7:G:85:ALA:CB      | 2.46        | 0.45     |
| 6:F:11:SER:HB2    | 6:F:14:VAL:HG23    | 1.98        | 0.45     |
| 2:P:45:GLY:HA2    | 2:P:146:TYR:CE1    | 2.52        | 0.45     |
| 6:T:79:SER:OG     | 6:T:165:THR:HG23   | 2.17        | 0.45     |
| 4:D:90:GLU:OE1    | 11:K:69:ARG:HD2    | 2.17        | 0.45     |
| 5:S:207:LEU:HD23  | 5:S:207:LEU:H      | 1.81        | 0.45     |

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| Atom-1              | Atom-2            | Distance(Å) | Clash(Å) |
|---------------------|-------------------|-------------|----------|
| 8:V:172:ASN:ND2     | 8:V:193:THR:HG22  | 2.32        | 0.45     |
| 7:G:151:THR:HG22    | 7:G:157:TYR:HB2   | 1.98        | 0.45     |
| 3:Q:97:GLN:HG3      | 10:X:65:LEU:HB2   | 1.97        | 0.45     |
| 9:I:165:ARG:NH2     | 12:Z:135:MET:HE2  | 2.32        | 0.45     |
| 13:1:120:TYR:HE1    | 13:1:135:THR:HG22 | 1.81        | 0.45     |
| 1:O:20:LYS:HA       | 1:O:20:LYS:HD3    | 1.78        | 0.45     |
| 4:R:163:LYS:HG3     | 4:R:164:ALA:N     | 2.32        | 0.45     |
| 4:D:45:GLY:HA2      | 4:D:146:TYR:CE1   | 2.52        | 0.45     |
| 8:V:3:ILE:HD11      | 8:V:127:LEU:HB2   | 1.99        | 0.45     |
| 10:X:44:SER:OG      | 10:X:100:LEU:HB2  | 2.17        | 0.45     |
| 7:U:151:THR:HG22    | 7:U:157:TYR:HB2   | 1.99        | 0.45     |
| 10:J:7:ARG:O        | 10:J:7:ARG:HG3    | 2.16        | 0.45     |
| 13:1:0:THR:HG23     | 13:1:1:SER:H      | 1.80        | 0.45     |
| 14:2:14:LEU:O       | 14:2:175:MET:HA   | 2.16        | 0.45     |
| 7:U:47:VAL:HG12     | 7:U:49:ILE:HD12   | 1.99        | 0.45     |
| 7:U:49:ILE:HD13     | 7:U:193:ALA:CB    | 2.48        | 0.45     |
| 5:E:92:LEU:HD11     | 5:E:112:ALA:HB1   | 1.98        | 0.45     |
| 1:O:152:ASP:HB3     | 1:O:153:PRO:HD2   | 1.99        | 0.45     |
| 3:C:17:PRO:HA       | 4:D:26:TYR:CD1    | 2.51        | 0.44     |
| 1:O:150:GLN:O       | 1:O:157:TYR:HA    | 2.17        | 0.44     |
| 5:E:103:PHE:HE2     | 13:M:61:LEU:HD21  | 1.82        | 0.44     |
| 13:1:39:ASN:H       | 13:1:39:ASN:HD22  | 1.65        | 0.44     |
| 10:X:90(A):ILE:HD12 | 10:X:90(A):ILE:HA | 1.81        | 0.44     |
| 13:1:120:TYR:CE1    | 13:1:135:THR:HG22 | 2.52        | 0.44     |
| 12:L:137:PHE:CE1    | 12:L:141:GLN:HG3  | 2.52        | 0.44     |
| 5:S:173:LYS:O       | 5:S:177:GLU:HB2   | 2.16        | 0.44     |
| 9:W:143:GLU:HG3     | 9:W:146:LEU:HD21  | 1.98        | 0.44     |
| 13:M:119:ARG:HH11   | 13:M:129:SER:HB2  | 1.82        | 0.44     |
| 7:G:152:ASP:HB2     | 7:G:153:PRO:CD    | 2.47        | 0.44     |
| 10:J:59:ILE:O       | 10:J:63:ILE:HG12  | 2.18        | 0.44     |
| 11:K:63:CYS:SG      | 11:K:74:ILE:HG21  | 2.58        | 0.44     |
| 7:U:180(A):ILE:CD1  | 7:U:184:ASN:HB2   | 2.48        | 0.44     |
| 9:I:48:LEU:HG       | 9:I:50:THR:HG22   | 2.00        | 0.44     |
| 6:F:127:ASN:HD22    | 6:F:127:ASN:C     | 2.20        | 0.44     |
| 1:A:118:LYS:O       | 1:A:122:GLU:HG3   | 2.17        | 0.44     |
| 6:T:22:PHE:HA       | 6:T:22:PHE:HD1    | 1.76        | 0.44     |
| 4:D:192:LEU:O       | 4:D:196:ILE:HG13  | 2.18        | 0.44     |
| 1:A:97:HIS:CD2      | 8:H:61:SER:OG     | 2.69        | 0.44     |
| 3:C:17:PRO:HA       | 4:D:26:TYR:CE1    | 2.53        | 0.44     |
| 2:P:60:GLU:O        | 2:P:63(A):SER:HB2 | 2.17        | 0.44     |
| 10:J:12:VAL:HG23    | 10:J:108:PRO:HB2  | 2.00        | 0.44     |
| 13:1:88:ALA:HA      | 13:1:121:VAL:HG21 | 2.00        | 0.44     |

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| Atom-1              | Atom-2              | Distance(Å) | Clash(Å) |
|---------------------|---------------------|-------------|----------|
| 6:T:43:ASN:HD22     | 6:T:44:ASP:H        | 1.65        | 0.44     |
| 11:Y:31:VAL:HG21    | 16:Y:302:3SD:H25    | 2.00        | 0.44     |
| 5:S:209(B):THR:N    | 5:S:209(E):ASN:HB2  | 2.32        | 0.44     |
| 6:T:13:SER:O        | 7:U:130:ARG:HB3     | 2.16        | 0.44     |
| 5:S:11:ASP:OD1      | 5:S:13:VAL:HG12     | 2.17        | 0.44     |
| 12:Z:51:ASP:OD1     | 12:Z:95:TYR:HA      | 2.17        | 0.44     |
| 11:K:86:LEU:C       | 11:K:86:LEU:HD13    | 2.38        | 0.44     |
| 14:2:32:ASP:OD1     | 14:2:186:ARG:NH2    | 2.51        | 0.44     |
| 7:G:151:THR:HG22    | 7:G:157:TYR:HB3     | 1.99        | 0.44     |
| 6:T:43:ASN:HD22     | 6:T:44:ASP:N        | 2.16        | 0.44     |
| 10:J:137:LEU:HD21   | 11:Y:140:SER:OG     | 2.18        | 0.44     |
| 9:I:33:LYS:O        | 9:I:44:GLY:HA2      | 2.17        | 0.44     |
| 13:M:39:ASN:N       | 13:M:39:ASN:HD22    | 2.16        | 0.44     |
| 13:1:152:ARG:NH1    | 13:1:152:ARG:CG     | 2.76        | 0.44     |
| 3:C:228:GLU:O       | 3:C:232:TYR:HD1     | 2.01        | 0.44     |
| 6:T:127:ASN:HD22    | 6:T:127:ASN:C       | 2.21        | 0.44     |
| 12:Z:129:ALA:HB1    | 12:Z:166:HIS:CE1    | 2.53        | 0.43     |
| 4:D:97:VAL:HG11     | 11:K:65:LEU:HD22    | 2.00        | 0.43     |
| 14:2:34:LEU:HD13    | 14:2:176:VAL:HG23   | 2.00        | 0.43     |
| 5:E:31:ILE:HD11     | 5:E:153:PRO:CD      | 2.48        | 0.43     |
| 1:A:78:TYR:HB3      | 1:A:85:TYR:CD1      | 2.52        | 0.43     |
| 7:U:38:LEU:HD12     | 7:U:38:LEU:C        | 2.38        | 0.43     |
| 6:F:12:ASN:C        | 6:F:14:VAL:H        | 2.21        | 0.43     |
| 8:H:165:ASN:HD22    | 13:1:147:ARG:HH11   | 1.65        | 0.43     |
| 5:S:198:SER:C       | 5:S:200:SER:H       | 2.21        | 0.43     |
| 12:L:144(A):LYS:HB3 | 12:L:144(A):LYS:HE3 | 1.81        | 0.43     |
| 2:P:116:LEU:HD23    | 2:P:116:LEU:HA      | 1.83        | 0.43     |
| 4:R:194:LEU:HD22    | 4:R:212:LEU:HD11    | 2.00        | 0.43     |
| 7:U:150:LYS:O       | 7:U:157:TYR:HA      | 2.17        | 0.43     |
| 3:C:35:THR:HB       | 3:C:51:GLU:HG3      | 2.00        | 0.43     |
| 6:F:35:THR:CG2      | 6:F:36:THR:N        | 2.81        | 0.43     |
| 8:H:172:ASN:ND2     | 8:H:193:THR:HA      | 2.34        | 0.43     |
| 3:Q:36:CYS:H        | 3:Q:51:GLU:HG2      | 1.83        | 0.43     |
| 3:Q:57:LYS:HD2      | 3:Q:58:LEU:N        | 2.33        | 0.43     |
| 2:B:37:ALA:O        | 2:B:164:SER:HA      | 2.19        | 0.43     |
| 11:K:87:VAL:HG13    | 11:K:115:SER:HA     | 2.00        | 0.43     |
| 2:B:125:GLN:HG3     | 3:C:130:ARG:HG2     | 2.01        | 0.43     |
| 10:J:34:THR:HG21    | 10:J:176:LYS:HZ3    | 1.83        | 0.43     |
| 5:S:76:LEU:HA       | 5:S:137:LEU:O       | 2.19        | 0.43     |
| 7:U:96:ALA:CA       | 7:U:107:MET:CE      | 2.93        | 0.43     |
| 4:D:75:GLY:HA3      | 4:D:221:PHE:CE2     | 2.54        | 0.43     |
| 14:N:8:PHE:HB2      | 14:N:146:MET:O      | 2.19        | 0.43     |

