# Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 05:47 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 2GPL |
| Title | : | TMC-95 based biphenyl-ether macrocycles: specific proteasome inhibitors |
| Authors | : | Groll, M.; Goetz, M.; Kaiser, M.; Weyher, E.; Moroder, M. |
| Deposited on | : | 2006-04-18 |
| Resolution | : | 2.81 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

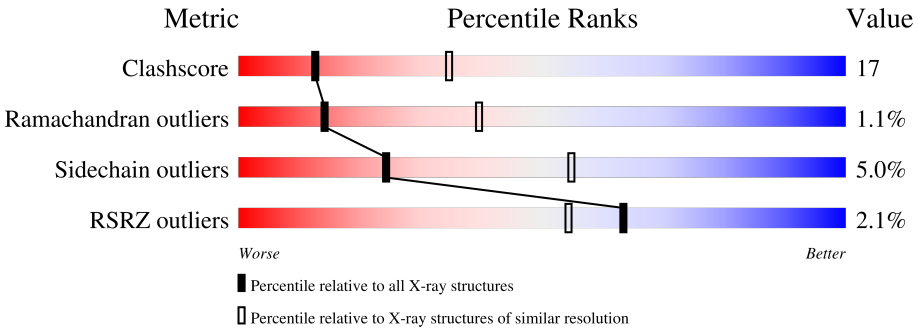
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 4060 (2.84-2.80) |
| Ramachandran outliers | 138981 | 3978 (2.84-2.80) |
| Sidechain outliers | 138945 | 3980 (2.84-2.80) |
| RSRZ outliers | 127900 | 3552 (2.84-2.80) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 250 | 78% 20% |
| 1 | O | 250 | 2% 76% 22% |
| 2 | B | 244 | 4% 63% 31% 6% |
| 2 | P | 244 | 6% 63% 31% 6% |
| 3 | C | 241 | 4% 60% 36% |
| 3 | Q | 241 | 5% 61% 35% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | D | 242 | 3% 76% 21% |
| 4 | R | 242 | 5% 71% 26% |
| 5 | E | 233 | 2% 60% 34% 6% |
| 5 | S | 233 | 7% 59% 35% 6% |
| 6 | F | 244 | 2% 65% 31% |
| 6 | T | 244 | 2% 65% 31% |
| 7 | G | 243 | % 65% 32% |
| 7 | U | 243 | % 65% 32% |
| 8 | H | 222 | % 71% 27% |
| 8 | V | 222 | % 73% 25% |
| 9 | I | 204 | 74% 25% |
| 9 | W | 204 | 71% 28% |
| 10 | J | 198 | 2% 68% 30% |
| 10 | X | 198 | 3% 67% 31% |
| 11 | K | 212 | 74% 24% |
| 11 | Y | 212 | 75% 23% |
| 12 | L | 222 | % 68% 29% |
| 12 | Z | 222 | 70% 27% |
| 13 | 1 | 233 | 70% 27% |
| 13 | M | 233 | 70% 27% |
| 14 | 2 | 196 | % 72% 26% |
| 14 | N | 196 | 71% 26% |

# 2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 50714 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome component Y7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |
| 1 | O | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |

- Molecule 2 is a protein called Proteasome component Y13.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |
| 2 | P | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1905 | 1201 | 321 | 380 | 3 | | | |

- Molecule 3 is a protein called Proteasome component PRE6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |
| 3 | Q | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1891 | 1181 | 331 | 375 | 4 | | | |

- Molecule 4 is a protein called Proteasome component PUP2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |
| 4 | R | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1862 | 1162 | 314 | 379 | 7 | | | |

- Molecule 5 is a protein called Proteasome component PRE5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |
| 5 | S | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |

- Molecule 6 is a protein called Proteasome component C1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |
| 6 | T | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1897 | 1205 | 330 | 358 | 4 | | | |

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

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |
| 7 | U | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 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 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | X | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

- 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 | | | |

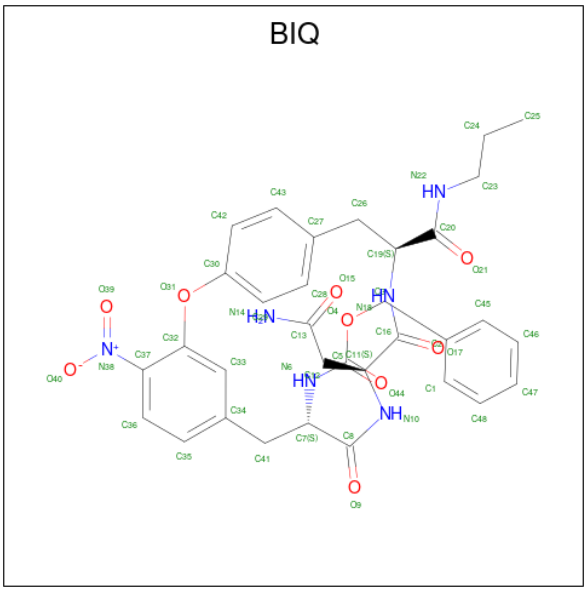
- Molecule 13 is a protein called Proteasome component PRE4.

| 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 BENZYL [12-(2-AMINO-2-OXOETHYL)-4-NITRO-10,13-DIOXO-15-[(PROPYLAMINO)CARBONYL]-2-OXA-11,14-DIAZATRICYCLO[15 .2.2.1 3,7 ]DOCOSA-1(19),3(22),4,6,17,20-HEXAEN-9-YL]CARBAMATE (three-letter code: BIQ) (formula: $C_{33}H_{36}N_6O_9$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 15 | H | 1 | Total C N O<br>48 33 6 9 | 7 | 0 |
| 15 | V | 1 | Total C N O<br>48 33 6 9 | 6 | 0 |

- Molecule 16 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 16 | A | 43 | Total O<br>43 43 | 0 | 0 |
| 16 | B | 27 | Total O<br>27 27 | 0 | 0 |
| 16 | C | 32 | Total O<br>32 32 | 0 | 0 |
| 16 | D | 30 | Total O<br>30 30 | 0 | 0 |
| 16 | E | 14 | Total O<br>14 14 | 0 | 0 |
| 16 | F | 38 | Total O<br>38 38 | 0 | 0 |
| 16 | G | 51 | Total O<br>51 51 | 0 | 0 |
| 16 | H | 37 | Total O<br>37 37 | 0 | 0 |
| 16 | I | 48 | Total O<br>48 48 | 0 | 0 |
| 16 | J | 44 | Total O<br>44 44 | 0 | 0 |

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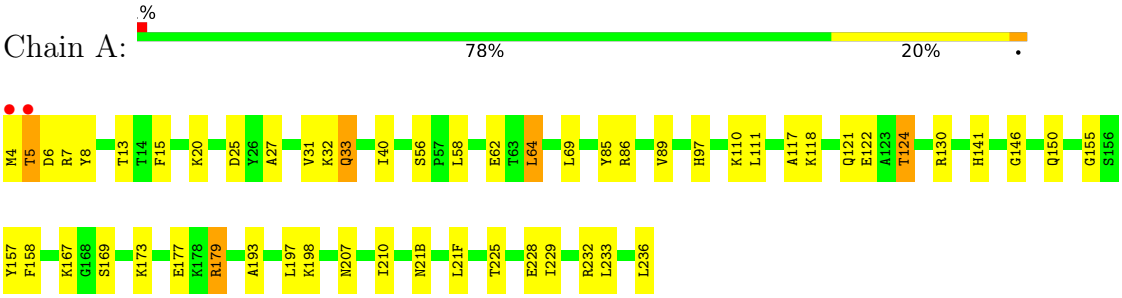
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 16 | K | 36 | Total O<br>36 36 | 0 | 0 |
| 16 | L | 49 | Total O<br>49 49 | 0 | 0 |
| 16 | M | 60 | Total O<br>60 60 | 0 | 0 |
| 16 | N | 48 | Total O<br>48 48 | 0 | 0 |
| 16 | O | 27 | Total O<br>27 27 | 0 | 0 |
| 16 | P | 24 | Total O<br>24 24 | 0 | 0 |
| 16 | Q | 22 | Total O<br>22 22 | 0 | 0 |
| 16 | R | 25 | Total O<br>25 25 | 0 | 0 |
| 16 | S | 16 | Total O<br>16 16 | 0 | 0 |
| 16 | T | 36 | Total O<br>36 36 | 0 | 0 |
| 16 | U | 47 | Total O<br>47 47 | 0 | 0 |
| 16 | V | 39 | Total O<br>39 39 | 0 | 0 |
| 16 | W | 44 | Total O<br>44 44 | 0 | 0 |
| 16 | X | 38 | Total O<br>38 38 | 0 | 0 |
| 16 | Y | 42 | Total O<br>42 42 | 0 | 0 |
| 16 | Z | 45 | Total O<br>45 45 | 0 | 0 |
| 16 | 1 | 59 | Total O<br>59 59 | 0 | 0 |
| 16 | 2 | 49 | Total O<br>49 49 | 0 | 0 |

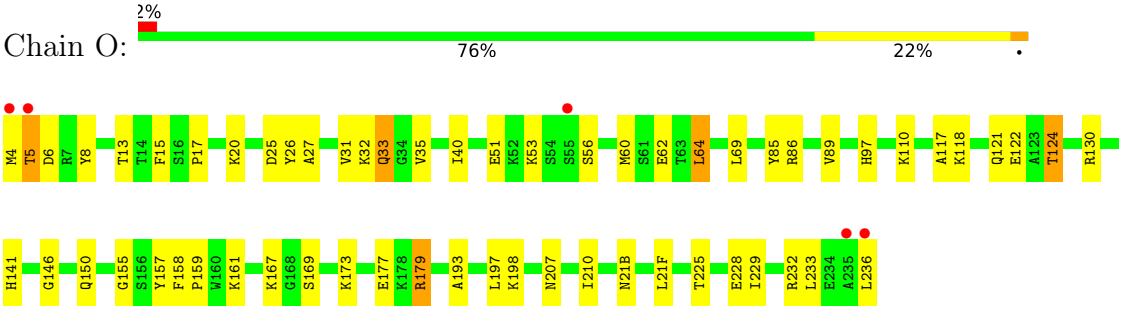
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

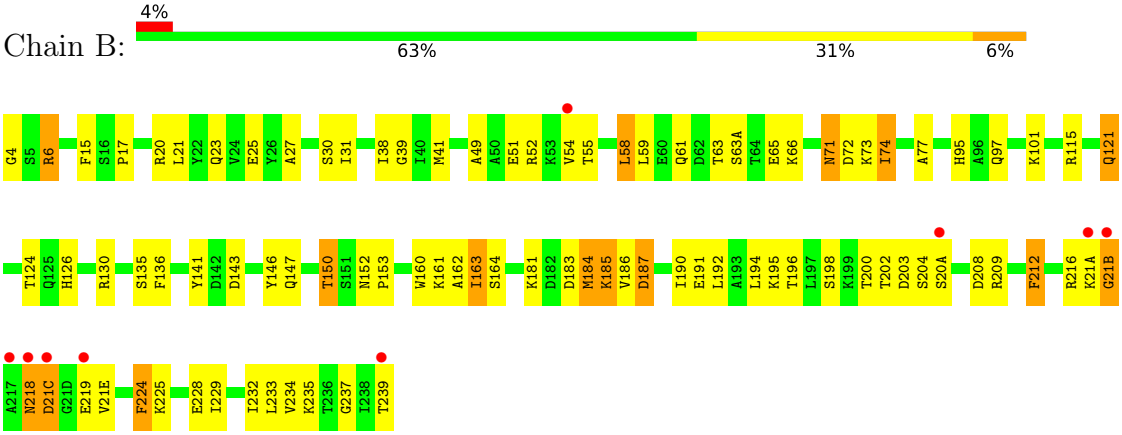
• Molecule 1: Proteasome component Y7



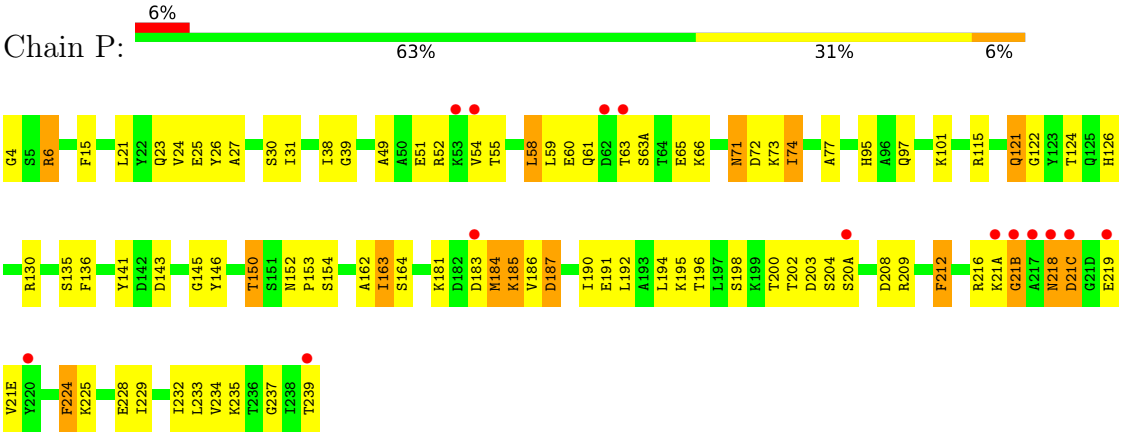

• Molecule 1: Proteasome component Y7



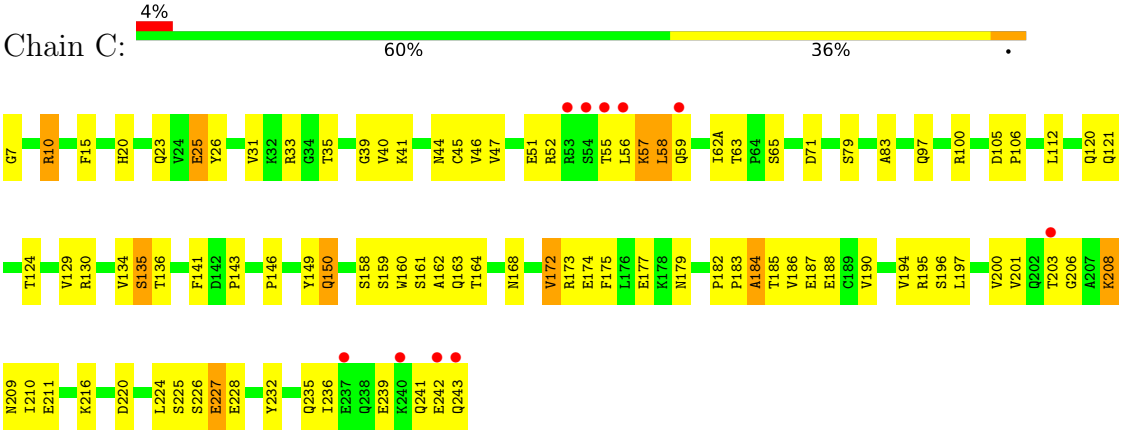

• Molecule 2: Proteasome component Y13



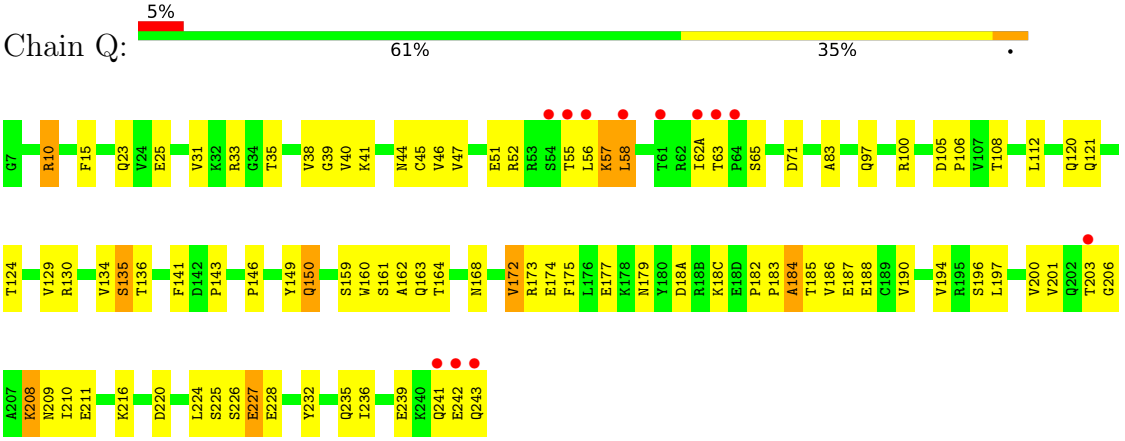

• Molecule 2: Proteasome component Y13



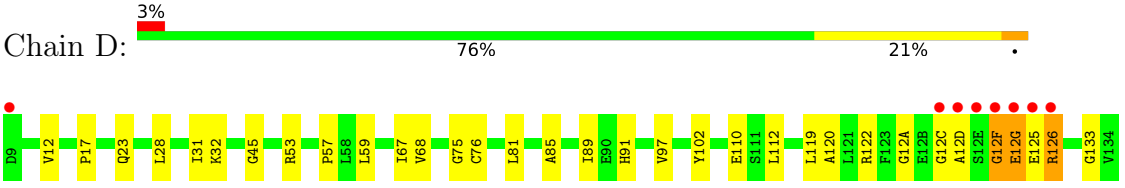

• Molecule 3: Proteasome component PRE6

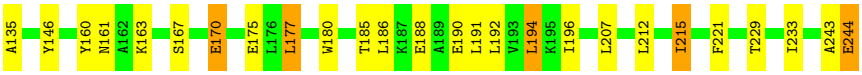



• Molecule 3: Proteasome component PRE6

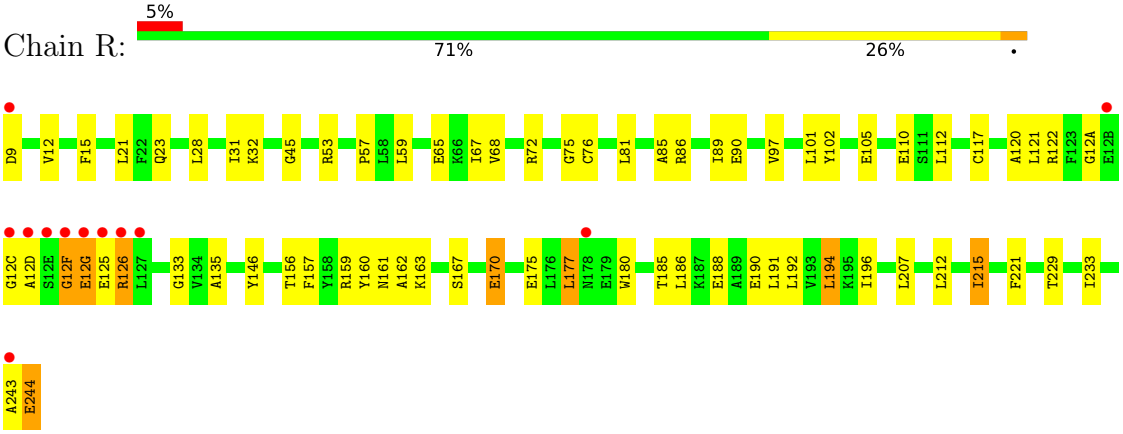



• Molecule 4: Proteasome component PUP2

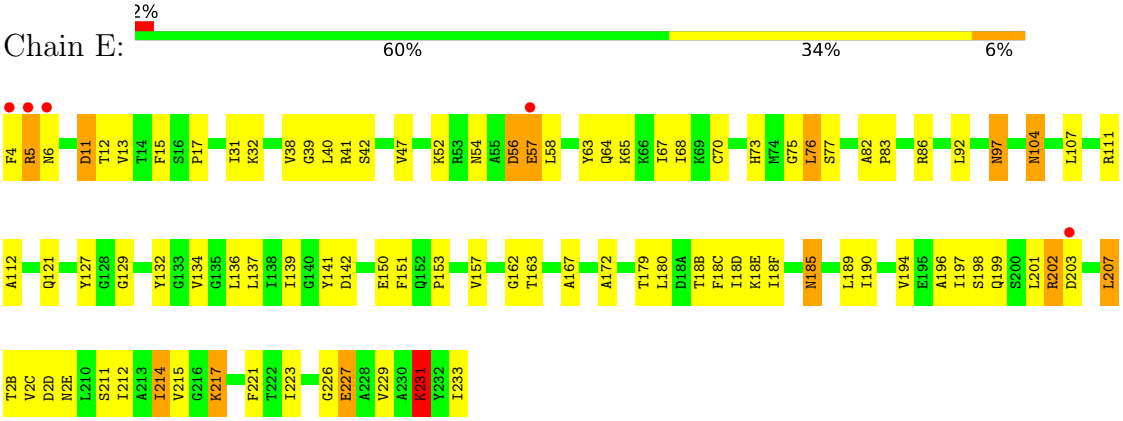




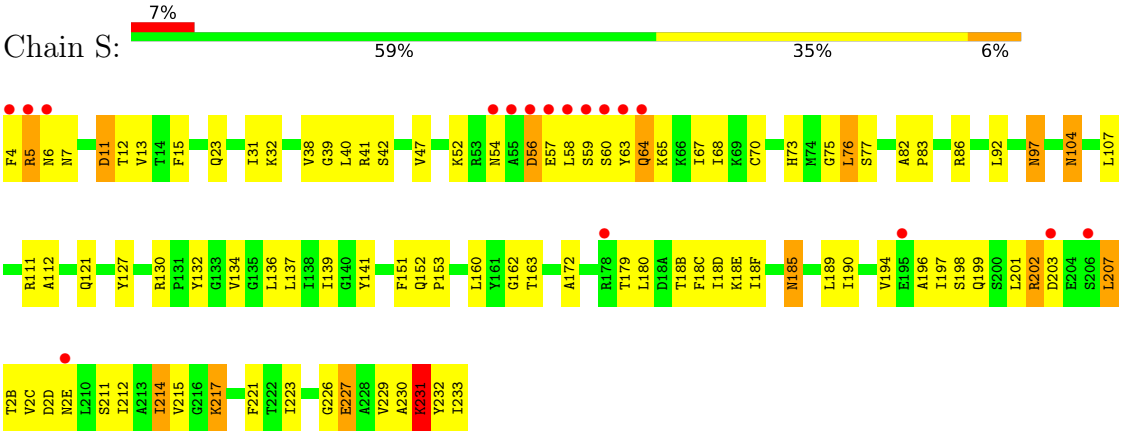

• Molecule 4: Proteasome component PUP2




• Molecule 5: Proteasome component PRE5

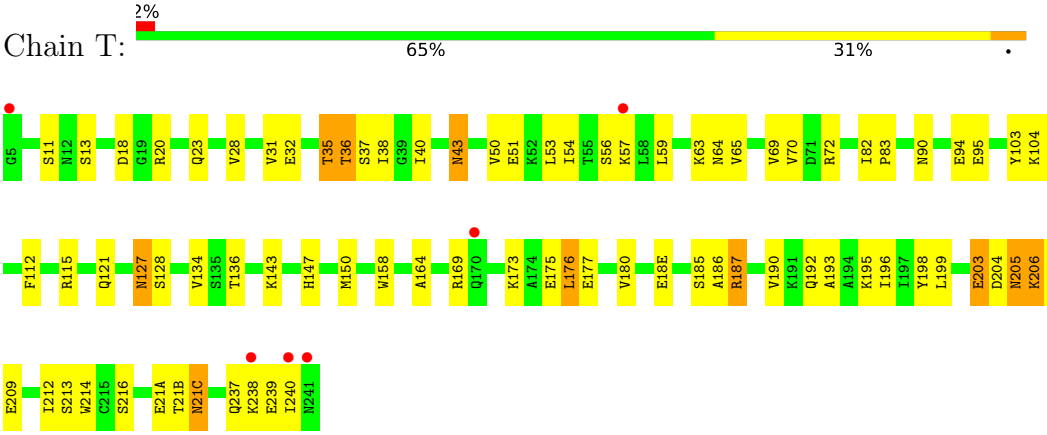



• Molecule 5: Proteasome component PRE5

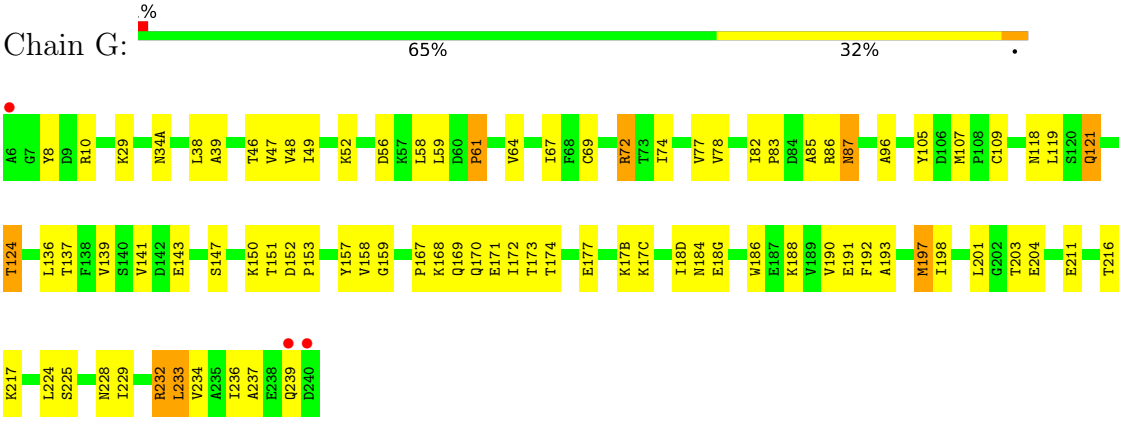



• Molecule 6: Proteasome component C1

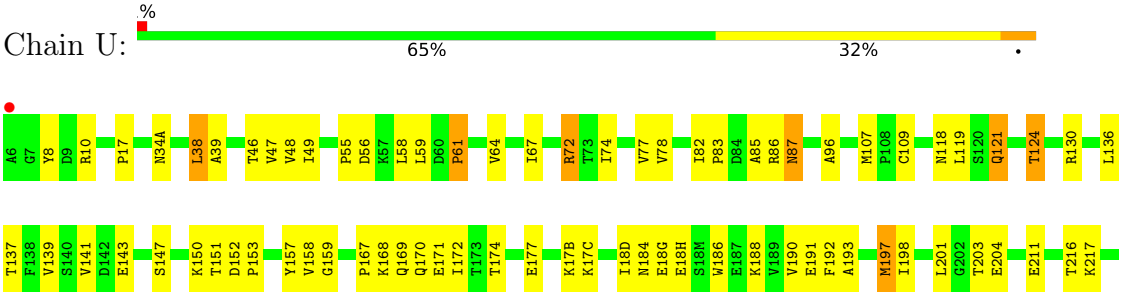

• Molecule 6: Proteasome component C1

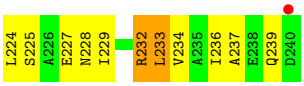



• Molecule 7: Proteasome component C7-alpha



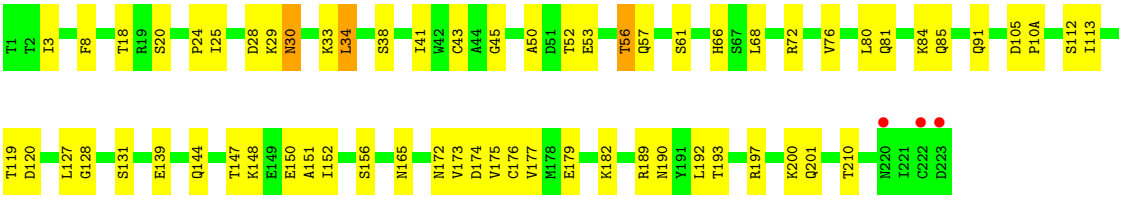

• Molecule 7: Proteasome component C7-alpha





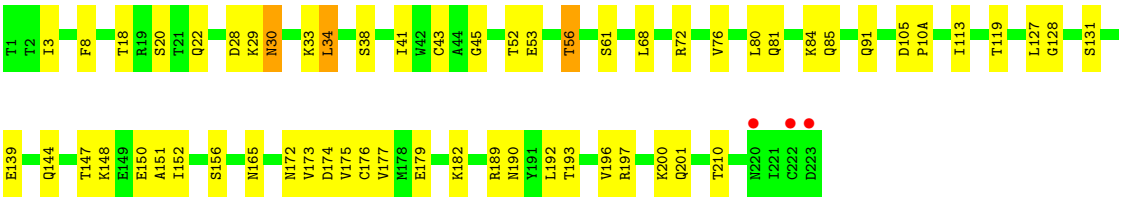

• Molecule 8: Proteasome component PUP1

Chain H:

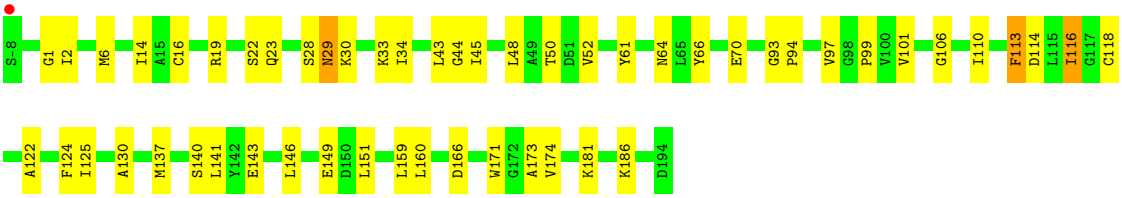

• Molecule 8: Proteasome component PUP1

Chain V:

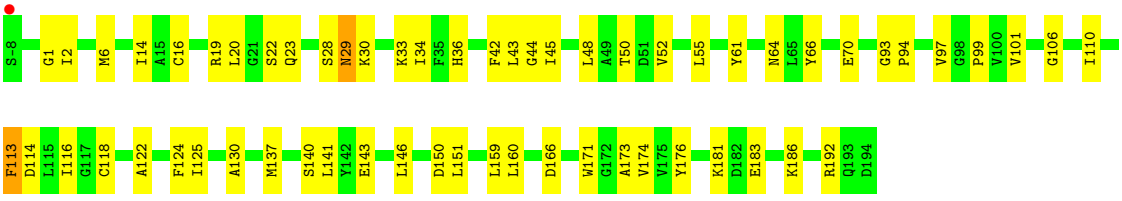

• Molecule 9: Proteasome component PUP3

Chain I:

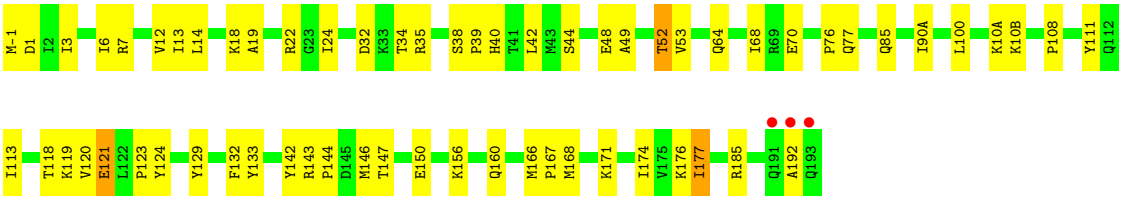

• Molecule 9: Proteasome component PUP3

Chain W:

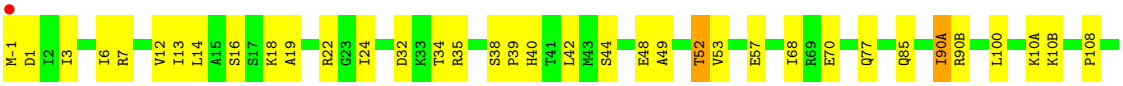

• Molecule 10: Proteasome component C11

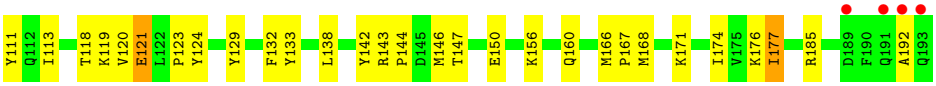
Chain J:



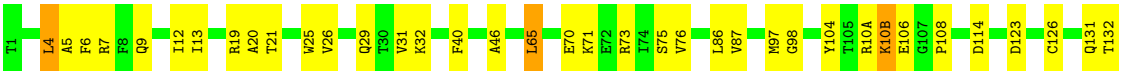


• Molecule 10: Proteasome component C11

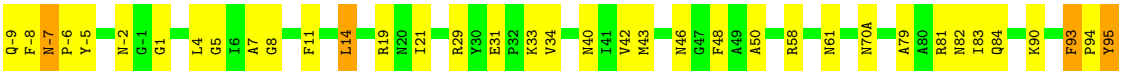


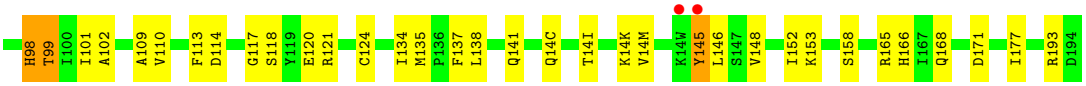
• Molecule 11: Proteasome component PRE2

• Molecule 11: Proteasome component PRE2

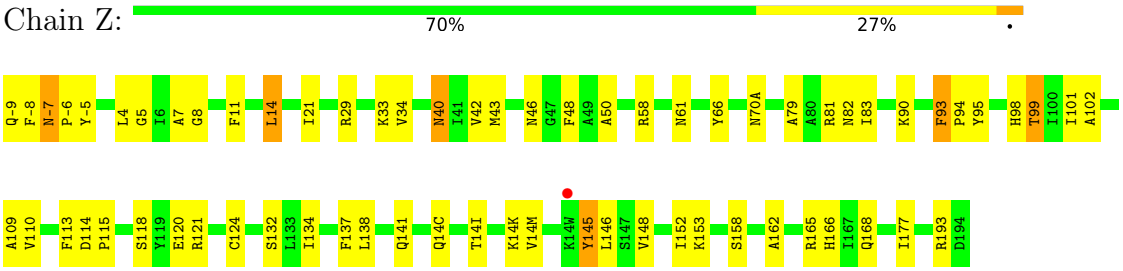

• Molecule 12: Proteasome component C5



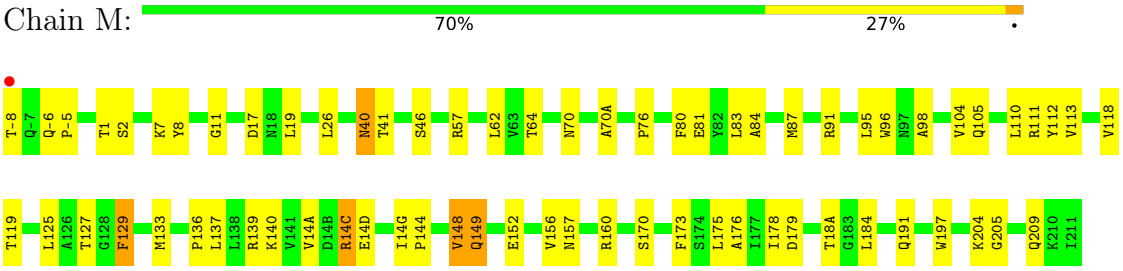
• Molecule 12: Proteasome component C5

Chain Z:



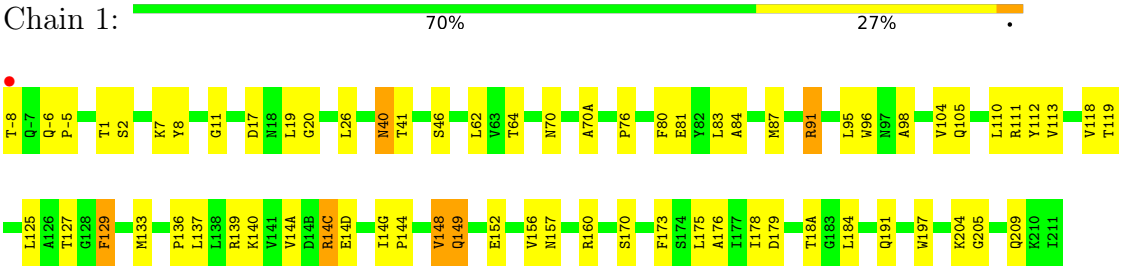

• Molecule 13: Proteasome component PRE4

Chain M:



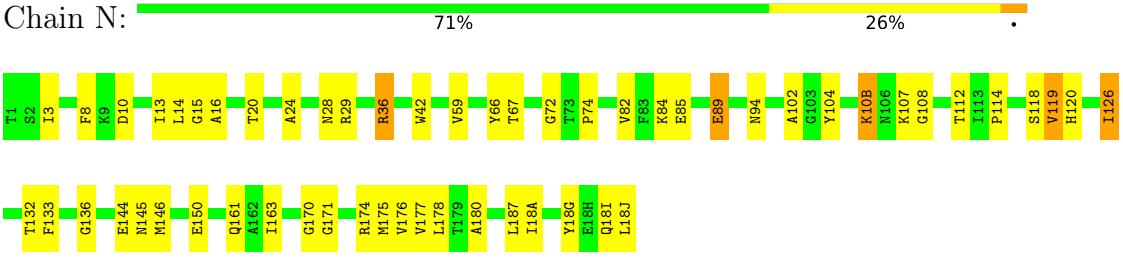

• Molecule 13: Proteasome component PRE4

Chain 1:




• Molecule 14: Proteasome component PRE3

Chain N:




• Molecule 14: Proteasome component PRE3

Chain 2:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 136.43Å 300.96Å 144.76Å<br>90.00° 113.17° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.81<br>20.04 – 2.82 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.8 (15.00-2.81)<br>97.9 (20.04-2.82) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.64 (at 2.83Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.217 , 0.241<br>0.204 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 52.7 | Xtriage |
| Anisotropy | 0.719 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 52.6 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.52$, $< L^2 > = 0.35$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 50714 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 53.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BIQ