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| Atom-1            | Atom-2             | Distance(Å) | Clash(Å) |
|-------------------|--------------------|-------------|----------|
| 13:M:7:TYR:CE2    | 13:M:161:VAL:HG22  | 2.54        | 0.43     |
| 13:1:71:LEU:O     | 13:1:73:ASP:N      | 2.52        | 0.43     |
| 9:W:11:CYS:HA     | 9:W:104:ILE:HD11   | 2.00        | 0.43     |
| 4:D:194:LEU:HD22  | 4:D:212:LEU:HD11   | 2.00        | 0.43     |
| 9:I:156:SER:O     | 9:I:160:LEU:HD22   | 2.19        | 0.43     |
| 5:S:75:GLY:HA3    | 5:S:221:PHE:CE2    | 2.54        | 0.43     |
| 4:D:67:ILE:HG22   | 4:D:221:PHE:HZ     | 1.82        | 0.43     |
| 6:F:187:ARG:NH1   | 6:F:187:ARG:HG2    | 2.34        | 0.43     |
| 4:D:85:ALA:O      | 4:D:89:ILE:HG12    | 2.18        | 0.43     |
| 10:J:140:HIS:HE1  | 11:Y:203:GLU:OE1   | 2.01        | 0.43     |
| 2:P:69:LYS:CG     | 2:P:221:GLN:OE1    | 2.66        | 0.43     |
| 7:U:152:ASP:HB2   | 7:U:153:PRO:HD2    | 1.98        | 0.43     |
| 3:C:215:VAL:HB    | 3:C:221:ILE:HG12   | 2.01        | 0.43     |
| 5:E:160:LEU:HD13  | 5:E:163:THR:HB     | 2.01        | 0.43     |
| 9:W:55:LEU:HD11   | 9:W:97:VAL:HG21    | 2.00        | 0.43     |
| 13:M:152:ARG:CG   | 13:M:152:ARG:HH11  | 2.29        | 0.42     |
| 13:M:39:ASN:H     | 13:M:39:ASN:HD22   | 1.66        | 0.42     |
| 8:V:109:HIS:HB3   | 8:V:111:PHE:CE2    | 2.54        | 0.42     |
| 13:M:16:ASP:HA    | 13:M:186:PHE:CB    | 2.49        | 0.42     |
| 2:P:97:GLN:NE2    | 9:W:61:TYR:HA      | 2.33        | 0.42     |
| 3:Q:71:ASP:OD1    | 3:Q:100:ARG:NH1    | 2.52        | 0.42     |
| 7:U:48:VAL:HG13   | 7:U:139:VAL:HG11   | 2.01        | 0.42     |
| 2:B:152:ASN:HB2   | 2:B:153:PRO:CD     | 2.48        | 0.42     |
| 1:A:58:LEU:HD12   | 7:G:173:THR:HG23   | 2.00        | 0.42     |
| 10:X:129:TYR:O    | 10:X:132:PHE:HB2   | 2.19        | 0.42     |
| 2:B:149:TYR:CZ    | 3:C:62(A):ILE:HD12 | 2.55        | 0.42     |
| 4:D:38:ILE:HD12   | 4:D:197:LEU:HG     | 2.00        | 0.42     |
| 3:C:206:GLY:HA3   | 3:C:209:ASN:HB2    | 2.00        | 0.42     |
| 3:Q:140:GLY:HA2   | 3:Q:215:VAL:HG21   | 2.01        | 0.42     |
| 14:2:15:GLY:HA2   | 14:2:174:ARG:O     | 2.19        | 0.42     |
| 6:F:24:VAL:HG11   | 6:F:154:SER:HB3    | 2.01        | 0.42     |
| 7:G:107:MET:HE1   | 7:G:112:LEU:HD13   | 2.01        | 0.42     |
| 5:E:160:LEU:HD23  | 6:F:59:LEU:HA      | 1.99        | 0.42     |
| 13:M:178:ARG:NH1  | 8:V:139:GLU:OE1    | 2.38        | 0.42     |
| 11:K:5:ALA:HA     | 11:K:13:ILE:O      | 2.20        | 0.42     |
| 7:G:172:ILE:H     | 7:G:172:ILE:HG13   | 1.71        | 0.42     |
| 8:V:112:SER:HB3   | 8:V:125:LEU:HD13   | 2.01        | 0.42     |
| 8:V:128:GLY:O     | 8:V:131:SER:HB2    | 2.19        | 0.42     |
| 11:Y:37:ILE:HB    | 11:Y:41:LEU:HB3    | 2.02        | 0.42     |
| 3:C:97:GLN:HA     | 3:C:97:GLN:NE2     | 2.35        | 0.42     |
| 5:S:111:ARG:HH11  | 5:S:111:ARG:HG2    | 1.84        | 0.42     |
| 14:N:161:GLN:HE22 | 14:2:139:ASP:HB3   | 1.85        | 0.42     |

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| Atom-1            | Atom-2           | Distance(Å) | Clash(Å) |
|-------------------|------------------|-------------|----------|
| 1:O:158:PHE:HD1   | 1:O:160:TRP:HE1  | 1.68        | 0.42     |
| 12:L:8:GLY:HA3    | 12:L:11:PHE:CE2  | 2.55        | 0.42     |
| 5:S:15:PHE:H      | 6:T:23:GLN:NE2   | 2.12        | 0.42     |
| 3:Q:215:VAL:HB    | 3:Q:221:ILE:HG12 | 2.02        | 0.42     |
| 8:V:128:GLY:O     | 8:V:131:SER:CB   | 2.67        | 0.42     |
| 4:D:40:ILE:CD1    | 4:D:193:VAL:HG23 | 2.47        | 0.42     |
| 10:J:44:SER:OG    | 10:J:100:LEU:HB2 | 2.20        | 0.42     |
| 2:B:234:VAL:HG22  | 2:B:239:THR:HA   | 2.02        | 0.42     |
| 10:X:112:GLN:HE22 | 10:X:126:ALA:H   | 1.68        | 0.42     |
| 6:T:210:LEU:HD21  | 6:T:212:ILE:HD11 | 2.01        | 0.42     |
| 11:Y:20:ALA:HA    | 16:Y:302:3SD:O19 | 2.20        | 0.42     |
| 12:Z:90:LYS:HD3   | 12:Z:95:TYR:CZ   | 2.55        | 0.42     |
| 9:W:55:LEU:HA     | 9:W:55:LEU:HD23  | 1.91        | 0.42     |
| 2:B:152:ASN:HB2   | 2:B:153:PRO:HD2  | 2.02        | 0.42     |
| 6:T:18:ASP:OD1    | 6:T:20:ARG:NH1   | 2.46        | 0.42     |
| 10:X:3:ILE:HD11   | 10:X:127:HIS:HD2 | 1.84        | 0.42     |
| 12:L:2:THR:HG23   | 12:L:127:GLY:O   | 2.20        | 0.42     |
| 1:A:41:LYS:HG3    | 1:A:46:VAL:HG22  | 2.02        | 0.42     |
| 4:R:46:VAL:HG11   | 4:R:139:ALA:HB1  | 2.01        | 0.42     |
| 3:C:57:LYS:CD     | 3:C:58:LEU:H     | 2.16        | 0.41     |
| 1:O:13:THR:O      | 2:P:130:ARG:HD3  | 2.20        | 0.41     |
| 5:E:134:VAL:O     | 5:E:153:PRO:HG3  | 2.20        | 0.41     |
| 13:1:73:ASP:CG    | 13:1:73:ASP:O    | 2.58        | 0.41     |
| 1:A:67:VAL:HG11   | 1:A:213:ALA:CB   | 2.50        | 0.41     |
| 1:A:111:LEU:HA    | 1:A:111:LEU:HD23 | 1.95        | 0.41     |
| 3:C:172:VAL:HG23  | 3:C:196:SER:HB2  | 2.01        | 0.41     |
| 5:E:226:GLY:O     | 5:E:229:VAL:HG22 | 2.20        | 0.41     |
| 7:G:96:ALA:CA     | 7:G:107:MET:CE   | 2.93        | 0.41     |
| 10:X:113:ILE:HG12 | 10:X:119:LYS:HG3 | 2.01        | 0.41     |
| 12:Z:113:PHE:CD1  | 12:Z:113:PHE:N   | 2.87        | 0.41     |
| 8:H:3:ILE:HD11    | 8:H:127:LEU:HB2  | 2.01        | 0.41     |
| 12:Z:146:LEU:HD22 | 12:Z:150:GLU:HG2 | 2.02        | 0.41     |
| 6:F:39:GLY:HA2    | 6:F:47:VAL:O     | 2.19        | 0.41     |
| 3:C:237:GLU:HA    | 3:C:240:LYS:HB2  | 2.01        | 0.41     |
| 11:K:112:TYR:O    | 11:K:119:ARG:HA  | 2.20        | 0.41     |
| 11:Y:19:ARG:HH21  | 11:Y:29:GLN:HE22 | 1.68        | 0.41     |
| 9:W:55:LEU:CD1    | 9:W:97:VAL:HG21  | 2.50        | 0.41     |
| 6:T:18:ASP:OD1    | 6:T:20:ARG:HD3   | 2.20        | 0.41     |
| 1:O:67:VAL:HG11   | 1:O:213:ALA:HB3  | 2.03        | 0.41     |
| 3:Q:17:PRO:HA     | 4:R:26:TYR:CD1   | 2.55        | 0.41     |
| 8:H:223:ASP:OD2   | 8:H:223:ASP:N    | 2.54        | 0.41     |
| 12:L:153:LYS:HG2  | 8:V:201:GLN:HG3  | 2.02        | 0.41     |