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 | 0.39 | 0/1952 | 0.64 | 0/2642 |
| 1 | O | 0.37 | 0/1952 | 0.63 | 0/2642 |
| 2 | B | 0.37 | 0/1935 | 0.63 | 0/2618 |
| 2 | P | 0.37 | 0/1935 | 0.64 | 0/2618 |
| 3 | C | 0.36 | 0/1920 | 0.61 | 0/2598 |
| 3 | Q | 0.35 | 0/1920 | 0.61 | 0/2598 |
| 4 | D | 0.36 | 0/1887 | 0.63 | 0/2541 |
| 4 | R | 0.36 | 0/1887 | 0.63 | 0/2541 |
| 5 | E | 0.35 | 0/1823 | 0.60 | 0/2463 |
| 5 | S | 0.36 | 0/1823 | 0.60 | 0/2463 |
| 6 | F | 0.37 | 0/1937 | 0.61 | 0/2614 |
| 6 | T | 0.37 | 0/1937 | 0.62 | 0/2614 |
| 7 | G | 0.40 | 0/1959 | 0.63 | 0/2652 |
| 7 | U | 0.40 | 0/1959 | 0.63 | 0/2652 |
| 8 | H | 0.38 | 0/1716 | 0.68 | 0/2326 |
| 8 | V | 0.37 | 0/1716 | 0.67 | 0/2326 |
| 9 | I | 0.39 | 0/1611 | 0.66 | 0/2174 |
| 9 | W | 0.40 | 0/1611 | 0.67 | 0/2174 |
| 10 | J | 0.38 | 0/1613 | 0.64 | 0/2173 |
| 10 | X | 0.39 | 0/1613 | 0.65 | 0/2173 |
| 11 | K | 0.41 | 0/1681 | 0.65 | 0/2274 |
| 11 | Y | 0.39 | 0/1681 | 0.64 | 0/2274 |
| 12 | L | 0.40 | 0/1795 | 0.67 | 1/2420 (0.0%) |
| 12 | Z | 0.40 | 0/1795 | 0.66 | 0/2420 |
| 13 | 1 | 0.41 | 0/1855 | 0.67 | 1/2514 (0.0%) |
| 13 | M | 0.39 | 0/1855 | 0.66 | 1/2514 (0.0%) |
| 14 | 2 | 0.40 | 0/1541 | 0.65 | 1/2087 (0.0%) |
| 14 | N | 0.40 | 0/1541 | 0.65 | 0/2087 |
| All | All | 0.38 | 0/50450 | 0.64 | 4/68192 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | 1 | 95 | LEU | N-CA-C | -5.48 | 96.21 | 111.00 |
| 13 | M | 95 | LEU | N-CA-C | -5.47 | 96.22 | 111.00 |
| 14 | 2 | 22 | THR | N-CA-C | -5.15 | 97.09 | 111.00 |
| 12 | L | 95 | TYR | N-CA-C | -5.13 | 97.16 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1915 | 0 | 1926 | 50 | 0 |
| 1 | O | 1915 | 0 | 1926 | 52 | 0 |
| 2 | B | 1905 | 0 | 1901 | 94 | 0 |
| 2 | P | 1905 | 0 | 1901 | 96 | 0 |
| 3 | C | 1891 | 0 | 1900 | 101 | 0 |
| 3 | Q | 1891 | 0 | 1900 | 91 | 0 |
| 4 | D | 1862 | 0 | 1836 | 52 | 0 |
| 4 | R | 1862 | 0 | 1836 | 70 | 0 |
| 5 | E | 1795 | 0 | 1797 | 91 | 0 |
| 5 | S | 1795 | 0 | 1797 | 103 | 0 |
| 6 | F | 1897 | 0 | 1886 | 77 | 0 |
| 6 | T | 1897 | 0 | 1886 | 74 | 0 |
| 7 | G | 1921 | 0 | 1910 | 78 | 0 |
| 7 | U | 1921 | 0 | 1910 | 82 | 0 |
| 8 | H | 1685 | 0 | 1688 | 53 | 0 |
| 8 | V | 1685 | 0 | 1688 | 47 | 0 |
| 9 | I | 1581 | 0 | 1574 | 49 | 0 |
| 9 | W | 1581 | 0 | 1574 | 55 | 0 |
| 10 | J | 1585 | 0 | 1590 | 69 | 0 |
| 10 | X | 1585 | 0 | 1590 | 75 | 0 |
| 11 | K | 1644 | 0 | 1595 | 42 | 0 |
| 11 | Y | 1644 | 0 | 1595 | 40 | 0 |
| 12 | L | 1757 | 0 | 1711 | 57 | 0 |
| 12 | Z | 1757 | 0 | 1711 | 57 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 13 | 1 | 1824 | 0 | 1832 | 57 | 0 |
| 13 | M | 1824 | 0 | 1832 | 56 | 0 |
| 14 | 2 | 1512 | 0 | 1481 | 44 | 0 |
| 14 | N | 1512 | 0 | 1481 | 46 | 0 |
| 15 | H | 48 | 0 | 35 | 4 | 0 |
| 15 | V | 48 | 0 | 35 | 5 | 0 |
| 16 | 1 | 59 | 0 | 0 | 2 | 0 |
| 16 | 2 | 49 | 0 | 0 | 2 | 0 |
| 16 | A | 43 | 0 | 0 | 1 | 0 |
| 16 | B | 27 | 0 | 0 | 2 | 0 |
| 16 | C | 32 | 0 | 0 | 4 | 0 |
| 16 | D | 30 | 0 | 0 | 2 | 0 |
| 16 | E | 14 | 0 | 0 | 2 | 0 |
| 16 | F | 38 | 0 | 0 | 2 | 0 |
| 16 | G | 51 | 0 | 0 | 3 | 0 |
| 16 | H | 37 | 0 | 0 | 2 | 0 |
| 16 | I | 48 | 0 | 0 | 0 | 0 |
| 16 | J | 44 | 0 | 0 | 2 | 0 |
| 16 | K | 36 | 0 | 0 | 1 | 0 |
| 16 | L | 49 | 0 | 0 | 5 | 0 |
| 16 | M | 60 | 0 | 0 | 4 | 0 |
| 16 | N | 48 | 0 | 0 | 2 | 0 |
| 16 | O | 27 | 0 | 0 | 2 | 0 |
| 16 | P | 24 | 0 | 0 | 0 | 0 |
| 16 | Q | 22 | 0 | 0 | 3 | 0 |
| 16 | R | 25 | 0 | 0 | 3 | 0 |
| 16 | S | 16 | 0 | 0 | 1 | 0 |
| 16 | T | 36 | 0 | 0 | 3 | 0 |
| 16 | U | 47 | 0 | 0 | 5 | 0 |
| 16 | V | 39 | 0 | 0 | 3 | 0 |
| 16 | W | 44 | 0 | 0 | 4 | 0 |
| 16 | X | 38 | 0 | 0 | 5 | 0 |
| 16 | Y | 42 | 0 | 0 | 2 | 0 |
| 16 | Z | 45 | 0 | 0 | 3 | 0 |
| All | All | 50714 | 0 | 49324 | 1654 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1654) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:Y:10(B):LYS:H | 11:Y:10(B):LYS:HD2 | 1.10 | 1.17 |
| 2:P:202:THR:HG22 | 2:P:204:SER:H | 1.13 | 1.12 |
| 14:N:161:GLN:HE21 | 14:2:136:GLY:HA2 | 1.11 | 1.10 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:HD2 | 1.09 | 1.08 |
| 2:B:202:THR:HG22 | 2:B:204:SER:H | 1.14 | 1.04 |
| 7:G:96:ALA:HA | 7:G:107:MET:HE2 | 1.35 | 1.04 |
| 2:B:190:ILE:HG21 | 2:B:232:ILE:HD11 | 1.36 | 1.03 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:HE21 | 1.13 | 1.03 |
| 7:U:96:ALA:HA | 7:U:107:MET:HE2 | 1.35 | 1.03 |
| 2:P:190:ILE:HG21 | 2:P:232:ILE:HD11 | 1.35 | 1.03 |
| 12:L:33:LYS:HD2 | 12:L:46:ASN:HD22 | 1.24 | 1.00 |
| 1:O:15:PHE:H | 2:P:23:GLN:HE22 | 1.09 | 0.97 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:HH21 | 1.28 | 0.97 |
| 12:Z:33:LYS:HD2 | 12:Z:46:ASN:HD22 | 1.26 | 0.96 |
| 3:Q:15:PHE:H | 4:R:23:GLN:HE22 | 1.12 | 0.94 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:NH1 | 1.65 | 0.93 |
| 13:1:157:ASN:ND2 | 13:1:160:ARG:HH11 | 1.67 | 0.92 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:NH1 | 1.68 | 0.92 |
| 3:C:185:THR:HG22 | 3:C:187:GLU:H | 1.33 | 0.92 |
| 3:Q:163:GLN:NE2 | 3:Q:164:THR:H | 1.69 | 0.91 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:H | 1.31 | 0.91 |
| 3:C:163:GLN:NE2 | 3:C:164:THR:H | 1.68 | 0.91 |
| 3:C:15:PHE:H | 4:D:23:GLN:HE22 | 1.18 | 0.91 |
| 3:Q:185:THR:HB | 3:Q:188:GLU:HG2 | 1.54 | 0.90 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:N | 1.68 | 0.90 |
| 13:M:157:ASN:ND2 | 13:M:160:ARG:HH11 | 1.70 | 0.90 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:N | 1.68 | 0.90 |
| 2:B:15:PHE:H | 3:C:23:GLN:HE22 | 1.19 | 0.89 |
| 1:A:15:PHE:H | 2:B:23:GLN:HE22 | 1.14 | 0.89 |
| 3:C:185:THR:HB | 3:C:188:GLU:HG2 | 1.55 | 0.88 |
| 4:R:162:ALA:HB3 | 5:S:58:LEU:HD23 | 1.57 | 0.87 |
| 1:O:130:ARG:HH21 | 7:U:124:THR:CG2 | 1.87 | 0.87 |
| 2:P:163:ILE:HD13 | 2:P:164:SER:H | 1.40 | 0.87 |
| 13:M:157:ASN:HD22 | 13:M:160:ARG:HH11 | 0.90 | 0.86 |
| 13:1:157:ASN:HD22 | 13:1:160:ARG:HH11 | 0.88 | 0.86 |
| 3:Q:163:GLN:HE21 | 3:Q:164:THR:H | 0.86 | 0.85 |
| 5:S:15:PHE:H | 6:T:23:GLN:HE22 | 1.23 | 0.85 |
| 14:N:161:GLN:NE2 | 14:2:136:GLY:HA2 | 1.91 | 0.85 |
| 2:B:163:ILE:HD13 | 2:B:164:SER:H | 1.42 | 0.85 |
| 8:H:165:ASN:HD22 | 13:1:139:ARG:HH11 | 1.25 | 0.84 |
| 3:C:163:GLN:HE21 | 3:C:164:THR:H | 0.86 | 0.84 |
| 1:O:86:ARG:HE | 7:U:118:ASN:HD21 | 1.25 | 0.84 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:130:ARG:HH21 | 7:U:124:THR:HG22 | 1.43 | 0.82 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:H | 1.44 | 0.82 |
| 1:O:124:THR:CG2 | 2:P:130:ARG:HH21 | 1.93 | 0.82 |
| 1:O:124:THR:HG22 | 2:P:130:ARG:HH21 | 1.42 | 0.82 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:HD22 | 1.26 | 0.82 |
| 5:S:207:LEU:HD23 | 5:S:207:LEU:H | 1.42 | 0.82 |
| 5:E:15:PHE:H | 6:F:23:GLN:HE22 | 1.28 | 0.81 |
| 2:P:124:THR:HG22 | 3:Q:130:ARG:HH21 | 1.44 | 0.81 |
| 3:Q:206:GLY:HA3 | 3:Q:209:ASN:HB2 | 1.62 | 0.81 |
| 14:N:136:GLY:HA2 | 14:2:161:GLN:NE2 | 1.93 | 0.80 |
| 2:P:61:GLN:OE1 | 2:P:208:ASP:HA | 1.80 | 0.80 |
| 2:B:71:ASN:ND2 | 2:B:72:ASP:H | 1.80 | 0.80 |
| 3:C:206:GLY:HA3 | 3:C:209:ASN:HB2 | 1.62 | 0.80 |
| 6:T:95:GLU:HG2 | 6:T:115:ARG:HB3 | 1.61 | 0.80 |
| 13:1:104:VAL:HG23 | 13:1:178:ILE:HG22 | 1.64 | 0.80 |
| 7:G:198:ILE:HG23 | 7:G:203:THR:O | 1.81 | 0.80 |
| 3:Q:65:SER:HB2 | 16:Q:247:HOH:O | 1.80 | 0.80 |
| 7:U:198:ILE:HG23 | 7:U:203:THR:O | 1.81 | 0.80 |
| 2:P:71:ASN:ND2 | 2:P:72:ASP:H | 1.79 | 0.80 |
| 2:B:124:THR:CG2 | 3:C:130:ARG:HH21 | 1.95 | 0.79 |
| 11:K:10(B):LYS:HD2 | 11:K:10(B):LYS:N | 1.94 | 0.79 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:HD22 | 1.64 | 0.79 |
| 6:F:95:GLU:HG2 | 6:F:115:ARG:HB3 | 1.64 | 0.79 |
| 2:B:61:GLN:OE1 | 2:B:208:ASP:HA | 1.81 | 0.78 |
| 5:E:198:SER:HA | 5:E:201:LEU:HG | 1.65 | 0.78 |
| 5:S:198:SER:HA | 5:S:201:LEU:HG | 1.65 | 0.78 |
| 13:M:104:VAL:HG23 | 13:M:178:ILE:HG22 | 1.66 | 0.78 |
| 1:A:124:THR:CG2 | 2:B:130:ARG:HH21 | 1.96 | 0.78 |
| 1:A:86:ARG:HE | 7:G:118:ASN:HD21 | 1.32 | 0.78 |
| 3:Q:33:ARG:NH1 | 3:Q:33:ARG:HB2 | 2.00 | 0.77 |
| 12:Z:114:ASP:HB2 | 12:Z:118:SER:HB3 | 1.64 | 0.77 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:HG22 | 1.48 | 0.77 |
| 12:L:114:ASP:HB2 | 12:L:118:SER:HB3 | 1.65 | 0.77 |
| 12:Z:33:LYS:HD2 | 12:Z:46:ASN:ND2 | 2.00 | 0.77 |
| 1:A:20:LYS:HE3 | 1:A:25:ASP:OD1 | 1.85 | 0.77 |
| 1:A:130:ARG:HH21 | 7:G:124:THR:CG2 | 1.97 | 0.76 |
| 4:R:12(D):ALA:HB3 | 4:R:126:ARG:HD3 | 1.67 | 0.76 |
| 11:K:10(B):LYS:H | 11:K:10(B):LYS:CD | 1.89 | 0.76 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:H | 1.49 | 0.76 |