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| Atom-1             | Atom-2             | Distance(Å) | Clash(Å) |
|--------------------|--------------------|-------------|----------|
| 6:F:95:GLU:HG3     | 6:F:115:ARG:HD2    | 2.03        | 0.41     |
| 7:U:65:SER:HA      | 7:U:211:GLU:OE2    | 2.21        | 0.41     |
| 11:K:196:PHE:CE1   | 9:W:193:GLN:HG3    | 2.55        | 0.41     |
| 13:1:87:LEU:O      | 13:1:91:MET:HG2    | 2.20        | 0.41     |
| 10:J:3:ILE:HD13    | 10:J:3:ILE:HA      | 1.94        | 0.41     |
| 10:J:36:GLN:HG3    | 10:J:184:ILE:CD1   | 2.51        | 0.41     |
| 5:S:92:LEU:HD11    | 5:S:112:ALA:HB1    | 2.02        | 0.41     |
| 7:G:96:ALA:CA      | 7:G:107:MET:HE2    | 2.23        | 0.41     |
| 12:Z:135:MET:N     | 12:Z:136:PRO:CD    | 2.83        | 0.41     |
| 2:B:163:ILE:HG13   | 2:B:164:SER:H      | 1.85        | 0.41     |
| 8:H:165:ASN:ND2    | 13:1:147:ARG:HH11  | 2.19        | 0.41     |
| 9:I:28:SER:CB      | 10:J:120:VAL:HG21  | 2.50        | 0.41     |
| 11:Y:100:MET:SD    | 11:Y:125:PHE:HB2   | 2.61        | 0.41     |
| 7:U:59:LEU:O       | 7:U:61:PRO:HD3     | 2.20        | 0.41     |
| 14:N:4:MET:HB3     | 14:N:126:ILE:HG22  | 2.02        | 0.41     |
| 12:Z:112:SER:CB    | 12:Z:125:ARG:HG2   | 2.51        | 0.41     |
| 7:G:152:ASP:HB2    | 7:G:153:PRO:HD2    | 2.01        | 0.41     |
| 10:X:112:GLN:NE2   | 10:X:126:ALA:H     | 2.19        | 0.41     |
| 11:K:7:ARG:HG3     | 11:K:12:ILE:HG12   | 2.01        | 0.41     |
| 13:M:110:VAL:HG12  | 13:M:111:GLN:O     | 2.20        | 0.41     |
| 2:B:44:ASP:N       | 2:B:44:ASP:OD2     | 2.54        | 0.41     |
| 7:U:69:CYS:O       | 7:U:93:LYS:HE2     | 2.21        | 0.41     |
| 2:P:144(A):TYR:HB2 | 2:P:147:GLN:NE2    | 2.36        | 0.41     |
| 6:F:126:TYR:HB2    | 6:F:129:VAL:CG2    | 2.51        | 0.41     |
| 14:2:146:MET:HE3   | 14:2:150:GLU:HB3   | 2.03        | 0.41     |
| 9:I:174:VAL:HG21   | 9:I:186:LYS:HE2    | 2.02        | 0.41     |
| 6:F:121:GLN:HE21   | 6:F:121:GLN:HB3    | 1.66        | 0.41     |
| 10:J:48:GLU:HB3    | 10:J:96:GLN:HB2    | 2.03        | 0.41     |
| 5:E:207(B):THR:H   | 5:E:209(E):ASN:HB2 | 1.84        | 0.41     |
| 6:F:166:GLY:O      | 6:F:169:ARG:HB3    | 2.21        | 0.41     |
| 5:S:13:VAL:HG21    | 6:T:128:SER:O      | 2.21        | 0.41     |
| 10:X:52:THR:CG2    | 10:X:53:VAL:N      | 2.83        | 0.41     |
| 1:O:11:SER:OG      | 2:P:129:LEU:HA     | 2.21        | 0.41     |
| 4:R:90:GLU:OE2     | 11:Y:69:ARG:NH1    | 2.54        | 0.41     |
| 3:Q:53:ARG:HD3     | 3:Q:55:THR:OG1     | 2.20        | 0.41     |
| 13:1:121:VAL:HA    | 13:1:126:VAL:O     | 2.22        | 0.41     |
| 5:S:13:VAL:HG13    | 5:S:13:VAL:O       | 2.21        | 0.41     |
| 2:P:218:ASN:O      | 2:P:218(C):ASP:HB2 | 2.22        | 0.41     |
| 1:O:217(K):GLY:HA3 | 8:V:186:TYR:HB3    | 2.04        | 0.41     |
| 1:O:33:GLN:HG2     | 1:O:33:GLN:H       | 1.69        | 0.41     |
| 3:C:57:LYS:CD      | 3:C:58:LEU:N       | 2.80        | 0.40     |
| 6:T:7:GLY:O        | 7:U:11:HIS:CE1     | 2.74        | 0.40     |

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| Atom-1              | Atom-2             | Distance(Å) | Clash(Å) |
|---------------------|--------------------|-------------|----------|
| 14:2:36:ARG:HG3     | 14:2:42:TRP:CZ2    | 2.57        | 0.40     |
| 2:P:149:TYR:CZ      | 3:Q:62(A):ILE:HD12 | 2.56        | 0.40     |
| 13:M:6:LYS:HB3      | 13:M:11:VAL:HG12   | 2.03        | 0.40     |
| 11:K:99:THR:HB      | 11:K:113:VAL:O     | 2.22        | 0.40     |
| 6:T:143:LYS:HB3     | 6:T:143:LYS:HE3    | 1.93        | 0.40     |
| 13:1:69:ASN:HA      | 13:1:70:PRO:HD2    | 1.97        | 0.40     |
| 7:U:192:PHE:C       | 7:U:192:PHE:CD1    | 2.94        | 0.40     |
| 13:1:69:ASN:HD21    | 13:1:72:ALA:HA     | 1.82        | 0.40     |
| 11:K:4:LEU:HD12     | 11:K:159:ILE:CD1   | 2.51        | 0.40     |
| 1:O:8:TYR:HE2       | 6:T:127:ASN:OD1    | 2.05        | 0.40     |
| 10:X:4:LEU:HD23     | 10:X:126:ALA:HB2   | 2.02        | 0.40     |
| 1:O:217(G):LEU:HD13 | 1:O:218:GLY:HA2    | 2.03        | 0.40     |
| 5:E:75:GLY:HA3      | 5:E:221:PHE:CE2    | 2.56        | 0.40     |
| 5:E:68:ILE:HB       | 5:E:76:LEU:CD2     | 2.51        | 0.40     |
| 2:B:46:ILE:HD11     | 2:B:146:TYR:HB3    | 2.01        | 0.40     |
| 6:T:180(E):GLU:H    | 6:T:180(E):GLU:HG3 | 1.32        | 0.40     |
| 2:P:215:ILE:HG12    | 2:P:221:GLN:HG2    | 2.03        | 0.40     |
| 11:Y:87:VAL:HG13    | 11:Y:115:SER:HA    | 2.03        | 0.40     |
| 13:M:178:ARG:HD3    | 8:V:139:GLU:OE1    | 2.22        | 0.40     |
| 9:I:94:PRO:HB3      | 9:I:116:ILE:HG22   | 2.04        | 0.40     |
| 11:Y:200:LYS:HG3    | 11:Y:206:PHE:HB2   | 2.03        | 0.40     |
| 7:U:161:LYS:HG2     | 7:U:180(B):ASP:HB2 | 2.03        | 0.40     |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 244/250 (98%) | 239 (98%) | 4 (2%)  | 1 (0%)   | 43 74       |
| 1   | O     | 244/250 (98%) | 232 (95%) | 10 (4%) | 2 (1%)   | 27 55       |
| 2   | B     | 233/235 (99%) | 218 (94%) | 12 (5%) | 3 (1%)   | 18 39       |
| 2   | P     | 233/235 (99%) | 217 (93%) | 12 (5%) | 4 (2%)   | 14 30       |
| 3   | C     | 236/241 (98%) | 227 (96%) | 5 (2%)  | 4 (2%)   | 14 30       |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 3   | Q     | 236/241 (98%)   | 226 (96%)  | 7 (3%)   | 3 (1%)   | 18          | 39  |
| 4   | D     | 224/260 (86%)   | 215 (96%)  | 8 (4%)   | 1 (0%)   | 43          | 74  |
| 4   | R     | 225/260 (86%)   | 216 (96%)  | 8 (4%)   | 1 (0%)   | 43          | 74  |
| 5   | E     | 228/233 (98%)   | 214 (94%)  | 12 (5%)  | 2 (1%)   | 25          | 52  |
| 5   | S     | 228/233 (98%)   | 211 (92%)  | 14 (6%)  | 3 (1%)   | 18          | 39  |
| 6   | F     | 240/242 (99%)   | 228 (95%)  | 11 (5%)  | 1 (0%)   | 43          | 74  |
| 6   | T     | 240/242 (99%)   | 225 (94%)  | 12 (5%)  | 3 (1%)   | 18          | 39  |
| 7   | G     | 238/243 (98%)   | 225 (94%)  | 13 (6%)  | 0        | 100         | 100 |
| 7   | U     | 238/243 (98%)   | 229 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 8   | H     | 220/222 (99%)   | 209 (95%)  | 11 (5%)  | 0        | 100         | 100 |
| 8   | V     | 220/222 (99%)   | 210 (96%)  | 10 (4%)  | 0        | 100         | 100 |
| 9   | I     | 202/204 (99%)   | 196 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 9   | W     | 202/204 (99%)   | 192 (95%)  | 10 (5%)  | 0        | 100         | 100 |
| 10  | J     | 196/198 (99%)   | 188 (96%)  | 7 (4%)   | 1 (0%)   | 38          | 68  |
| 10  | X     | 196/198 (99%)   | 188 (96%)  | 7 (4%)   | 1 (0%)   | 38          | 68  |
| 11  | K     | 210/212 (99%)   | 204 (97%)  | 5 (2%)   | 1 (0%)   | 38          | 68  |
| 11  | Y     | 210/212 (99%)   | 201 (96%)  | 9 (4%)   | 0        | 100         | 100 |
| 12  | L     | 220/222 (99%)   | 214 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 12  | Z     | 220/222 (99%)   | 217 (99%)  | 3 (1%)   | 0        | 100         | 100 |
| 13  | 1     | 231/233 (99%)   | 221 (96%)  | 8 (4%)   | 2 (1%)   | 25          | 52  |
| 13  | M     | 231/233 (99%)   | 221 (96%)  | 9 (4%)   | 1 (0%)   | 43          | 74  |
| 14  | 2     | 194/196 (99%)   | 186 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 14  | N     | 194/196 (99%)   | 189 (97%)  | 5 (3%)   | 0        | 100         | 100 |
| All | All   | 6233/6382 (98%) | 5958 (96%) | 241 (4%) | 34 (0%)  | 38          | 68  |

All (34) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | C     | 58     | LEU  |
| 4   | D     | 180(E) | SER  |
| 11  | K     | 180    | GLU  |
| 2   | P     | 218(C) | ASP  |
| 3   | Q     | 58     | LEU  |
| 3   | Q     | 203    | THR  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 6   | T     | 13     | SER  |
| 2   | B     | 54     | VAL  |
| 2   | B     | 218(C) | ASP  |
| 6   | F     | 13     | SER  |
| 13  | M     | 1      | SER  |
| 1   | O     | 167    | LYS  |
| 5   | S     | 199    | GLN  |
| 5   | S     | 202    | ARG  |
| 1   | A     | 167    | LYS  |
| 3   | C     | 183    | PRO  |
| 3   | C     | 203    | THR  |
| 5   | E     | 203    | ASP  |
| 5   | E     | 217    | LYS  |
| 1   | O     | 53     | LYS  |
| 2   | P     | 54     | VAL  |
| 2   | P     | 218(D) | GLY  |
| 3   | Q     | 183    | PRO  |
| 6   | T     | 8      | TYR  |
| 3   | C     | 55     | THR  |
| 2   | P     | 62     | ASP  |
| 4   | R     | 180(D) | SER  |
| 10  | X     | 8      | VAL  |
| 10  | J     | 8      | VAL  |
| 6   | T     | 206    | LYS  |
| 13  | 1     | 72     | ALA  |
| 5   | S     | 186    | PRO  |
| 2   | B     | 218(D) | GLY  |
| 13  | 1     | 220    | GLY  |

### 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     | 205/209 (98%)  | 199 (97%) | 6 (3%)   | 55          | 83 |
| 1   | O     | 205/209 (98%)  | 197 (96%) | 8 (4%)   | 43          | 74 |
| 2   | B     | 194/195 (100%) | 179 (92%) | 15 (8%)  | 18          | 38 |
| 2   | P     | 194/195 (100%) | 179 (92%) | 15 (8%)  | 18          | 38 |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 3   | C     | 210/213 (99%)   | 192 (91%)  | 18 (9%)  | 15          | 31 |
| 3   | Q     | 210/213 (99%)   | 195 (93%)  | 15 (7%)  | 21          | 43 |
| 4   | D     | 186/215 (86%)   | 171 (92%)  | 15 (8%)  | 17          | 34 |
| 4   | R     | 186/215 (86%)   | 173 (93%)  | 13 (7%)  | 21          | 44 |
| 5   | E     | 187/191 (98%)   | 167 (89%)  | 20 (11%) | 10          | 20 |
| 5   | S     | 187/191 (98%)   | 167 (89%)  | 20 (11%) | 10          | 20 |
| 6   | F     | 200/200 (100%)  | 179 (90%)  | 21 (10%) | 10          | 21 |
| 6   | T     | 200/200 (100%)  | 179 (90%)  | 21 (10%) | 10          | 21 |
| 7   | G     | 205/207 (99%)   | 190 (93%)  | 15 (7%)  | 20          | 41 |
| 7   | U     | 205/207 (99%)   | 193 (94%)  | 12 (6%)  | 28          | 54 |
| 8   | H     | 181/181 (100%)  | 171 (94%)  | 10 (6%)  | 30          | 57 |
| 8   | V     | 181/181 (100%)  | 173 (96%)  | 8 (4%)   | 39          | 69 |
| 9   | I     | 172/172 (100%)  | 161 (94%)  | 11 (6%)  | 25          | 49 |
| 9   | W     | 172/172 (100%)  | 165 (96%)  | 7 (4%)   | 41          | 72 |
| 10  | J     | 174/175 (99%)   | 164 (94%)  | 10 (6%)  | 29          | 56 |
| 10  | X     | 174/175 (99%)   | 158 (91%)  | 16 (9%)  | 13          | 27 |
| 11  | K     | 169/169 (100%)  | 153 (90%)  | 16 (10%) | 12          | 25 |
| 11  | Y     | 169/169 (100%)  | 159 (94%)  | 10 (6%)  | 28          | 54 |
| 12  | L     | 185/185 (100%)  | 172 (93%)  | 13 (7%)  | 21          | 44 |
| 12  | Z     | 185/185 (100%)  | 176 (95%)  | 9 (5%)   | 35          | 64 |
| 13  | 1     | 199/199 (100%)  | 191 (96%)  | 8 (4%)   | 42          | 73 |
| 13  | M     | 199/199 (100%)  | 189 (95%)  | 10 (5%)  | 34          | 63 |
| 14  | 2     | 162/162 (100%)  | 151 (93%)  | 11 (7%)  | 22          | 46 |
| 14  | N     | 162/162 (100%)  | 155 (96%)  | 7 (4%)   | 40          | 70 |
| All | All   | 5258/5346 (98%) | 4898 (93%) | 360 (7%) | 22          | 46 |