| 12:L:33:LYS:HD2 | 12:L:46:ASN:ND2 | 1.99 | 0.75 |
| 2:P:65:GLU:HG3 | 2:P:66:LYS:HG3 | 1.68 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:121:LEU:HB2 | 16:R:853:HOH:O | 1.85 | 0.75 |
| 3:C:33:ARG:NH1 | 3:C:33:ARG:HB2 | 2.00 | 0.75 |
| 7:U:217:LYS:HE3 | 7:U:217:LYS:HA | 1.68 | 0.75 |
| 1:A:124:THR:HG22 | 2:B:130:ARG:HH21 | 1.53 | 0.74 |
| 2:B:65:GLU:HG3 | 2:B:66:LYS:HG3 | 1.70 | 0.74 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:H | 1.51 | 0.74 |
| 2:B:202:THR:HG22 | 2:B:204:SER:N | 1.98 | 0.74 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:CD2 | 2.17 | 0.74 |
| 3:C:33:ARG:HB2 | 3:C:33:ARG:HH11 | 1.53 | 0.74 |
| 9:W:192:ARG:HG3 | 16:W:200:HOH:O | 1.87 | 0.73 |
| 12:L:166:HIS:HD2 | 12:L:168:GLN:H | 1.36 | 0.73 |
| 3:Q:33:ARG:HB2 | 3:Q:33:ARG:HH11 | 1.52 | 0.73 |
| 3:Q:55:THR:HG22 | 3:Q:56:LEU:HD22 | 1.70 | 0.73 |
| 5:S:97:ASN:HD21 | 12:Z:61:ASN:HD21 | 1.34 | 0.73 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:ND2 | 2.03 | 0.73 |
| 4:D:12(D):ALA:HB3 | 4:D:126:ARG:HD3 | 1.68 | 0.73 |
| 14:N:146:MET:HE3 | 14:N:150:GLU:HB3 | 1.70 | 0.73 |
| 2:P:101:LYS:NZ | 10:X:85:GLN:NE2 | 2.36 | 0.73 |
| 5:E:207:LEU:HA | 5:E:2(E):ASN:ND2 | 2.03 | 0.73 |
| 2:P:202:THR:HG22 | 2:P:204:SER:N | 1.97 | 0.73 |
| 4:D:177:LEU:HD13 | 5:E:58:LEU:HD11 | 1.71 | 0.72 |
| 4:R:156:THR:HG22 | 5:S:83:PRO:HD3 | 1.71 | 0.72 |
| 11:Y:10(B):LYS:HD2 | 11:Y:10(B):LYS:N | 1.96 | 0.72 |
| 7:G:217:LYS:HE3 | 7:G:217:LYS:HA | 1.70 | 0.72 |
| 1:O:20:LYS:HE3 | 1:O:25:ASP:OD1 | 1.89 | 0.72 |
| 8:V:52:THR:O | 8:V:56:THR:HB | 1.90 | 0.71 |
| 8:V:128:GLY:O | 8:V:131:SER:HB2 | 1.89 | 0.71 |
| 12:L:-9:GLN:HE21 | 13:M:-8:THR:HG21 | 1.54 | 0.71 |
| 13:1:40:ASN:H | 13:1:40:ASN:HD22 | 1.37 | 0.71 |
| 5:E:201:LEU:HD11 | 5:E:207:LEU:HD22 | 1.72 | 0.71 |
| 6:F:43:ASN:N | 6:F:43:ASN:HD22 | 1.88 | 0.71 |
| 14:2:112:THR:HG22 | 14:2:120:HIS:HB2 | 1.72 | 0.71 |
| 3:C:55:THR:HG22 | 3:C:56:LEU:HD22 | 1.71 | 0.71 |
| 4:D:175:GLU:HG2 | 4:D:196:ILE:HD12 | 1.72 | 0.71 |
| 3:Q:185:THR:HG22 | 3:Q:187:GLU:N | 2.05 | 0.70 |
| 3:Q:33:ARG:HH11 | 3:Q:33:ARG:CB | 2.04 | 0.70 |
| 2:P:190:ILE:HG21 | 2:P:232:ILE:CD1 | 2.18 | 0.70 |
| 13:1:76:PRO:HD2 | 13:1:105:GLN:OE1 | 1.91 | 0.70 |
| 3:C:185:THR:HG22 | 3:C:187:GLU:N | 2.06 | 0.70 |
| 12:Z:166:HIS:HD2 | 12:Z:168:GLN:H | 1.38 | 0.70 |
| 14:N:112:THR:HG22 | 14:N:120:HIS:HB2 | 1.73 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:HE | 1.40 | 0.70 |
| 12:Z:-9:GLN:HE21 | 13:1:-8:THR:HG21 | 1.56 | 0.70 |
| 5:E:18(D):ILE:HG23 | 5:E:18(E):LYS:HG3 | 1.73 | 0.70 |
| 8:H:52:THR:O | 8:H:56:THR:HB | 1.91 | 0.70 |
| 11:Y:10(B):LYS:H | 11:Y:10(B):LYS:CD | 1.90 | 0.70 |
| 3:C:33:ARG:HH11 | 3:C:33:ARG:CB | 2.04 | 0.70 |
| 2:B:181:LYS:O | 2:B:184:MET:HG3 | 1.92 | 0.70 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:H | 1.57 | 0.70 |
| 6:T:43:ASN:N | 6:T:43:ASN:HD22 | 1.88 | 0.70 |
| 4:R:175:GLU:HG2 | 4:R:196:ILE:HD12 | 1.73 | 0.69 |
| 5:S:75:GLY:HA3 | 5:S:221:PHE:CE2 | 2.26 | 0.69 |
| 5:S:201:LEU:HD11 | 5:S:207:LEU:HD22 | 1.72 | 0.69 |
| 2:B:190:ILE:HG21 | 2:B:232:ILE:CD1 | 2.19 | 0.69 |
| 11:K:142:TYR:O | 11:K:143:LYS:HD2 | 1.92 | 0.69 |
| 5:S:18(D):ILE:HG23 | 5:S:18(E):LYS:HG3 | 1.73 | 0.69 |
| 8:H:128:GLY:O | 8:H:131:SER:HB2 | 1.93 | 0.69 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:HG13 | 1.75 | 0.69 |
| 12:L:134:ILE:HD12 | 12:L:158:SER:HB3 | 1.73 | 0.69 |
| 12:Z:134:ILE:HD12 | 12:Z:158:SER:HB3 | 1.75 | 0.69 |
| 12:Z:4:LEU:HD11 | 12:Z:138:LEU:HD21 | 1.75 | 0.69 |
| 5:E:167:ALA:HB3 | 16:E:246:HOH:O | 1.93 | 0.68 |
| 13:1:14(C):ARG:HG3 | 13:1:14(C):ARG:HH11 | 1.58 | 0.68 |
| 5:E:75:GLY:HA3 | 5:E:221:PHE:CE2 | 2.28 | 0.68 |
| 13:M:40:ASN:H | 13:M:40:ASN:HD22 | 1.39 | 0.68 |
| 5:S:18(C):PHE:HA | 5:S:18(F):ILE:HG13 | 1.75 | 0.68 |
| 14:2:10(B):LYS:O | 14:2:10(B):LYS:HD3 | 1.93 | 0.68 |
| 3:C:41:LYS:HG2 | 3:C:161:SER:O | 1.92 | 0.68 |
| 12:L:4:LEU:HD11 | 12:L:138:LEU:HD21 | 1.73 | 0.68 |
| 11:Y:143:LYS:HB2 | 11:Y:146:LEU:CD1 | 2.23 | 0.68 |
| 9:W:29:ASN:ND2 | 9:W:30:LYS:HG3 | 2.09 | 0.68 |
| 7:G:170:GLN:HE21 | 7:G:174:THR:HG23 | 1.59 | 0.68 |
| 9:I:29:ASN:ND2 | 9:I:30:LYS:HG3 | 2.08 | 0.68 |
| 5:S:207:LEU:H | 5:S:207:LEU:CD2 | 2.06 | 0.68 |
| 2:B:51:GLU:OE2 | 2:B:202:THR:HG23 | 1.94 | 0.68 |
| 5:S:92:LEU:HD11 | 5:S:112:ALA:HB1 | 1.75 | 0.68 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:H | 1.58 | 0.68 |
| 3:C:163:GLN:HE22 | 3:C:173:ARG:HE | 1.41 | 0.67 |
| 5:S:207:LEU:HA | 5:S:2(E):ASN:HD22 | 1.58 | 0.67 |
| 6:F:35:THR:HG21 | 6:F:51:GLU:O | 1.94 | 0.67 |
| 7:U:59:LEU:O | 7:U:61:PRO:HD3 | 1.94 | 0.67 |
| 5:E:92:LEU:HD11 | 5:E:112:ALA:HB1 | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:86:ARG:HD2 | 16:G:256:HOH:O | 1.95 | 0.67 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:CB | 2.24 | 0.67 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:NH1 | 2.10 | 0.67 |
| 14:N:10(B):LYS:O | 14:N:10(B):LYS:HD3 | 1.95 | 0.67 |
| 3:Q:41:LYS:HG2 | 3:Q:161:SER:O | 1.95 | 0.67 |
| 11:Y:142:TYR:O | 11:Y:143:LYS:HD2 | 1.94 | 0.67 |
| 13:M:14(C):ARG:HG3 | 13:M:14(C):ARG:HH11 | 1.60 | 0.67 |
| 4:R:161:ASN:N | 5:S:58:LEU:O | 2.26 | 0.67 |
| 5:S:207:LEU:HD23 | 5:S:207:LEU:N | 2.10 | 0.67 |
| 3:Q:187:GLU:HG3 | 3:Q:232:TYR:OH | 1.95 | 0.66 |
| 14:2:13:ILE:HG12 | 14:2:177:VAL:HG13 | 1.77 | 0.66 |
| 11:K:143:LYS:HB2 | 11:K:146:LEU:CD1 | 2.25 | 0.66 |
| 1:O:159:PRO:O | 2:P:59:LEU:HD12 | 1.95 | 0.66 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:CB | 2.25 | 0.66 |
| 7:G:59:LEU:O | 7:G:61:PRO:HD3 | 1.95 | 0.66 |
| 2:P:181:LYS:O | 2:P:184:MET:HG3 | 1.94 | 0.66 |
| 3:Q:52:ARG:HD2 | 3:Q:208:LYS:O | 1.95 | 0.66 |
| 4:R:207:LEU:C | 4:R:207:LEU:HD23 | 2.16 | 0.66 |
| 6:F:192:GLN:O | 6:F:196:ILE:HG12 | 1.95 | 0.66 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:HD22 | 1.43 | 0.66 |
| 6:T:192:GLN:HE21 | 6:T:195:LYS:HE3 | 1.61 | 0.66 |
| 7:U:72:ARG:HB2 | 7:U:72:ARG:HH11 | 1.60 | 0.66 |
| 11:K:21:THR:HG22 | 11:K:26:VAL:HA | 1.77 | 0.66 |
| 5:E:207:LEU:H | 5:E:207:LEU:CD2 | 2.08 | 0.66 |
| 2:P:51:GLU:OE2 | 2:P:202:THR:HG23 | 1.96 | 0.66 |
| 9:W:45:ILE:HB | 9:W:52:VAL:HG13 | 1.76 | 0.66 |
| 2:B:141:TYR:CD1 | 2:B:21(E):VAL:HG21 | 2.31 | 0.66 |
| 2:B:190:ILE:CG2 | 2:B:232:ILE:HD11 | 2.20 | 0.66 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:CG | 2.26 | 0.66 |
| 13:M:149:GLN:NE2 | 13:M:149:GLN:H | 1.92 | 0.66 |
| 2:P:190:ILE:CG2 | 2:P:232:ILE:HD11 | 2.19 | 0.66 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:HB2 | 1.78 | 0.66 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:H | 1.60 | 0.66 |
| 6:T:192:GLN:O | 6:T:196:ILE:HG12 | 1.96 | 0.66 |
| 7:G:34(A):ASN:HD22 | 7:G:167:PRO:HG2 | 1.61 | 0.66 |
| 7:G:72:ARG:HB2 | 7:G:72:ARG:NH1 | 2.11 | 0.65 |
| 13:1:149:GLN:H | 13:1:149:GLN:NE2 | 1.94 | 0.65 |
| 3:C:52:ARG:HD2 | 3:C:208:LYS:O | 1.97 | 0.65 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:HB2 | 1.77 | 0.65 |
| 12:Z:29:ARG:NH1 | 12:Z:193:ARG:HB3 | 2.11 | 0.65 |
| 5:E:207:LEU:HD23 | 5:E:207:LEU:N | 2.11 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:121:GLN:O | 1:O:124:THR:HB | 1.95 | 0.65 |
| 10:X:32:ASP:OD2 | 10:X:34:THR:HG22 | 1.96 | 0.65 |
| 2:B:219:GLU:HG2 | 2:B:21(E):VAL:N | 2.12 | 0.65 |
| 5:E:97:ASN:HD21 | 12:L:61:ASN:HD21 | 1.43 | 0.65 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:HG21 | 1.79 | 0.65 |
| 14:2:14:LEU:HD11 | 14:2:102:ALA:HB3 | 1.77 | 0.65 |
| 13:M:76:PRO:HD2 | 13:M:105:GLN:OE1 | 1.96 | 0.65 |
| 6:T:35:THR:HG21 | 6:T:51:GLU:O | 1.95 | 0.65 |
| 4:D:207:LEU:CD2 | 4:D:233:ILE:HD12 | 2.27 | 0.65 |
| 5:E:226:GLY:O | 5:E:229:VAL:HG22 | 1.97 | 0.65 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:CG | 2.25 | 0.65 |
| 5:S:226:GLY:O | 5:S:229:VAL:HG22 | 1.97 | 0.65 |
| 7:U:170:GLN:HE21 | 7:U:174:THR:HG23 | 1.60 | 0.65 |
| 8:V:38:SER:OG | 8:V:41:ILE:HD13 | 1.96 | 0.65 |
| 11:Y:21:THR:HG22 | 11:Y:26:VAL:HA | 1.78 | 0.65 |
| 12:Z:14(I):THR:HG21 | 12:Z:14(M):VAL:HB | 1.79 | 0.65 |
| 5:E:132:TYR:O | 5:E:153:PRO:HB3 | 1.97 | 0.65 |
| 5:S:132:TYR:O | 5:S:153:PRO:HB3 | 1.97 | 0.65 |
| 2:B:21:LEU:HD13 | 2:B:124:THR:HG23 | 1.78 | 0.65 |
| 5:E:207:LEU:HA | 5:E:2(E):ASN:HD22 | 1.59 | 0.65 |
| 12:Z:114:ASP:HB3 | 12:Z:118:SER:H | 1.62 | 0.65 |
| 8:H:34:LEU:HB2 | 16:H:1021:HOH:O | 1.97 | 0.65 |
| 16:T:244:HOH:O | 7:U:86:ARG:HD2 | 1.97 | 0.65 |
| 14:N:107:LYS:HG2 | 14:N:108:GLY:N | 2.12 | 0.64 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:HD2 | 1.61 | 0.64 |
| 1:O:86:ARG:HE | 7:U:118:ASN:ND2 | 1.94 | 0.64 |