All (360) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 62     | GLU  |
| 1   | A     | 64     | LEU  |
| 1   | A     | 147(A) | SER  |
| 1   | A     | 158    | PHE  |
| 1   | A     | 212    | LEU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | A     | 222    | ARG  |
| 2   | B     | 58     | LEU  |
| 2   | B     | 61     | GLN  |
| 2   | B     | 62     | ASP  |
| 2   | B     | 63     | THR  |
| 2   | B     | 71     | ASN  |
| 2   | B     | 91     | THR  |
| 2   | B     | 104    | ASN  |
| 2   | B     | 121    | GLN  |
| 2   | B     | 150    | THR  |
| 2   | B     | 185    | LYS  |
| 2   | B     | 187    | ASP  |
| 2   | B     | 192    | LEU  |
| 2   | B     | 202    | THR  |
| 2   | B     | 216    | ARG  |
| 2   | B     | 218(C) | ASP  |
| 3   | C     | 18     | ASP  |
| 3   | C     | 44     | ASN  |
| 3   | C     | 55     | THR  |
| 3   | C     | 57     | LYS  |
| 3   | C     | 66     | LYS  |
| 3   | C     | 82     | ASN  |
| 3   | C     | 87     | ILE  |
| 3   | C     | 121    | GLN  |
| 3   | C     | 150    | GLN  |
| 3   | C     | 156    | ILE  |
| 3   | C     | 163    | GLN  |
| 3   | C     | 172    | VAL  |
| 3   | C     | 174    | GLU  |
| 3   | C     | 178    | LYS  |
| 3   | C     | 208    | LYS  |
| 3   | C     | 209    | ASN  |
| 3   | C     | 215    | VAL  |
| 3   | C     | 226    | SER  |
| 4   | D     | 27     | SER  |
| 4   | D     | 28     | LEU  |
| 4   | D     | 52     | LYS  |
| 4   | D     | 59     | LEU  |
| 4   | D     | 76     | CYS  |
| 4   | D     | 86     | ARG  |
| 4   | D     | 110    | GLU  |
| 4   | D     | 119    | LEU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 4   | D     | 170    | GLU  |
| 4   | D     | 177    | LEU  |
| 4   | D     | 184    | LEU  |
| 4   | D     | 191    | LEU  |
| 4   | D     | 194    | LEU  |
| 4   | D     | 215    | ILE  |
| 4   | D     | 238    | LYS  |
| 5   | E     | 12     | THR  |
| 5   | E     | 13     | VAL  |
| 5   | E     | 28     | LEU  |
| 5   | E     | 58     | LEU  |
| 5   | E     | 64     | GLN  |
| 5   | E     | 76     | LEU  |
| 5   | E     | 90     | ASN  |
| 5   | E     | 111    | ARG  |
| 5   | E     | 121    | GLN  |
| 5   | E     | 149    | LEU  |
| 5   | E     | 168    | ARG  |
| 5   | E     | 185    | ASN  |
| 5   | E     | 189    | LEU  |
| 5   | E     | 198    | SER  |
| 5   | E     | 207    | LEU  |
| 5   | E     | 208(C) | VAL  |
| 5   | E     | 209(D) | ASP  |
| 5   | E     | 219    | THR  |
| 5   | E     | 222    | THR  |
| 5   | E     | 231    | LYS  |
| 6   | F     | 9      | ASP  |
| 6   | F     | 18     | ASP  |
| 6   | F     | 43     | ASN  |
| 6   | F     | 98     | SER  |
| 6   | F     | 121    | GLN  |
| 6   | F     | 127    | ASN  |
| 6   | F     | 129    | VAL  |
| 6   | F     | 135    | SER  |
| 6   | F     | 136    | THR  |
| 6   | F     | 167    | LYS  |
| 6   | F     | 169    | ARG  |
| 6   | F     | 171    | SER  |
| 6   | F     | 176    | LEU  |
| 6   | F     | 180(E) | GLU  |
| 6   | F     | 187    | ARG  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 6   | F     | 192    | GLN  |
| 6   | F     | 203    | GLU  |
| 6   | F     | 205    | ASN  |
| 6   | F     | 206(B) | GLU  |
| 6   | F     | 214    | TRP  |
| 6   | F     | 240    | ILE  |
| 7   | G     | 29     | LYS  |
| 7   | G     | 38     | LEU  |
| 7   | G     | 72     | ARG  |
| 7   | G     | 87     | ASN  |
| 7   | G     | 119    | LEU  |
| 7   | G     | 121    | GLN  |
| 7   | G     | 124    | THR  |
| 7   | G     | 169    | GLN  |
| 7   | G     | 197    | MET  |
| 7   | G     | 203    | THR  |
| 7   | G     | 204    | GLU  |
| 7   | G     | 217    | LYS  |
| 7   | G     | 232    | ARG  |
| 7   | G     | 233    | LEU  |
| 7   | G     | 240    | ASP  |
| 8   | H     | 7      | LYS  |
| 8   | H     | 30     | ASN  |
| 8   | H     | 34     | LEU  |
| 8   | H     | 55     | VAL  |
| 8   | H     | 63     | ILE  |
| 8   | H     | 68     | LEU  |
| 8   | H     | 101    | VAL  |
| 8   | H     | 113    | ILE  |
| 8   | H     | 144    | GLN  |
| 8   | H     | 223    | ASP  |
| 9   | I     | -8     | SER  |
| 9   | I     | 4      | VAL  |
| 9   | I     | 29     | ASN  |
| 9   | I     | 104    | ILE  |
| 9   | I     | 122(A) | LYS  |
| 9   | I     | 144    | PRO  |
| 9   | I     | 159    | LEU  |
| 9   | I     | 160    | LEU  |
| 9   | I     | 171    | TRP  |
| 9   | I     | 174    | VAL  |
| 9   | I     | 182    | ASP  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 10  | J     | 6      | ILE  |
| 10  | J     | 34     | THR  |
| 10  | J     | 52     | THR  |
| 10  | J     | 68     | ILE  |
| 10  | J     | 70     | GLU  |
| 10  | J     | 77     | GLN  |
| 10  | J     | 90     | SER  |
| 10  | J     | 105(B) | LYS  |
| 10  | J     | 130    | SER  |
| 10  | J     | 166    | MET  |
| 11  | K     | 4      | LEU  |
| 11  | K     | 7      | ARG  |
| 11  | K     | 9      | GLN  |
| 11  | K     | 31     | VAL  |
| 11  | K     | 41     | LEU  |
| 11  | K     | 65     | LEU  |
| 11  | K     | 73     | ARG  |
| 11  | K     | 87     | VAL  |
| 11  | K     | 91     | LYS  |
| 11  | K     | 99     | THR  |
| 11  | K     | 105(A) | ARG  |
| 11  | K     | 105(B) | LYS  |
| 11  | K     | 121    | LYS  |
| 11  | K     | 143    | LYS  |
| 11  | K     | 175    | LEU  |
| 11  | K     | 201    | GLU  |
| 12  | L     | -9     | GLN  |
| 12  | L     | -7     | ASN  |
| 12  | L     | 4      | LEU  |
| 12  | L     | 14     | LEU  |
| 12  | L     | 25     | SER  |
| 12  | L     | 40     | ASN  |
| 12  | L     | 58     | ARG  |
| 12  | L     | 99     | THR  |
| 12  | L     | 118    | SER  |
| 12  | L     | 123    | GLN  |
| 12  | L     | 138    | LEU  |
| 12  | L     | 144(K) | LYS  |
| 12  | L     | 144(P) | LEU  |
| 13  | M     | 39     | ASN  |
| 13  | M     | 61     | LEU  |
| 13  | M     | 64     | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 13  | M     | 95     | ARG  |
| 13  | M     | 152    | ARG  |
| 13  | M     | 162    | GLN  |
| 13  | M     | 178    | ARG  |
| 13  | M     | 185    | ASN  |
| 13  | M     | 195    | THR  |
| 13  | M     | 217    | LYS  |
| 14  | N     | 20     | THR  |
| 14  | N     | 105    | ASP  |
| 14  | N     | 105(A) | ASP  |
| 14  | N     | 105(B) | LYS  |
| 14  | N     | 119    | VAL  |
| 14  | N     | 149    | GLU  |
| 14  | N     | 178    | LEU  |
| 1   | O     | 32     | LYS  |
| 1   | O     | 33     | GLN  |
| 1   | O     | 54     | SER  |
| 1   | O     | 64     | LEU  |
| 1   | O     | 65     | SER  |
| 1   | O     | 110    | LYS  |
| 1   | O     | 158    | PHE  |
| 1   | O     | 212    | LEU  |
| 2   | P     | 55     | THR  |
| 2   | P     | 57     | THR  |
| 2   | P     | 58     | LEU  |
| 2   | P     | 90     | ASN  |
| 2   | P     | 91     | THR  |
| 2   | P     | 121    | GLN  |
| 2   | P     | 150    | THR  |
| 2   | P     | 156    | ASN  |
| 2   | P     | 170    | SER  |
| 2   | P     | 181    | LYS  |
| 2   | P     | 185    | LYS  |
| 2   | P     | 192    | LEU  |
| 2   | P     | 203    | ASP  |
| 2   | P     | 204(A) | SER  |
| 2   | P     | 212    | PHE  |
| 3   | Q     | 18     | ASP  |
| 3   | Q     | 35     | THR  |
| 3   | Q     | 57     | LYS  |
| 3   | Q     | 61     | THR  |
| 3   | Q     | 75     | VAL  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 3   | Q     | 82     | ASN  |
| 3   | Q     | 121    | GLN  |
| 3   | Q     | 150    | GLN  |
| 3   | Q     | 156    | ILE  |
| 3   | Q     | 163    | GLN  |
| 3   | Q     | 172    | VAL  |
| 3   | Q     | 208    | LYS  |
| 3   | Q     | 209    | ASN  |
| 3   | Q     | 215    | VAL  |
| 3   | Q     | 240    | LYS  |
| 4   | R     | 48     | LEU  |
| 4   | R     | 59     | LEU  |
| 4   | R     | 62     | ASP  |
| 4   | R     | 76     | CYS  |
| 4   | R     | 86     | ARG  |
| 4   | R     | 119    | LEU  |
| 4   | R     | 177    | LEU  |
| 4   | R     | 180(E) | SER  |
| 4   | R     | 184    | LEU  |
| 4   | R     | 191    | LEU  |
| 4   | R     | 194    | LEU  |
| 4   | R     | 207    | LEU  |
| 4   | R     | 215    | ILE  |
| 5   | S     | 11     | ASP  |
| 5   | S     | 12     | THR  |
| 5   | S     | 13     | VAL  |
| 5   | S     | 32     | LYS  |
| 5   | S     | 33     | GLN  |
| 5   | S     | 43     | ASN  |
| 5   | S     | 58     | LEU  |
| 5   | S     | 76     | LEU  |
| 5   | S     | 111    | ARG  |
| 5   | S     | 121    | GLN  |
| 5   | S     | 168    | ARG  |
| 5   | S     | 185    | ASN  |
| 5   | S     | 189    | LEU  |
| 5   | S     | 198    | SER  |
| 5   | S     | 199    | GLN  |
| 5   | S     | 209(D) | ASP  |
| 5   | S     | 211    | SER  |
| 5   | S     | 219    | THR  |
| 5   | S     | 227    | GLU  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 5   | S     | 231    | LYS  |
| 6   | T     | 20     | ARG  |
| 6   | T     | 22     | PHE  |
| 6   | T     | 36     | THR  |
| 6   | T     | 43     | ASN  |
| 6   | T     | 98     | SER  |
| 6   | T     | 121    | GLN  |
| 6   | T     | 127    | ASN  |
| 6   | T     | 135    | SER  |
| 6   | T     | 143    | LYS  |
| 6   | T     | 169    | ARG  |
| 6   | T     | 170    | GLN  |
| 6   | T     | 171    | SER  |
| 6   | T     | 176    | LEU  |
| 6   | T     | 180(E) | GLU  |
| 6   | T     | 187    | ARG  |
| 6   | T     | 192    | GLN  |
| 6   | T     | 203    | GLU  |
| 6   | T     | 205    | ASN  |
| 6   | T     | 206(B) | GLU  |
| 6   | T     | 206(C) | LYS  |
| 6   | T     | 214    | TRP  |
| 7   | U     | 29     | LYS  |
| 7   | U     | 38     | LEU  |
| 7   | U     | 72     | ARG  |
| 7   | U     | 76     | MET  |
| 7   | U     | 87     | ASN  |
| 7   | U     | 119    | LEU  |
| 7   | U     | 121    | GLN  |
| 7   | U     | 204    | GLU  |
| 7   | U     | 217    | LYS  |
| 7   | U     | 232    | ARG  |
| 7   | U     | 233    | LEU  |
| 7   | U     | 239    | GLN  |
| 8   | V     | 13     | VAL  |
| 8   | V     | 30     | ASN  |
| 8   | V     | 34     | LEU  |
| 8   | V     | 55     | VAL  |
| 8   | V     | 68     | LEU  |
| 8   | V     | 113    | ILE  |
| 8   | V     | 144    | GLN  |
| 8   | V     | 221    | ILE  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 9   | W     | -8     | SER  |
| 9   | W     | 16     | CYS  |
| 9   | W     | 29     | ASN  |
| 9   | W     | 160    | LEU  |
| 9   | W     | 171    | TRP  |
| 9   | W     | 181    | LYS  |
| 9   | W     | 182    | ASP  |
| 10  | X     | 6      | ILE  |
| 10  | X     | 9      | GLN  |
| 10  | X     | 24     | ILE  |
| 10  | X     | 34     | THR  |
| 10  | X     | 52     | THR  |
| 10  | X     | 68     | ILE  |
| 10  | X     | 70     | GLU  |
| 10  | X     | 77     | GLN  |
| 10  | X     | 90     | SER  |
| 10  | X     | 90(A)  | ILE  |
| 10  | X     | 90(B)  | ARG  |
| 10  | X     | 105(B) | LYS  |
| 10  | X     | 120    | VAL  |
| 10  | X     | 137    | LEU  |
| 10  | X     | 166    | MET  |
| 10  | X     | 191    | GLN  |
| 11  | Y     | 4      | LEU  |
| 11  | Y     | 9      | GLN  |
| 11  | Y     | 41     | LEU  |
| 11  | Y     | 65     | LEU  |
| 11  | Y     | 87     | VAL  |
| 11  | Y     | 105(A) | ARG  |
| 11  | Y     | 145    | ASP  |
| 11  | Y     | 146    | LEU  |
| 11  | Y     | 208    | ASN  |
| 11  | Y     | 210    | ILE  |
| 12  | Z     | -9     | GLN  |
| 12  | Z     | -7     | ASN  |
| 12  | Z     | 2      | THR  |
| 12  | Z     | 14     | LEU  |
| 12  | Z     | 25     | SER  |
| 12  | Z     | 40     | ASN  |
| 12  | Z     | 118    | SER  |
| 12  | Z     | 138    | LEU  |
| 12  | Z     | 144(J) | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 13  | 1     | 39     | ASN  |
| 13  | 1     | 61     | LEU  |
| 13  | 1     | 95     | ARG  |
| 13  | 1     | 152    | ARG  |
| 13  | 1     | 161    | VAL  |
| 13  | 1     | 195    | THR  |
| 13  | 1     | 203    | LEU  |
| 13  | 1     | 217    | LYS  |
| 14  | 2     | 20     | THR  |
| 14  | 2     | 22     | THR  |
| 14  | 2     | 36     | ARG  |
| 14  | 2     | 105    | ASP  |
| 14  | 2     | 105(A) | ASP  |
| 14  | 2     | 105(B) | LYS  |
| 14  | 2     | 119    | VAL  |
| 14  | 2     | 132    | THR  |
| 14  | 2     | 149    | GLU  |
| 14  | 2     | 186    | ARG  |
| 14  | 2     | 187(I) | GLN  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 97  | HIS  |
| 2   | B     | 23  | GLN  |
| 2   | B     | 71  | ASN  |
| 2   | B     | 97  | GLN  |
| 2   | B     | 121 | GLN  |
| 2   | B     | 125 | GLN  |
| 2   | B     | 156 | ASN  |
| 2   | B     | 177 | GLN  |
| 3   | C     | 20  | HIS  |
| 3   | C     | 23  | GLN  |
| 3   | C     | 82  | ASN  |
| 3   | C     | 97  | GLN  |
| 3   | C     | 121 | GLN  |
| 3   | C     | 125 | GLN  |
| 3   | C     | 150 | GLN  |
| 3   | C     | 163 | GLN  |
| 3   | C     | 209 | ASN  |
| 4   | D     | 23  | GLN  |
| 4   | D     | 108 | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 4   | D     | 141    | HIS  |
| 4   | D     | 199    | GLN  |
| 4   | D     | 226    | ASN  |
| 5   | E     | 73     | HIS  |
| 5   | E     | 97     | ASN  |
| 5   | E     | 121    | GLN  |
| 5   | E     | 125    | GLN  |
| 5   | E     | 185    | ASN  |
| 5   | E     | 199    | GLN  |
| 5   | E     | 209(E) | ASN  |
| 6   | F     | 12     | ASN  |
| 6   | F     | 23     | GLN  |
| 6   | F     | 43     | ASN  |
| 6   | F     | 90     | ASN  |
| 6   | F     | 121    | GLN  |
| 6   | F     | 127    | ASN  |
| 6   | F     | 192    | GLN  |
| 7   | G     | 11     | HIS  |
| 7   | G     | 34(A)  | ASN  |
| 7   | G     | 87     | ASN  |
| 7   | G     | 118    | ASN  |
| 7   | G     | 121    | GLN  |
| 7   | G     | 125    | GLN  |
| 7   | G     | 169    | GLN  |
| 7   | G     | 170    | GLN  |
| 7   | G     | 178    | ASN  |
| 7   | G     | 184    | ASN  |
| 8   | H     | 66     | HIS  |
| 8   | H     | 144    | GLN  |
| 8   | H     | 165    | ASN  |
| 8   | H     | 172    | ASN  |
| 10  | J     | 54     | GLN  |
| 10  | J     | 77     | GLN  |
| 10  | J     | 85     | GLN  |
| 10  | J     | 112    | GLN  |
| 10  | J     | 140    | HIS  |
| 10  | J     | 186    | GLN  |
| 11  | K     | 9      | GLN  |
| 11  | K     | 85     | ASN  |
| 11  | K     | 131    | GLN  |
| 11  | K     | 174    | ASN  |
| 11  | K     | 208    | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 12  | L     | -7     | ASN  |
| 12  | L     | 40     | ASN  |
| 12  | L     | 67     | HIS  |
| 12  | L     | 70(A)  | ASN  |
| 12  | L     | 123    | GLN  |
| 12  | L     | 144(B) | ASN  |
| 12  | L     | 166    | HIS  |
| 13  | M     | 9      | ASN  |
| 13  | M     | 39     | ASN  |
| 13  | M     | 93     | GLN  |
| 13  | M     | 162    | GLN  |
| 13  | M     | 170    | ASN  |
| 13  | M     | 204    | GLN  |
| 14  | N     | 145    | ASN  |
| 14  | N     | 157    | HIS  |
| 14  | N     | 161    | GLN  |
| 1   | O     | 97     | HIS  |
| 2   | P     | 23     | GLN  |
| 2   | P     | 71     | ASN  |
| 2   | P     | 97     | GLN  |
| 2   | P     | 121    | GLN  |
| 2   | P     | 125    | GLN  |
| 2   | P     | 156    | ASN  |
| 2   | P     | 177    | GLN  |
| 2   | P     | 218    | ASN  |
| 3   | Q     | 23     | GLN  |
| 3   | Q     | 82     | ASN  |
| 3   | Q     | 121    | GLN  |
| 3   | Q     | 125    | GLN  |
| 3   | Q     | 150    | GLN  |
| 3   | Q     | 163    | GLN  |
| 3   | Q     | 179    | ASN  |
| 3   | Q     | 243    | GLN  |
| 4   | R     | 23     | GLN  |
| 4   | R     | 108    | ASN  |
| 4   | R     | 147    | GLN  |
| 4   | R     | 199    | GLN  |
| 4   | R     | 226    | ASN  |
| 5   | S     | 73     | HIS  |
| 5   | S     | 104    | ASN  |
| 5   | S     | 121    | GLN  |
| 5   | S     | 123    | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 5   | S     | 125    | GLN  |
| 5   | S     | 185    | ASN  |
| 5   | S     | 199    | GLN  |
| 5   | S     | 209(E) | ASN  |
| 6   | T     | 23     | GLN  |
| 6   | T     | 43     | ASN  |
| 6   | T     | 90     | ASN  |
| 6   | T     | 121    | GLN  |
| 6   | T     | 127    | ASN  |
| 6   | T     | 147    | HIS  |
| 6   | T     | 192    | GLN  |
| 6   | T     | 237    | GLN  |
| 7   | U     | 11     | HIS  |
| 7   | U     | 34(A)  | ASN  |
| 7   | U     | 87     | ASN  |
| 7   | U     | 118    | ASN  |
| 7   | U     | 121    | GLN  |
| 7   | U     | 125    | GLN  |
| 7   | U     | 170    | GLN  |
| 7   | U     | 178    | ASN  |
| 7   | U     | 180(C) | HIS  |
| 7   | U     | 184    | ASN  |
| 8   | V     | 30     | ASN  |
| 8   | V     | 35     | HIS  |
| 8   | V     | 66     | HIS  |
| 8   | V     | 86     | HIS  |
| 8   | V     | 144    | GLN  |
| 8   | V     | 165    | ASN  |
| 8   | V     | 172    | ASN  |
| 8   | V     | 190    | ASN  |
| 9   | W     | 81     | GLN  |
| 9   | W     | 145    | ASN  |
| 10  | X     | 54     | GLN  |
| 10  | X     | 77     | GLN  |
| 10  | X     | 85     | GLN  |
| 10  | X     | 112    | GLN  |
| 10  | X     | 127    | HIS  |
| 10  | X     | 186    | GLN  |
| 11  | Y     | 85     | ASN  |
| 11  | Y     | 141    | ASN  |
| 11  | Y     | 174    | ASN  |
| 11  | Y     | 208    | ASN  |