| 2:P:101:LYS:HZ1 | 10:X:85:GLN:HE22 | 1.46 | 0.64 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:HE22 | 1.61 | 0.64 |
| 10:X:113:ILE:HG12 | 10:X:119:LYS:HG3 | 1.80 | 0.64 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:HD2 | 1.61 | 0.64 |
| 2:B:121:GLN:O | 2:B:124:THR:HB | 1.98 | 0.64 |
| 13:M:14(D):GLU:O | 13:M:14(G):ILE:HG12 | 1.98 | 0.64 |
| 8:H:45:GLY:O | 15:H:1000:BIQ:H251 | 1.97 | 0.64 |
| 5:S:214:ILE:HG13 | 5:S:215:VAL:N | 2.13 | 0.64 |
| 10:X:156:LYS:O | 10:X:160:GLN:HG3 | 1.98 | 0.64 |
| 7:U:96:ALA:CA | 7:U:107:MET:HE2 | 2.21 | 0.64 |
| 5:E:214:ILE:HG13 | 5:E:215:VAL:N | 2.12 | 0.64 |
| 14:N:14:LEU:HD11 | 14:N:102:ALA:HB3 | 1.78 | 0.64 |
| 2:P:121:GLN:HG3 | 3:Q:83:ALA:HB1 | 1.79 | 0.64 |
| 2:P:126:HIS:HB3 | 3:Q:129:VAL:HG12 | 1.80 | 0.64 |
| 14:2:84:LYS:HG3 | 14:2:119:VAL:HG22 | 1.79 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:102:TYR:O | 12:L:81:ARG:HG3 | 1.97 | 0.64 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:HB2 | 1.79 | 0.64 |
| 10:J:133:TYR:HD1 | 16:Y:236:HOH:O | 1.81 | 0.64 |
| 2:P:121:GLN:O | 2:P:124:THR:HB | 1.97 | 0.64 |
| 4:D:207:LEU:HD23 | 4:D:207:LEU:C | 2.18 | 0.64 |
| 14:N:84:LYS:HG3 | 14:N:119:VAL:HG22 | 1.79 | 0.64 |
| 3:Q:235:GLN:O | 3:Q:239:GLU:HG2 | 1.98 | 0.64 |
| 4:R:102:TYR:O | 12:Z:81:ARG:HG3 | 1.98 | 0.64 |
| 1:A:86:ARG:HH21 | 7:G:118:ASN:HD22 | 1.45 | 0.64 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:H | 1.62 | 0.64 |
| 2:B:71:ASN:HD22 | 2:B:72:ASP:H | 1.47 | 0.63 |
| 3:C:71:ASP:HA | 10:J:68:ILE:HD13 | 1.80 | 0.63 |
| 3:C:187:GLU:HG3 | 3:C:232:TYR:OH | 1.98 | 0.63 |
| 7:G:72:ARG:HB2 | 7:G:72:ARG:HH11 | 1.63 | 0.63 |
| 13:M:110:LEU:HG | 13:M:125:LEU:HD12 | 1.79 | 0.63 |
| 2:P:71:ASN:HD22 | 2:P:72:ASP:H | 1.46 | 0.63 |
| 4:R:207:LEU:CD2 | 4:R:233:ILE:HD12 | 2.28 | 0.63 |
| 10:X:38:SER:HB2 | 10:X:39:PRO:HD2 | 1.80 | 0.63 |
| 13:1:84:ALA:HA | 13:1:113:VAL:HG21 | 1.81 | 0.63 |
| 13:1:110:LEU:HG | 13:1:125:LEU:HD12 | 1.79 | 0.63 |
| 12:L:14(I):THR:HG21 | 12:L:14(M):VAL:HB | 1.80 | 0.63 |
| 2:P:141:TYR:CD1 | 2:P:21(E):VAL:HG21 | 2.33 | 0.63 |
| 2:P:219:GLU:HG2 | 2:P:21(E):VAL:N | 2.13 | 0.63 |
| 13:1:19:LEU:HD21 | 13:1:26:LEU:HD22 | 1.79 | 0.63 |
| 8:H:80:LEU:HD12 | 8:H:113:ILE:HD11 | 1.80 | 0.63 |
| 13:1:19:LEU:HB2 | 13:1:170:SER:HB2 | 1.80 | 0.63 |
| 9:I:45:ILE:HB | 9:I:52:VAL:HG13 | 1.80 | 0.63 |
| 12:L:90:LYS:HD3 | 12:L:95:TYR:CE1 | 2.33 | 0.63 |
| 11:K:143:LYS:HB2 | 11:K:146:LEU:HD13 | 1.80 | 0.63 |
| 4:R:192:LEU:O | 4:R:196:ILE:HG12 | 1.99 | 0.63 |
| 7:U:34(A):ASN:HD22 | 7:U:167:PRO:HG2 | 1.62 | 0.63 |
| 14:N:13:ILE:HG12 | 14:N:177:VAL:HG13 | 1.80 | 0.63 |
| 5:S:141:TYR:CE2 | 5:S:217:LYS:HA | 2.34 | 0.63 |
| 2:P:101:LYS:HZ1 | 10:X:85:GLN:NE2 | 1.96 | 0.63 |
| 6:F:187:ARG:HG3 | 6:F:187:ARG:HH11 | 1.64 | 0.63 |
| 10:J:156:LYS:O | 10:J:160:GLN:HG3 | 1.99 | 0.63 |
| 4:R:12(G):GLU:HG2 | 4:R:125:GLU:H | 1.63 | 0.63 |
| 14:2:107:LYS:HG2 | 14:2:108:GLY:N | 2.13 | 0.63 |
| 10:X:44:SER:OG | 10:X:100:LEU:HB2 | 1.99 | 0.62 |
| 1:A:121:GLN:O | 1:A:124:THR:HB | 2.00 | 0.62 |
| 8:H:38:SER:OG | 8:H:41:ILE:HD13 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:32:ASP:OD2 | 10:J:34:THR:HG22 | 1.99 | 0.62 |
| 2:B:97:GLN:HE22 | 9:I:64:ASN:HD22 | 1.47 | 0.62 |
| 3:C:235:GLN:O | 3:C:239:GLU:HG2 | 2.00 | 0.62 |
| 4:D:97:VAL:HG11 | 11:K:65:LEU:HD22 | 1.81 | 0.62 |
| 5:E:141:TYR:CE2 | 5:E:217:LYS:HA | 2.33 | 0.62 |
| 11:K:126:CYS:HB2 | 11:K:135:TYR:CE1 | 2.34 | 0.62 |
| 12:L:14(C):GLN:HG2 | 8:V:210:THR:CG2 | 2.29 | 0.62 |
| 12:Z:14:LEU:HD13 | 12:Z:34:VAL:HG13 | 1.80 | 0.62 |
| 12:Z:90:LYS:HD3 | 12:Z:95:TYR:CE1 | 2.34 | 0.62 |
| 14:2:10(B):LYS:HD3 | 14:2:10(B):LYS:C | 2.19 | 0.62 |
| 8:V:80:LEU:HD12 | 8:V:113:ILE:HD11 | 1.79 | 0.62 |
| 3:C:232:TYR:O | 3:C:236:ILE:HG13 | 1.98 | 0.62 |
| 7:G:96:ALA:CA | 7:G:107:MET:HE2 | 2.22 | 0.62 |
| 13:M:84:ALA:HA | 13:M:113:VAL:HG21 | 1.80 | 0.62 |
| 7:U:8:TYR:C | 7:U:10:ARG:H | 2.03 | 0.62 |
| 4:D:12(G):GLU:HG2 | 4:D:125:GLU:H | 1.63 | 0.62 |
| 5:S:201:LEU:O | 5:S:202:ARG:HB2 | 1.98 | 0.62 |
| 11:Y:143:LYS:HB2 | 11:Y:146:LEU:HD13 | 1.79 | 0.62 |
| 13:1:14(D):GLU:O | 13:1:14(G):ILE:HG12 | 2.00 | 0.62 |
| 6:F:43:ASN:ND2 | 6:F:185:SER:HA | 2.15 | 0.62 |
| 8:V:45:GLY:O | 15:V:1001:BIQ:H251 | 2.00 | 0.62 |
| 2:P:15:PHE:H | 3:Q:23:GLN:HE22 | 1.47 | 0.62 |
| 3:Q:173:ARG:O | 3:Q:177:GLU:HG3 | 2.00 | 0.62 |
| 7:U:39:ALA:HB2 | 7:U:48:VAL:HG12 | 1.82 | 0.62 |
| 3:C:71:ASP:HA | 10:J:68:ILE:CD1 | 2.29 | 0.62 |
| 10:J:-1:MET:HG2 | 10:J:1:ASP:N | 2.14 | 0.62 |
| 1:O:225:THR:OG1 | 1:O:228:GLU:HG3 | 2.00 | 0.62 |
| 6:T:43:ASN:ND2 | 6:T:185:SER:HA | 2.14 | 0.62 |
| 10:X:133:TYR:CE2 | 10:X:166:MET:HG3 | 2.35 | 0.62 |
| 13:M:57:ARG:NE | 16:M:247:HOH:O | 2.33 | 0.62 |
| 4:R:97:VAL:HG11 | 11:Y:65:LEU:HD22 | 1.81 | 0.62 |
| 7:U:121:GLN:O | 7:U:124:THR:HB | 2.00 | 0.62 |
| 15:V:1001:BIQ:HN6 | 9:W:114:ASP:HB2 | 1.64 | 0.61 |
| 6:F:192:GLN:HE21 | 6:F:195:LYS:HE3 | 1.64 | 0.61 |
| 13:M:19:LEU:HD21 | 13:M:26:LEU:HD22 | 1.82 | 0.61 |
| 2:P:21:LEU:HD13 | 2:P:124:THR:HG23 | 1.80 | 0.61 |
| 4:D:192:LEU:O | 4:D:196:ILE:HG12 | 2.00 | 0.61 |
| 11:Y:7:ARG:HD2 | 11:Y:108:PRO:O | 2.00 | 0.61 |
| 5:E:201:LEU:O | 5:E:202:ARG:HB2 | 2.00 | 0.61 |
| 3:Q:232:TYR:O | 3:Q:236:ILE:HG13 | 1.99 | 0.61 |
| 11:Y:126:CYS:HB2 | 11:Y:135:TYR:CE1 | 2.35 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:38:SER:HB2 | 10:J:39:PRO:HD2 | 1.83 | 0.61 |
| 10:J:167:PRO:HB2 | 10:X:168:MET:HE1 | 1.82 | 0.61 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:HB2 | 1.81 | 0.61 |
| 2:P:163:ILE:HD13 | 2:P:164:SER:N | 2.11 | 0.61 |
| 3:Q:177:GLU:OE2 | 4:R:57:PRO:HD2 | 2.01 | 0.61 |
| 12:Z:93:PHE:N | 12:Z:94:PRO:HD3 | 2.15 | 0.61 |
| 10:J:44:SER:OG | 10:J:100:LEU:HB2 | 2.01 | 0.61 |
| 9:W:43:LEU:HD21 | 9:W:45:ILE:HD11 | 1.82 | 0.61 |
| 10:X:-1:MET:HG2 | 10:X:1:ASP:N | 2.15 | 0.61 |
| 3:Q:52:ARG:HB2 | 3:Q:209:ASN:HA | 1.82 | 0.61 |
| 3:C:226:SER:HB2 | 3:C:227:GLU:OE1 | 2.00 | 0.61 |
| 5:E:15:PHE:HB2 | 6:F:23:GLN:NE2 | 2.16 | 0.61 |
| 13:M:19:LEU:HB2 | 13:M:170:SER:HB2 | 1.81 | 0.61 |
| 14:N:36:ARG:HG3 | 14:N:42:TRP:CE2 | 2.36 | 0.61 |
| 2:P:185:LYS:HD3 | 2:P:186:VAL:N | 2.16 | 0.60 |
| 3:Q:241:GLN:C | 3:Q:243:GLN:H | 2.03 | 0.60 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:HB2 | 1.83 | 0.60 |
| 6:T:186:ALA:O | 6:T:190:VAL:HG23 | 2.02 | 0.60 |
| 6:T:187:ARG:HH11 | 6:T:187:ARG:HG3 | 1.64 | 0.60 |
| 5:E:2(B):THR:H | 5:E:2(E):ASN:HD22 | 1.49 | 0.60 |
| 9:W:6:MET:HB3 | 9:W:151:LEU:HD11 | 1.84 | 0.60 |
| 3:C:241:GLN:C | 3:C:243:GLN:H | 2.03 | 0.60 |
| 4:D:175:GLU:CG | 4:D:196:ILE:HD12 | 2.31 | 0.60 |
| 12:L:29:ARG:NH1 | 12:L:193:ARG:HB3 | 2.16 | 0.60 |
| 7:G:39:ALA:HB2 | 7:G:48:VAL:HG12 | 1.82 | 0.60 |
| 14:N:10(B):LYS:HD3 | 14:N:10(B):LYS:C | 2.22 | 0.60 |
| 2:B:185:LYS:HD3 | 2:B:186:VAL:N | 2.17 | 0.60 |
| 6:F:69:VAL:HG12 | 16:F:248:HOH:O | 2.01 | 0.60 |
| 6:T:54:ILE:HG12 | 6:T:208:PHE:HA | 1.84 | 0.60 |
| 6:T:147:HIS:HD2 | 16:T:242:HOH:O | 1.84 | 0.60 |
| 7:G:8:TYR:C | 7:G:10:ARG:H | 2.03 | 0.60 |
| 1:A:225:THR:OG1 | 1:A:228:GLU:HG3 | 2.01 | 0.60 |
| 2:B:163:ILE:HD13 | 2:B:164:SER:N | 2.13 | 0.60 |
| 3:C:40:VAL:HG12 | 3:C:162:ALA:HB1 | 1.83 | 0.60 |
| 10:J:113:ILE:HG12 | 10:J:119:LYS:HG3 | 1.84 | 0.60 |
| 12:L:14:LEU:HD13 | 12:L:34:VAL:HG13 | 1.81 | 0.60 |
| 3:Q:40:VAL:HG12 | 3:Q:162:ALA:HB1 | 1.81 | 0.60 |
| 14:2:36:ARG:HG3 | 14:2:42:TRP:CE2 | 2.36 | 0.60 |
| 1:A:173:LYS:O | 1:A:177:GLU:HG3 | 2.03 | 0.59 |
| 4:D:45:GLY:HA2 | 4:D:146:TYR:CE1 | 2.37 | 0.59 |
| 1:O:110:LYS:HG2 | 16:O:245:HOH:O | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:45:GLY:HA2 | 4:R:146:TYR:CE1 | 2.37 | 0.59 |
| 8:V:196:VAL:HG23 | 16:V:1021:HOH:O | 2.01 | 0.59 |
| 14:N:175:MET:HB2 | 14:N:187:LEU:HB2 | 1.83 | 0.59 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:HD13 | 1.83 | 0.59 |
| 8:H:165:ASN:ND2 | 13:1:139:ARG:HH11 | 1.99 | 0.59 |
| 3:Q:226:SER:HB2 | 3:Q:227:GLU:OE1 | 2.01 | 0.59 |
| 2:B:121:GLN:HG3 | 3:C:83:ALA:HB1 | 1.85 | 0.59 |
| 10:J:133:TYR:HE1 | 16:X:220:HOH:O | 1.86 | 0.59 |
| 8:H:210:THR:HG21 | 12:Z:14(C):GLN:HG2 | 1.85 | 0.59 |
| 9:I:43:LEU:HD21 | 9:I:45:ILE:HD11 | 1.85 | 0.59 |
| 6:T:82:ILE:HB | 6:T:83:PRO:HD3 | 1.83 | 0.59 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:HD2 | 1.82 | 0.59 |
| 6:F:82:ILE:HB | 6:F:83:PRO:HD3 | 1.84 | 0.59 |
| 9:W:106:GLY:HA2 | 9:W:181:LYS:HD3 | 1.85 | 0.59 |
| 4:D:243:ALA:O | 4:D:244:GLU:HB2 | 2.01 | 0.59 |
| 5:E:31:ILE:HD11 | 5:E:153:PRO:CD | 2.33 | 0.59 |
| 6:F:186:ALA:O | 6:F:190:VAL:HG23 | 2.03 | 0.59 |
| 1:O:179:ARG:NH1 | 1:O:179:ARG:HB3 | 2.17 | 0.59 |