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| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 12  | Z     | -9     | GLN  |
| 12  | Z     | -7     | ASN  |
| 12  | Z     | 40     | ASN  |
| 12  | Z     | 61     | ASN  |
| 12  | Z     | 67     | HIS  |
| 12  | Z     | 70(A)  | ASN  |
| 12  | Z     | 144(B) | ASN  |
| 12  | Z     | 144(J) | ASN  |
| 12  | Z     | 166    | HIS  |
| 13  | 1     | 9      | ASN  |
| 13  | 1     | 39     | ASN  |
| 13  | 1     | 69     | ASN  |
| 13  | 1     | 93     | GLN  |
| 13  | 1     | 162    | GLN  |
| 13  | 1     | 170    | ASN  |
| 13  | 1     | 185    | ASN  |
| 13  | 1     | 204    | GLN  |
| 14  | 2     | 69     | GLN  |
| 14  | 2     | 141    | ASN  |
| 14  | 2     | 157    | HIS  |
| 14  | 2     | 161    | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 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  | 3SD  | K     | 302 | -    | 44,44,44     | 0.89 | 3 (6%)      | 60,60,60    | 1.42 | 4 (6%)      |
| 17  | MES  | K     | 303 | -    | 12,12,12     | 1.88 | 1 (8%)      | 16,16,16    | 1.30 | 2 (12%)     |
| 16  | 3SD  | Y     | 302 | -    | 44,44,44     | 1.11 | 4 (9%)      | 60,60,60    | 1.54 | 4 (6%)      |
| 17  | MES  | Y     | 303 | -    | 12,12,12     | 2.11 | 1 (8%)      | 16,16,16    | 1.37 | 3 (18%)     |