| 8:V:18:THR:HB | 8:V:30:ASN:HA | 1.83 | 0.59 |
| 1:A:179:ARG:HB3 | 1:A:179:ARG:NH1 | 2.18 | 0.59 |
| 12:L:93:PHE:N | 12:L:94:PRO:HD3 | 2.17 | 0.59 |
| 4:R:243:ALA:O | 4:R:244:GLU:HB2 | 2.02 | 0.59 |
| 6:T:203:GLU:O | 6:T:206:LYS:HD2 | 2.03 | 0.59 |
| 4:D:12(D):ALA:HA | 5:E:129:GLY:HA2 | 1.84 | 0.59 |
| 4:D:207:LEU:HD21 | 4:D:233:ILE:HD12 | 1.84 | 0.59 |
| 10:J:168:MET:HE3 | 10:X:168:MET:HE3 | 1.85 | 0.59 |
| 13:M:139:ARG:HH11 | 8:V:165:ASN:ND2 | 1.97 | 0.59 |
| 5:S:2(B):THR:H | 5:S:2(E):ASN:HD22 | 1.49 | 0.59 |
| 3:C:173:ARG:O | 3:C:177:GLU:HG3 | 2.03 | 0.59 |
| 14:2:175:MET:HB2 | 14:2:187:LEU:HB2 | 1.85 | 0.59 |
| 6:F:173:LYS:O | 6:F:177:GLU:HG3 | 2.02 | 0.58 |
| 15:H:1000:BIQ:HN6 | 9:I:114:ASP:HB2 | 1.68 | 0.58 |
| 3:Q:41:LYS:HD3 | 3:Q:161:SER:HA | 1.85 | 0.58 |
| 4:R:207:LEU:HD21 | 4:R:233:ILE:HD12 | 1.84 | 0.58 |
| 6:T:43:ASN:N | 6:T:43:ASN:ND2 | 2.52 | 0.58 |
| 3:C:177:GLU:OE2 | 4:D:57:PRO:HD2 | 2.03 | 0.58 |
| 9:I:6:MET:HB3 | 9:I:151:LEU:HD11 | 1.85 | 0.58 |
| 2:B:126:HIS:HB3 | 3:C:129:VAL:HG12 | 1.86 | 0.58 |
| 5:S:201:LEU:HD11 | 5:S:207:LEU:CD2 | 2.34 | 0.58 |
| 1:A:97:HIS:HD2 | 8:H:61:SER:OG | 1.87 | 0.58 |
| 3:C:52:ARG:HB2 | 3:C:209:ASN:HA | 1.85 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:194:LEU:HD22 | 4:D:212:LEU:HD11 | 1.84 | 0.58 |
| 6:F:54:ILE:HG12 | 6:F:208:PHE:HA | 1.85 | 0.58 |
| 4:R:85:ALA:O | 4:R:89:ILE:HG12 | 2.03 | 0.58 |
| 1:O:33:GLN:HE21 | 1:O:33:GLN:HA | 1.68 | 0.58 |
| 9:W:137:MET:HE3 | 9:W:141:LEU:HD11 | 1.84 | 0.58 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:HD2 | 1.85 | 0.58 |
| 10:X:7:ARG:HG2 | 10:X:7:ARG:HH11 | 1.69 | 0.58 |
| 2:B:15:PHE:H | 3:C:23:GLN:NE2 | 1.96 | 0.58 |
| 14:N:107:LYS:CG | 14:N:108:GLY:H | 2.17 | 0.58 |
| 6:F:43:ASN:N | 6:F:43:ASN:ND2 | 2.51 | 0.58 |
| 6:F:72:ARG:HD2 | 13:M:64:THR:OG1 | 2.04 | 0.58 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:HG3 | 1.85 | 0.58 |
| 1:A:33:GLN:HE21 | 1:A:33:GLN:HA | 1.69 | 0.57 |
| 3:C:160:TRP:CE2 | 4:D:59:LEU:HD23 | 2.38 | 0.57 |
| 9:I:106:GLY:HA2 | 9:I:181:LYS:HD3 | 1.86 | 0.57 |
| 4:R:175:GLU:CG | 4:R:196:ILE:HD12 | 2.33 | 0.57 |
| 1:A:179:ARG:HB3 | 1:A:179:ARG:HH11 | 1.69 | 0.57 |
| 4:D:85:ALA:O | 4:D:89:ILE:HG12 | 2.04 | 0.57 |
| 8:H:210:THR:CG2 | 12:Z:14(C):GLN:HG2 | 2.34 | 0.57 |
| 12:L:114:ASP:HB3 | 12:L:118:SER:H | 1.69 | 0.57 |
| 1:O:179:ARG:HB3 | 1:O:179:ARG:HH11 | 1.69 | 0.57 |
| 3:C:7:GLY:N | 16:C:268:HOH:O | 2.37 | 0.57 |
| 10:J:147:THR:OG1 | 10:J:150:GLU:HG3 | 2.04 | 0.57 |
| 3:C:41:LYS:HD3 | 3:C:161:SER:HA | 1.85 | 0.57 |
| 2:P:101:LYS:HZ2 | 10:X:85:GLN:NE2 | 2.02 | 0.57 |
| 5:S:47:VAL:HG22 | 5:S:214:ILE:HD12 | 1.86 | 0.57 |
| 6:T:95:GLU:CG | 6:T:115:ARG:HB3 | 2.33 | 0.57 |
| 12:Z:43:MET:HB2 | 12:Z:101:ILE:HG22 | 1.85 | 0.57 |
| 8:H:72:ARG:HG3 | 8:H:72:ARG:HH11 | 1.69 | 0.57 |
| 4:R:194:LEU:HD22 | 4:R:212:LEU:HD11 | 1.86 | 0.57 |
| 3:Q:182:PRO:O | 3:Q:184:ALA:N | 2.38 | 0.57 |
| 7:G:172:ILE:HD12 | 7:G:197:MET:CE | 2.35 | 0.57 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:HB2 | 1.86 | 0.57 |
| 1:A:86:ARG:HE | 7:G:118:ASN:ND2 | 2.03 | 0.57 |
| 9:I:29:ASN:H | 9:I:29:ASN:HD22 | 1.52 | 0.57 |
| 9:W:29:ASN:HD22 | 9:W:29:ASN:H | 1.53 | 0.57 |
| 14:2:176:VAL:HG12 | 14:2:178:LEU:HD13 | 1.87 | 0.57 |
| 12:L:148:VAL:O | 12:L:152:ILE:HG13 | 2.05 | 0.57 |
| 5:E:47:VAL:HG22 | 5:E:214:ILE:HD12 | 1.87 | 0.56 |
| 10:J:133:TYR:CE2 | 10:J:166:MET:HG3 | 2.40 | 0.56 |
| 11:K:19:ARG:HH21 | 11:K:29:GLN:HE22 | 1.52 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:177:LEU:HA | 5:S:58:LEU:HD11 | 1.86 | 0.56 |
| 5:S:31:ILE:HD11 | 5:S:153:PRO:CD | 2.34 | 0.56 |
| 6:F:237:GLN:O | 6:F:240:ILE:HG22 | 2.06 | 0.56 |
| 7:G:121:GLN:O | 7:G:124:THR:HB | 2.04 | 0.56 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:CD | 2.17 | 0.56 |
| 2:P:225:LYS:HG3 | 2:P:228:GLU:OE1 | 2.04 | 0.56 |
| 7:U:67:ILE:HD12 | 7:U:211:GLU:HG2 | 1.86 | 0.56 |
| 2:B:218:ASN:O | 2:B:21(C):ASP:HB2 | 2.06 | 0.56 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:HG3 | 1.87 | 0.56 |
| 3:C:182:PRO:O | 3:C:184:ALA:N | 2.38 | 0.56 |
| 6:F:203:GLU:O | 6:F:206:LYS:HD2 | 2.05 | 0.56 |
| 8:H:18:THR:HB | 8:H:30:ASN:HA | 1.86 | 0.56 |
| 11:K:7:ARG:HD2 | 11:K:108:PRO:O | 2.05 | 0.56 |
| 12:L:8:GLY:HA3 | 12:L:11:PHE:CE2 | 2.40 | 0.56 |
| 3:Q:160:TRP:CE2 | 4:R:59:LEU:HD23 | 2.40 | 0.56 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:CD | 2.18 | 0.56 |
| 2:P:6:ARG:HD2 | 4:R:9:ASP:N | 2.20 | 0.56 |
| 6:T:237:GLN:O | 6:T:240:ILE:HG22 | 2.05 | 0.56 |
| 7:G:141:VAL:HG21 | 7:G:216:THR:HA | 1.87 | 0.56 |
| 1:O:60:MET:HE2 | 16:U:255:HOH:O | 2.06 | 0.56 |
| 2:P:97:GLN:HE22 | 9:W:64:ASN:HD22 | 1.51 | 0.56 |
| 4:R:121:LEU:HD13 | 5:S:130:ARG:HH21 | 1.71 | 0.56 |
| 5:S:73:HIS:HE1 | 5:S:107:LEU:O | 1.87 | 0.56 |
| 6:T:72:ARG:HD2 | 13:1:64:THR:OG1 | 2.04 | 0.56 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:HG3 | 1.87 | 0.56 |
| 7:U:83:PRO:HG2 | 16:U:262:HOH:O | 2.06 | 0.56 |
| 11:Y:156:LYS:HB2 | 11:Y:175:LEU:HD11 | 1.87 | 0.56 |
| 2:B:225:LYS:HG3 | 2:B:228:GLU:OE1 | 2.06 | 0.56 |
| 14:N:176:VAL:HG12 | 14:N:178:LEU:HD13 | 1.86 | 0.56 |
| 2:B:55:THR:HG22 | 2:B:59:LEU:HD23 | 1.88 | 0.56 |
| 9:W:29:ASN:ND2 | 9:W:29:ASN:H | 2.04 | 0.56 |
| 11:Y:12:ILE:HB | 11:Y:178:VAL:HB | 1.88 | 0.56 |
| 11:Y:19:ARG:HH21 | 11:Y:29:GLN:HE22 | 1.52 | 0.56 |
| 12:L:43:MET:HB2 | 12:L:101:ILE:HG22 | 1.87 | 0.56 |
| 6:T:173:LYS:O | 6:T:177:GLU:HG3 | 2.05 | 0.56 |
| 8:V:72:ARG:HG3 | 8:V:72:ARG:HH11 | 1.71 | 0.56 |
| 13:1:7:LYS:HG3 | 13:1:14(G):ILE:HD12 | 1.88 | 0.56 |
| 2:B:152:ASN:HB2 | 2:B:153:PRO:CD | 2.36 | 0.56 |
| 9:I:43:LEU:CG | 9:I:45:ILE:HD11 | 2.36 | 0.56 |
| 9:W:14:ILE:HG13 | 9:W:34:ILE:HD12 | 1.88 | 0.56 |
| 9:W:43:LEU:CG | 9:W:45:ILE:HD11 | 2.36 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Z:-7:ASN:ND2 | 12:Z:-5:TYR:H | 2.03 | 0.56 |
| 11:K:156:LYS:HB2 | 11:K:175:LEU:HD11 | 1.88 | 0.56 |
| 2:P:124:THR:CG2 | 3:Q:130:ARG:HH21 | 2.16 | 0.56 |
| 6:F:95:GLU:CG | 6:F:115:ARG:HB3 | 2.35 | 0.55 |
| 7:G:152:ASP:HB2 | 7:G:153:PRO:CD | 2.36 | 0.55 |
| 9:I:28:SER:HB2 | 10:J:120:VAL:HG21 | 1.86 | 0.55 |
| 9:I:29:ASN:ND2 | 9:I:29:ASN:H | 2.03 | 0.55 |
| 10:J:52:THR:CG2 | 10:J:53:VAL:N | 2.69 | 0.55 |
| 14:N:126:ILE:HD13 | 14:N:126:ILE:H | 1.72 | 0.55 |
| 16:D:268:HOH:O | 5:E:86:ARG:HD3 | 2.07 | 0.55 |
| 5:E:73:HIS:HE1 | 5:E:107:LEU:O | 1.89 | 0.55 |
| 2:P:97:GLN:NE2 | 9:W:64:ASN:HD22 | 2.04 | 0.55 |
| 8:V:53:GLU:O | 8:V:56:THR:HG22 | 2.06 | 0.55 |
| 4:R:53:ARG:O | 4:R:53:ARG:HG2 | 2.05 | 0.55 |
| 4:R:72:ARG:HG3 | 16:R:1302:HOH:O | 2.05 | 0.55 |
| 6:T:37:SER:HB3 | 6:T:50:VAL:HG23 | 1.88 | 0.55 |
| 2:P:218:ASN:O | 2:P:21(C):ASP:HB2 | 2.07 | 0.55 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:HG3 | 1.87 | 0.55 |
| 13:1:46:SER:OG | 13:1:98:ALA:HB3 | 2.06 | 0.55 |
| 2:B:196:THR:O | 2:B:200:THR:HG23 | 2.07 | 0.55 |
| 5:E:201:LEU:HD11 | 5:E:207:LEU:CD2 | 2.34 | 0.55 |
| 12:L:14(I):THR:O | 12:L:14(K):LYS:HB2 | 2.07 | 0.55 |
| 7:U:141:VAL:HG21 | 7:U:216:THR:HA | 1.88 | 0.55 |
| 8:V:34:LEU:HD22 | 8:V:174:ASP:HB3 | 1.88 | 0.55 |
| 10:J:168:MET:HE1 | 10:X:167:PRO:CB | 2.37 | 0.55 |
| 7:U:87:ASN:C | 7:U:87:ASN:HD22 | 2.09 | 0.55 |
| 13:1:113:VAL:HG23 | 13:1:119:THR:HG22 | 1.87 | 0.55 |
| 6:F:36:THR:HG22 | 6:F:51:GLU:OE2 | 2.07 | 0.55 |
| 13:M:7:LYS:HG3 | 13:M:14(G):ILE:HD12 | 1.89 | 0.55 |
| 2:P:71:ASN:ND2 | 2:P:72:ASP:N | 2.52 | 0.55 |
| 4:R:160:TYR:CE2 | 5:S:59:SER:HB3 | 2.41 | 0.55 |
| 5:S:15:PHE:H | 6:T:23:GLN:NE2 | 2.01 | 0.55 |
| 9:W:14:ILE:CG1 | 9:W:34:ILE:HD12 | 2.36 | 0.55 |
| 1:A:197:LEU:HD23 | 1:A:210:ILE:HD12 | 1.87 | 0.55 |
| 11:K:40:PHE:HB3 | 11:K:73:ARG:NH2 | 2.21 | 0.55 |
| 8:V:172:ASN:HD22 | 8:V:193:THR:HA | 1.71 | 0.55 |
| 12:Z:79:ALA:O | 12:Z:83:ILE:HG12 | 2.07 | 0.55 |
| 12:Z:14(I):THR:O | 12:Z:14(K):LYS:HB2 | 2.07 | 0.55 |
| 14:2:107:LYS:CG | 14:2:108:GLY:H | 2.18 | 0.55 |
| 2:P:239:THR:OXT | 2:P:239:THR:HG22 | 2.07 | 0.55 |
| 9:W:174:VAL:HG21 | 9:W:186:LYS:HE3 | 1.88 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Z:5:GLY:O | 12:Z:124:CYS:HA | 2.07 | 0.55 |
| 2:B:124:THR:HG22 | 3:C:130:ARG:NH2 | 2.10 | 0.55 |
| 3:C:190:VAL:O | 3:C:194:VAL:HG23 | 2.07 | 0.55 |
| 6:T:216:SER:HB3 | 6:T:21(A):GLU:HB2 | 1.89 | 0.55 |
| 7:U:172:ILE:HD12 | 7:U:197:MET:CE | 2.36 | 0.55 |
| 12:L:79:ALA:O | 12:L:83:ILE:HG12 | 2.07 | 0.54 |
| 1:O:173:LYS:O | 1:O:177:GLU:HG3 | 2.06 | 0.54 |
| 2:P:55:THR:HG22 | 2:P:59:LEU:HD23 | 1.88 | 0.54 |
| 4:R:12(D):ALA:HB3 | 4:R:126:ARG:CD | 2.36 | 0.54 |
| 4:R:160:TYR:HA | 5:S:59:SER:HA | 1.88 | 0.54 |