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  | 3SD  | K     | 302 | -    | -       | 1/39/40/40 | 0/3/3/3 |
| 17  | MES  | K     | 303 | -    | -       | 0/6/14/14  | 0/1/1/1 |
| 16  | 3SD  | Y     | 302 | -    | -       | 1/39/40/40 | 0/3/3/3 |
| 17  | MES  | Y     | 303 | -    | -       | 0/6/14/14  | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 17  | Y     | 303 | MES  | C8-S  | -6.63 | 1.66        | 1.78     |
| 17  | K     | 303 | MES  | C8-S  | -5.83 | 1.67        | 1.78     |
| 16  | Y     | 302 | 3SD  | C6-C5 | 3.58  | 1.53        | 1.48     |
| 16  | Y     | 302 | 3SD  | O1-N2 | 3.57  | 1.45        | 1.42     |
| 16  | K     | 302 | 3SD  | C6-C5 | 3.39  | 1.53        | 1.48     |
| 16  | Y     | 302 | 3SD  | C4-C3 | -2.95 | 1.34        | 1.40     |
| 16  | K     | 302 | 3SD  | C4-C3 | -2.70 | 1.34        | 1.40     |
| 16  | Y     | 302 | 3SD  | C3-N2 | -2.40 | 1.33        | 1.38     |
| 16  | K     | 302 | 3SD  | C3-N2 | -2.33 | 1.33        | 1.38     |

All (13) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 16  | Y     | 302 | 3SD  | C5-O1-N2 | -8.89 | 104.77      | 107.66   |
| 16  | K     | 302 | 3SD  | C5-O1-N2 | -7.22 | 105.31      | 107.66   |
| 16  | Y     | 302 | 3SD  | O1-C5-C6 | 4.19  | 125.61      | 117.16   |
| 16  | K     | 302 | 3SD  | O1-C5-C6 | 3.80  | 124.83      | 117.16   |

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| Mol | Chain | Res | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 16  | Y     | 302 | 3SD  | C3-C4-C5   | 3.61  | 108.38      | 105.90   |
| 17  | K     | 303 | MES  | O3S-S-C8   | 2.74  | 113.07      | 105.99   |
| 16  | K     | 302 | 3SD  | C9-C8-C10  | -2.74 | 103.70      | 110.40   |
| 16  | K     | 302 | 3SD  | C9-C33-N34 | -2.64 | 112.20      | 116.02   |
| 17  | Y     | 303 | MES  | C8-C7-N4   | -2.60 | 107.99      | 112.44   |
| 17  | Y     | 303 | MES  | O1-C6-C5   | -2.48 | 108.39      | 111.34   |
| 17  | K     | 303 | MES  | O1-C6-C5   | -2.24 | 108.67      | 111.34   |
| 17  | Y     | 303 | MES  | O3S-S-C8   | 2.08  | 111.36      | 105.99   |
| 16  | Y     | 302 | 3SD  | C9-C8-C10  | -2.05 | 105.38      | 110.40   |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms        |
|-----|-------|-----|------|--------------|
| 16  | K     | 302 | 3SD  | C4-C3-C41-N7 |
| 16  | Y     | 302 | 3SD  | C4-C3-C41-N7 |

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed       | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 246/250 (98%)  | -0.26  | 3 (1%) 75 79  | 31, 43, 64, 89        | 0     |
| 1   | O     | 246/250 (98%)  | -0.06  | 3 (1%) 75 79  | 32, 50, 74, 94        | 0     |
| 2   | B     | 235/235 (100%) | 0.14   | 13 (5%) 24 25 | 26, 51, 82, 90        | 0     |
| 2   | P     | 235/235 (100%) | 0.14   | 8 (3%) 43 46  | 27, 51, 85, 94        | 0     |
| 3   | C     | 238/241 (98%)  | 0.23   | 17 (7%) 16 16 | 31, 59, 103, 118      | 0     |
| 3   | Q     | 238/241 (98%)  | 0.54   | 22 (9%) 9 8   | 34, 63, 111, 127      | 0     |
| 4   | D     | 228/260 (87%)  | -0.16  | 1 (0%) 90 93  | 28, 51, 73, 95        | 0     |
| 4   | R     | 229/260 (88%)  | 0.03   | 6 (2%) 53 56  | 29, 53, 77, 102       | 0     |
| 5   | E     | 230/233 (98%)  | -0.08  | 5 (2%) 59 63  | 37, 52, 78, 92        | 0     |
| 5   | S     | 230/233 (98%)  | 0.20   | 13 (5%) 23 24 | 34, 54, 89, 99        | 0     |
| 6   | F     | 242/242 (100%) | 0.10   | 12 (4%) 28 29 | 29, 49, 85, 109       | 0     |
| 6   | T     | 242/242 (100%) | 0.19   | 9 (3%) 39 42  | 29, 48, 76, 109       | 0     |
| 7   | G     | 240/243 (98%)  | -0.28  | 2 (0%) 83 86  | 28, 42, 68, 99        | 0     |
| 7   | U     | 240/243 (98%)  | -0.32  | 2 (0%) 83 86  | 26, 42, 63, 85        | 0     |
| 8   | H     | 222/222 (100%) | -0.28  | 2 (0%) 81 84  | 27, 37, 56, 85        | 0     |
| 8   | V     | 222/222 (100%) | -0.27  | 2 (0%) 81 84  | 29, 41, 59, 87        | 0     |
| 9   | I     | 204/204 (100%) | -0.36  | 1 (0%) 88 91  | 25, 37, 53, 61        | 0     |
| 9   | W     | 204/204 (100%) | -0.38  | 1 (0%) 88 91  | 28, 38, 56, 62        | 0     |
| 10  | J     | 198/198 (100%) | -0.08  | 6 (3%) 48 51  | 28, 41, 57, 114       | 0     |
| 10  | X     | 198/198 (100%) | -0.09  | 5 (2%) 54 58  | 30, 42, 55, 115       | 0     |
| 11  | K     | 212/212 (100%) | -0.32  | 0 100 100     | 26, 37, 54, 63        | 0     |
| 11  | Y     | 212/212 (100%) | -0.26  | 1 (0%) 88 91  | 29, 39, 57, 61        | 0     |
| 12  | L     | 222/222 (100%) | -0.37  | 1 (0%) 88 91  | 27, 39, 58, 65        | 0     |
| 12  | Z     | 222/222 (100%) | -0.32  | 2 (0%) 81 84  | 24, 38, 57, 65        | 0     |

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| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2  |     |     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|----------|-----|-----|-----------------------|-------|
| 13  | 1     | 233/233 (100%)  | -0.34  | 3 (1%)   | 74  | 78  | 23, 35, 53, 62        | 0     |
| 13  | M     | 233/233 (100%)  | -0.35  | 2 (0%)   | 81  | 84  | 25, 39, 55, 61        | 0     |
| 14  | 2     | 196/196 (100%)  | -0.36  | 0        | 100 | 100 | 27, 35, 52, 69        | 0     |
| 14  | N     | 196/196 (100%)  | -0.37  | 0        | 100 | 100 | 26, 36, 52, 64        | 0     |
| All | All   | 6293/6382 (98%) | -0.13  | 142 (2%) | 57  | 61  | 23, 44, 80, 127       | 0     |

All (142) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 6   | T     | 8      | TYR  | 18.5 |
| 6   | T     | 10     | LEU  | 17.0 |
| 6   | T     | 9      | ASP  | 14.3 |
| 6   | F     | 9      | ASP  | 13.8 |
| 6   | F     | 10     | LEU  | 12.7 |
| 6   | T     | 7      | GLY  | 10.8 |
| 6   | T     | 11     | SER  | 10.7 |
| 6   | F     | 8      | TYR  | 9.9  |
| 10  | J     | 192    | ALA  | 9.8  |
| 6   | F     | 11     | SER  | 9.3  |
| 6   | F     | 7      | GLY  | 9.1  |
| 2   | B     | 217    | ALA  | 8.8  |
| 2   | B     | 218    | ASN  | 8.2  |
| 3   | C     | 55     | THR  | 8.1  |
| 2   | B     | 216(B) | GLY  | 8.1  |
| 2   | P     | 217    | ALA  | 8.0  |
| 2   | P     | 218    | ASN  | 7.1  |
| 3   | Q     | 54     | SER  | 6.7  |
| 6   | F     | 12     | ASN  | 6.7  |
| 3   | Q     | 56     | LEU  | 6.5  |
| 10  | X     | 193    | GLN  | 6.1  |
| 10  | J     | 193    | GLN  | 6.1  |
| 3   | Q     | 207    | ALA  | 6.0  |
| 5   | S     | 57     | GLU  | 5.9  |
| 7   | G     | 240    | ASP  | 5.7  |
| 3   | Q     | 55     | THR  | 5.3  |
| 10  | X     | 192    | ALA  | 5.2  |
| 10  | J     | 191    | GLN  | 5.0  |
| 3   | C     | 207    | ALA  | 5.0  |
| 10  | X     | 191    | GLN  | 5.0  |
| 13  | M     | -8     | THR  | 4.9  |
| 11  | Y     | 211    | GLY  | 4.9  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 3   | C     | 208    | LYS  | 4.7  |
| 3   | C     | 56     | LEU  | 4.6  |
| 5   | E     | 203    | ASP  | 4.5  |
| 3   | Q     | 203    | THR  | 4.4  |
| 3   | Q     | 243    | GLN  | 4.4  |
| 3   | Q     | 53     | ARG  | 4.2  |
| 3   | C     | 11     | ALA  | 4.1  |
| 5   | S     | 58     | LEU  | 4.0  |
| 10  | X     | 189    | ASP  | 3.9  |
| 3   | Q     | 242    | GLU  | 3.9  |
| 3   | C     | 203    | THR  | 3.9  |
| 5   | S     | 206    | SER  | 3.9  |
| 5   | S     | 203    | ASP  | 3.9  |
| 6   | F     | 204    | ASP  | 3.8  |
| 2   | P     | 63     | THR  | 3.7  |
| 2   | P     | 54     | VAL  | 3.7  |
| 9   | W     | -8     | SER  | 3.6  |
| 4   | D     | 22     | PHE  | 3.6  |
| 3   | Q     | 64     | PRO  | 3.5  |
| 2   | B     | 216(A) | LYS  | 3.5  |
| 3   | Q     | 202    | GLN  | 3.5  |
| 5   | S     | 63     | TYR  | 3.5  |
| 8   | V     | 223    | ASP  | 3.5  |
| 3   | Q     | 208    | LYS  | 3.4  |
| 10  | J     | 189    | ASP  | 3.4  |
| 3   | Q     | 209    | ASN  | 3.4  |
| 3   | Q     | 240    | LYS  | 3.4  |
| 3   | Q     | 241    | GLN  | 3.4  |
| 3   | C     | 54     | SER  | 3.4  |
| 3   | Q     | 63     | THR  | 3.4  |
| 13  | 1     | -8     | THR  | 3.4  |
| 5   | E     | 206    | SER  | 3.4  |
| 2   | B     | 54     | VAL  | 3.3  |
| 10  | J     | 168    | MET  | 3.3  |
| 9   | I     | -8     | SER  | 3.2  |
| 5   | S     | 8      | TYR  | 3.2  |
| 2   | B     | 218(C) | ASP  | 3.2  |
| 2   | P     | 216(B) | GLY  | 3.2  |
| 1   | O     | 236    | LEU  | 3.2  |
| 2   | B     | 127    | GLY  | 3.1  |
| 3   | Q     | 206    | GLY  | 3.1  |
| 5   | E     | 204    | GLU  | 3.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 8   | V     | 222    | CYS  | 3.0  |
| 5   | S     | 178    | ARG  | 3.0  |
| 8   | H     | 222    | CYS  | 2.9  |
| 2   | B     | 239    | THR  | 2.9  |
| 3   | C     | 53     | ARG  | 2.9  |
| 6   | F     | 206(B) | GLU  | 2.9  |
| 3   | Q     | 180(C) | LYS  | 2.8  |
| 6   | F     | 205    | ASN  | 2.8  |
| 4   | R     | 178    | ASN  | 2.8  |
| 5   | E     | 202    | ARG  | 2.8  |
| 12  | L     | -9     | GLN  | 2.8  |
| 2   | P     | 220    | TYR  | 2.8  |
| 7   | U     | 240    | ASP  | 2.8  |
| 2   | P     | 62     | ASP  | 2.8  |
| 7   | U     | 218    | ASP  | 2.8  |
| 6   | T     | 241    | ASN  | 2.7  |
| 13  | M     | 112    | SER  | 2.7  |
| 8   | H     | 223    | ASP  | 2.7  |
| 3   | C     | 202    | GLN  | 2.7  |
| 2   | B     | 220    | TYR  | 2.7  |
| 3   | Q     | 144(B) | ASP  | 2.7  |
| 2   | B     | 62     | ASP  | 2.6  |
| 3   | C     | 180(C) | LYS  | 2.6  |
| 5   | S     | 233    | ILE  | 2.6  |
| 4   | R     | 177    | LEU  | 2.5  |
| 2   | B     | 204(A) | SER  | 2.5  |
| 1   | A     | 9      | SER  | 2.5  |
| 4   | R     | 123    | PHE  | 2.5  |
| 5   | S     | 9      | ASP  | 2.5  |
| 3   | C     | 49     | GLY  | 2.4  |
| 3   | Q     | 238    | GLN  | 2.4  |
| 5   | S     | 202    | ARG  | 2.4  |
| 4   | R     | 231    | GLU  | 2.4  |
| 5   | E     | 57     | GLU  | 2.4  |
| 6   | F     | 203    | GLU  | 2.4  |
| 3   | C     | 22     | PHE  | 2.4  |
| 3   | Q     | 49     | GLY  | 2.3  |
| 1   | O     | 234    | GLU  | 2.3  |
| 1   | A     | 236    | LEU  | 2.3  |
| 7   | G     | 239    | GLN  | 2.3  |
| 3   | C     | 180(D) | GLU  | 2.3  |
| 1   | O     | 39     | GLY  | 2.3  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 3   | C     | 12     | LEU  | 2.3  |
| 13  | 1     | 72     | ALA  | 2.3  |
| 3   | Q     | 237    | GLU  | 2.3  |
| 4   | R     | 57     | PRO  | 2.3  |
| 5   | S     | 56     | ASP  | 2.3  |
| 12  | Z     | -9     | GLN  | 2.2  |
| 6   | T     | 12     | ASN  | 2.2  |
| 5   | S     | 51     | LEU  | 2.2  |
| 10  | X     | 168    | MET  | 2.2  |
| 12  | Z     | 144(R) | LYS  | 2.2  |
| 13  | 1     | 224    | ILE  | 2.2  |
| 6   | F     | 13     | SER  | 2.2  |
| 2   | P     | 218(C) | ASP  | 2.2  |
| 2   | B     | 22     | TYR  | 2.2  |
| 5   | S     | 180(E) | LYS  | 2.2  |
| 3   | C     | 142    | ASP  | 2.2  |
| 2   | B     | 218(D) | GLY  | 2.1  |
| 1   | A     | 183    | GLU  | 2.1  |
| 3   | C     | 242    | GLU  | 2.1  |
| 3   | C     | 227    | GLU  | 2.1  |
| 6   | T     | 180(E) | GLU  | 2.1  |
| 6   | T     | 206    | LYS  | 2.1  |
| 6   | F     | 241    | ASN  | 2.0  |
| 4   | R     | 235    | LYS  | 2.0  |
| 10  | J     | 188    | ASP  | 2.0  |
| 3   | Q     | 201    | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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 | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 15  | MG   | V     | 301  | 1/1   | 0.08 | -    | 42,42,42,42                 | 0     |
| 15  | MG   | T     | 302  | 1/1   | 0.44 | -    | 110,110,110,110             | 0     |
| 15  | MG   | W     | 201  | 1/1   | 0.16 | -    | 53,53,53,53                 | 0     |
| 15  | MG   | 2     | 201  | 1/1   | 0.13 | -    | 30,30,30,30                 | 0     |
| 15  | MG   | G     | 9001 | 1/1   | 0.07 | -    | 45,45,45,45                 | 0     |
| 15  | MG   | I     | 201  | 1/1   | 0.10 | -    | 46,46,46,46                 | 0     |
| 15  | MG   | I     | 202  | 1/1   | 0.25 | -    | 50,50,50,50                 | 0     |
| 17  | MES  | K     | 303  | 12/12 | 0.17 | -    | 55,57,58,58                 | 0     |
| 17  | MES  | Y     | 303  | 12/12 | 0.14 | -    | 57,61,64,64                 | 0     |
| 15  | MG   | W     | 202  | 1/1   | 0.13 | -    | 50,50,50,50                 | 0     |
| 15  | MG   | Z     | 202  | 1/1   | 0.14 | -    | 49,49,49,49                 | 0     |
| 15  | MG   | K     | 301  | 1/1   | 0.14 | -    | 50,50,50,50                 | 0     |
| 15  | MG   | T     | 301  | 1/1   | 0.28 | -    | 69,69,69,69                 | 0     |
| 15  | MG   | L     | 202  | 1/1   | 0.10 | -    | 46,46,46,46                 | 0     |
| 15  | MG   | F     | 301  | 1/1   | 1.08 | -    | 74,74,74,74                 | 0     |
| 16  | 3SD  | Y     | 302  | 42/42 | 0.17 | -    | 37,39,48,50                 | 0     |
| 15  | MG   | Z     | 201  | 1/1   | 0.13 | -    | 65,65,65,65                 | 0     |
| 16  | 3SD  | K     | 302  | 42/42 | 0.16 | -    | 28,35,49,50                 | 0     |
| 15  | MG   | N     | 201  | 1/1   | 0.15 | -    | 41,41,41,41                 | 0     |
| 15  | MG   | H     | 301  | 1/1   | 0.06 | -    | 47,47,47,47                 | 0     |
| 15  | MG   | L     | 201  | 1/1   | 0.11 | -    | 52,52,52,52                 | 0     |
| 15  | MG   | Y     | 301  | 1/1   | 0.12 | -    | 53,53,53,53                 | 0     |
| 15  | MG   | U     | 301  | 1/1   | 0.07 | -    | 38,38,38,38                 | 0     |
| 15  | MG   | F     | 302  | 1/1   | 0.59 | -    | 120,120,120,120             | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.