| 5:S:68:ILE:HB | 5:S:76:LEU:CD2 | 2.37 | 0.54 |
| 7:U:152:ASP:HB2 | 7:U:153:PRO:CD | 2.37 | 0.54 |
| 9:W:43:LEU:CD2 | 9:W:45:ILE:HD11 | 2.36 | 0.54 |
| 7:G:225:SER:O | 7:G:229:ILE:HG13 | 2.06 | 0.54 |
| 12:L:5:GLY:O | 12:L:124:CYS:HA | 2.07 | 0.54 |
| 13:M:113:VAL:HG23 | 13:M:119:THR:HG22 | 1.88 | 0.54 |
| 3:Q:168:ASN:HB2 | 3:Q:200:VAL:HG11 | 1.89 | 0.54 |
| 10:X:143:ARG:O | 10:X:146:MET:HG3 | 2.07 | 0.54 |
| 12:Z:8:GLY:HA3 | 12:Z:11:PHE:CE2 | 2.41 | 0.54 |
| 2:B:97:GLN:NE2 | 9:I:64:ASN:HD22 | 2.06 | 0.54 |
| 3:C:206:GLY:CA | 3:C:209:ASN:HB2 | 2.36 | 0.54 |
| 8:H:34:LEU:HD22 | 8:H:174:ASP:HB3 | 1.89 | 0.54 |
| 14:N:163:ILE:HG23 | 14:N:170:GLY:HA2 | 1.89 | 0.54 |
| 7:U:225:SER:O | 7:U:229:ILE:HG13 | 2.08 | 0.54 |
| 10:X:52:THR:CG2 | 10:X:53:VAL:N | 2.70 | 0.54 |
| 7:G:233:LEU:O | 7:G:236:ILE:HG13 | 2.08 | 0.54 |
| 1:O:197:LEU:HD23 | 1:O:210:ILE:HD12 | 1.89 | 0.54 |
| 13:1:40:ASN:HD22 | 13:1:40:ASN:N | 1.99 | 0.54 |
| 5:E:65:LYS:HG3 | 5:E:65:LYS:O | 2.07 | 0.54 |
| 5:S:190:ILE:CG2 | 5:S:212:ILE:HD13 | 2.38 | 0.54 |
| 6:T:43:ASN:ND2 | 6:T:43:ASN:H | 2.04 | 0.54 |
| 6:T:54:ILE:HD11 | 6:T:209:GLU:HB2 | 1.89 | 0.54 |
| 7:U:224:LEU:HB3 | 7:U:228:ASN:HB2 | 1.90 | 0.54 |
| 1:A:69:LEU:C | 1:A:69:LEU:HD23 | 2.27 | 0.54 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:CD | 2.38 | 0.54 |
| 13:M:40:ASN:HD22 | 13:M:40:ASN:N | 1.99 | 0.54 |
| 2:P:71:ASN:HD22 | 2:P:72:ASP:N | 2.06 | 0.54 |
| 5:S:68:ILE:HB | 5:S:76:LEU:HD21 | 1.89 | 0.54 |
| 6:T:20(B):GLU:CD | 6:T:20(C):LYS:HE3 | 2.28 | 0.54 |
| 7:U:168:LYS:O | 7:U:172:ILE:HG12 | 2.07 | 0.54 |
| 11:Y:7:ARG:HG2 | 11:Y:108:PRO:HB2 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Z:40:ASN:ND2 | 16:Z:219:HOH:O | 2.39 | 0.54 |
| 16:B:254:HOH:O | 3:C:33:ARG:HD2 | 2.07 | 0.54 |
| 3:C:216:LYS:HD2 | 3:C:220:ASP:OD1 | 2.08 | 0.54 |
| 4:D:53:ARG:O | 4:D:53:ARG:HG2 | 2.08 | 0.54 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:HB2 | 1.89 | 0.54 |
| 10:J:7:ARG:HH11 | 10:J:7:ARG:HG2 | 1.73 | 0.54 |
| 11:K:195:LEU:O | 11:K:199:VAL:HG23 | 2.07 | 0.54 |
| 3:Q:216:LYS:HD2 | 3:Q:220:ASP:OD1 | 2.07 | 0.54 |
| 4:R:186:LEU:O | 4:R:190:GLU:HG3 | 2.08 | 0.54 |
| 7:G:38:LEU:C | 7:G:38:LEU:HD12 | 2.28 | 0.54 |
| 11:K:207:ASN:HD21 | 10:X:144:PRO:CG | 2.21 | 0.54 |
| 1:O:86:ARG:HH21 | 7:U:118:ASN:ND2 | 2.05 | 0.54 |
| 5:S:190:ILE:HG23 | 5:S:212:ILE:HD13 | 1.89 | 0.54 |
| 10:X:113:ILE:HA | 10:X:118:THR:O | 2.08 | 0.54 |
| 1:A:86:ARG:HH21 | 7:G:118:ASN:ND2 | 2.05 | 0.54 |
| 2:B:21:LEU:O | 2:B:25:GLU:HG2 | 2.07 | 0.54 |
| 3:C:168:ASN:HB2 | 3:C:200:VAL:HG11 | 1.90 | 0.54 |
| 9:I:2:ILE:HG21 | 9:I:130:ALA:HB3 | 1.90 | 0.54 |
| 1:O:232:ARG:HG3 | 1:O:232:ARG:HH11 | 1.71 | 0.54 |
| 3:Q:172:VAL:HG23 | 3:Q:196:SER:HB2 | 1.88 | 0.54 |
| 6:F:20(B):GLU:CD | 6:F:20(C):LYS:HE3 | 2.29 | 0.54 |
| 9:I:14:ILE:CG1 | 9:I:34:ILE:HD12 | 2.38 | 0.54 |
| 10:J:18:LYS:HG2 | 10:J:174:ILE:HG13 | 1.90 | 0.54 |
| 7:U:233:LEU:O | 7:U:236:ILE:HG13 | 2.08 | 0.54 |
| 12:Z:114:ASP:CB | 12:Z:118:SER:HB3 | 2.37 | 0.54 |
| 5:E:190:ILE:HG23 | 5:E:212:ILE:HD13 | 1.90 | 0.53 |
| 6:F:37:SER:HB3 | 6:F:50:VAL:HG23 | 1.89 | 0.53 |
| 6:F:54:ILE:HD11 | 6:F:209:GLU:HB2 | 1.91 | 0.53 |
| 7:G:224:LEU:HB3 | 7:G:228:ASN:HB2 | 1.90 | 0.53 |
| 8:H:105:ASP:HB2 | 8:H:10(A):PRO:HD2 | 1.90 | 0.53 |
| 9:I:43:LEU:HG | 9:I:45:ILE:HD11 | 1.88 | 0.53 |
| 9:I:174:VAL:HG21 | 9:I:186:LYS:HE3 | 1.90 | 0.53 |
| 11:K:12:ILE:HB | 11:K:178:VAL:HB | 1.89 | 0.53 |
| 13:M:197:TRP:CH2 | 14:2:171:GLY:HA2 | 2.43 | 0.53 |
| 10:X:147:THR:OG1 | 10:X:150:GLU:HG3 | 2.08 | 0.53 |
| 1:A:232:ARG:HG3 | 1:A:232:ARG:HH11 | 1.73 | 0.53 |
| 2:B:71:ASN:ND2 | 2:B:72:ASP:N | 2.53 | 0.53 |
| 4:D:12(F):GLY:HA3 | 16:E:243:HOH:O | 2.08 | 0.53 |
| 5:E:68:ILE:HB | 5:E:76:LEU:HD21 | 1.91 | 0.53 |
| 6:F:43:ASN:ND2 | 6:F:43:ASN:H | 2.06 | 0.53 |
| 7:G:18(G):GLU:HG2 | 7:G:188:LYS:HB3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:I:48:LEU:HG | 9:I:50:THR:HG22 | 1.91 | 0.53 |
| 14:N:14:LEU:O | 14:N:175:MET:HA | 2.07 | 0.53 |
| 9:W:28:SER:HB2 | 10:X:120:VAL:HG21 | 1.90 | 0.53 |
| 4:D:75:GLY:HA3 | 4:D:221:PHE:CD2 | 2.43 | 0.53 |
| 4:D:186:LEU:O | 4:D:190:GLU:HG3 | 2.09 | 0.53 |
| 7:U:136:LEU:O | 7:U:150:LYS:HA | 2.07 | 0.53 |
| 12:Z:148:VAL:O | 12:Z:152:ILE:HG13 | 2.08 | 0.53 |
| 2:P:196:THR:O | 2:P:200:THR:HG23 | 2.08 | 0.53 |
| 11:Y:195:LEU:O | 11:Y:199:VAL:HG23 | 2.08 | 0.53 |
| 6:F:203:GLU:C | 6:F:205:ASN:H | 2.11 | 0.53 |
| 9:I:43:LEU:CD2 | 9:I:45:ILE:HD11 | 2.38 | 0.53 |
| 10:J:111:TYR:CE1 | 10:J:121:GLU:HG3 | 2.43 | 0.53 |
| 14:2:84:LYS:HG3 | 14:2:119:VAL:CG2 | 2.39 | 0.53 |
| 10:X:24:ILE:HD13 | 11:Y:132:THR:HG21 | 1.90 | 0.53 |
| 14:2:14:LEU:O | 14:2:175:MET:HA | 2.08 | 0.53 |
| 14:2:146:MET:CE | 14:2:150:GLU:HB3 | 2.38 | 0.53 |
| 7:G:236:ILE:HD12 | 7:G:237:ALA:N | 2.24 | 0.53 |
| 1:O:69:LEU:C | 1:O:69:LEU:HD23 | 2.29 | 0.53 |
| 5:S:65:LYS:O | 5:S:65:LYS:HG3 | 2.08 | 0.53 |
| 7:U:236:ILE:HD12 | 7:U:237:ALA:N | 2.24 | 0.53 |
| 9:W:43:LEU:HG | 9:W:45:ILE:HD11 | 1.90 | 0.53 |
| 3:C:227:GLU:OE1 | 3:C:227:GLU:N | 2.41 | 0.53 |
| 6:F:216:SER:HB3 | 6:F:21(A):GLU:HB2 | 1.89 | 0.53 |
| 12:L:99:THR:HG23 | 12:L:113:PHE:HB2 | 1.90 | 0.53 |
| 2:B:239:THR:HG22 | 2:B:239:THR:OXT | 2.09 | 0.53 |
| 4:D:170:GLU:OE1 | 4:D:170:GLU:N | 2.40 | 0.53 |
| 10:J:6:ILE:HD11 | 10:J:142:TYR:CD1 | 2.44 | 0.53 |
| 11:K:7:ARG:HG2 | 11:K:108:PRO:HB2 | 1.91 | 0.53 |
| 12:L:-7:ASN:ND2 | 12:L:-5:TYR:H | 2.07 | 0.53 |
| 6:T:127:ASN:HD22 | 6:T:128:SER:N | 2.07 | 0.53 |
| 6:F:127:ASN:HD22 | 6:F:128:SER:N | 2.07 | 0.52 |
| 7:G:177:GLU:O | 7:G:17(B):LYS:HG3 | 2.09 | 0.52 |
| 12:L:145:TYR:CD1 | 12:L:146:LEU:N | 2.77 | 0.52 |
| 3:Q:190:VAL:O | 3:Q:194:VAL:HG23 | 2.08 | 0.52 |
| 4:R:170:GLU:OE1 | 4:R:170:GLU:N | 2.40 | 0.52 |
| 14:2:146:MET:HE3 | 14:2:150:GLU:HB3 | 1.91 | 0.52 |
| 5:S:40:LEU:N | 5:S:40:LEU:HD23 | 2.24 | 0.52 |
| 6:T:43:ASN:HD21 | 6:T:185:SER:HA | 1.74 | 0.52 |
| 12:Z:83:ILE:HB | 12:Z:113:PHE:CE2 | 2.44 | 0.52 |
| 5:E:194:VAL:O | 5:E:197:ILE:HG22 | 2.10 | 0.52 |
| 7:G:87:ASN:C | 7:G:87:ASN:HD22 | 2.13 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:G:158:VAL:HG22 | 7:G:159:GLY:N | 2.24 | 0.52 |
| 8:H:179:GLU:OE2 | 8:H:182:LYS:HE2 | 2.10 | 0.52 |
| 8:V:172:ASN:ND2 | 8:V:193:THR:HA | 2.25 | 0.52 |
| 16:V:1036:HOH:O | 9:W:150:ASP:HA | 2.09 | 0.52 |
| 10:X:6:ILE:HD11 | 10:X:142:TYR:CE1 | 2.44 | 0.52 |
| 14:2:126:ILE:HD13 | 14:2:126:ILE:H | 1.73 | 0.52 |
| 2:B:121:GLN:CG | 3:C:83:ALA:HB1 | 2.38 | 0.52 |
| 5:E:40:LEU:N | 5:E:40:LEU:HD23 | 2.25 | 0.52 |
| 5:E:190:ILE:CG2 | 5:E:212:ILE:HD13 | 2.39 | 0.52 |
| 6:F:21(B):THR:O | 6:F:21(C):ASN:HB2 | 2.09 | 0.52 |
| 8:H:33:LYS:HD3 | 15:H:1000:BIQ:H253 | 1.92 | 0.52 |
| 14:N:8:PHE:CE1 | 14:N:10:ASP:HB2 | 2.44 | 0.52 |
| 7:U:186:TRP:O | 7:U:190:VAL:HG23 | 2.10 | 0.52 |
| 9:W:130:ALA:HB2 | 9:W:166:ASP:HB2 | 1.91 | 0.52 |
| 3:C:186:VAL:O | 3:C:190:VAL:HG23 | 2.10 | 0.52 |
| 7:G:136:LEU:O | 7:G:150:LYS:HA | 2.08 | 0.52 |
| 7:G:168:LYS:O | 7:G:172:ILE:HG12 | 2.10 | 0.52 |
| 2:P:152:ASN:HB2 | 2:P:153:PRO:CD | 2.40 | 0.52 |
| 3:Q:55:THR:C | 3:Q:56:LEU:HD22 | 2.30 | 0.52 |
| 4:R:177:LEU:HD22 | 5:S:58:LEU:CD1 | 2.40 | 0.52 |
| 10:X:6:ILE:HD11 | 10:X:142:TYR:CD1 | 2.45 | 0.52 |
| 1:A:32:LYS:HA | 1:A:32:LYS:HE2 | 1.91 | 0.52 |
| 5:E:15:PHE:H | 6:F:23:GLN:NE2 | 2.02 | 0.52 |
| 9:I:44:GLY:O | 9:I:45:ILE:HD13 | 2.09 | 0.52 |
| 4:R:75:GLY:HA3 | 4:R:221:PHE:CD2 | 2.45 | 0.52 |
| 12:Z:145:TYR:CD1 | 12:Z:146:LEU:N | 2.77 | 0.52 |
| 2:B:6:ARG:HB2 | 5:E:127:TYR:OH | 2.10 | 0.52 |
| 2:B:95:HIS:CD2 | 2:B:115:ARG:HG2 | 2.44 | 0.52 |
| 6:F:43:ASN:HD21 | 6:F:185:SER:HA | 1.75 | 0.52 |
| 10:J:6:ILE:HD11 | 10:J:142:TYR:CE1 | 2.45 | 0.52 |
| 10:J:24:ILE:HD13 | 11:K:132:THR:HG21 | 1.92 | 0.52 |
| 14:N:66:TYR:CD2 | 14:N:74:PRO:HB3 | 2.45 | 0.52 |
| 4:R:229:THR:O | 4:R:233:ILE:HG12 | 2.09 | 0.52 |
| 6:T:203:GLU:C | 6:T:205:ASN:H | 2.12 | 0.52 |
| 10:X:3:ILE:HG22 | 10:X:100:LEU:CD1 | 2.39 | 0.52 |
| 9:I:130:ALA:HB2 | 9:I:166:ASP:HB2 | 1.92 | 0.52 |
| 2:P:95:HIS:CD2 | 2:P:115:ARG:HG2 | 2.44 | 0.52 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:CD | 2.39 | 0.52 |
| 10:X:111:TYR:CE1 | 10:X:121:GLU:HG3 | 2.45 | 0.52 |
| 9:I:1:GLY:HA3 | 9:I:33:LYS:HE2 | 1.91 | 0.52 |
| 14:N:146:MET:CE | 14:N:150:GLU:HB3 | 2.38 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:O:97:HIS:HD2 | 8:V:61:SER:OG | 1.92 | 0.52 |
| 3:Q:163:GLN:HE22 | 3:Q:173:ARG:NE | 2.08 | 0.52 |
| 2:B:41:MET:HE3 | 16:B:240:HOH:O | 2.10 | 0.52 |
| 5:E:227:GLU:N | 5:E:227:GLU:CD | 2.63 | 0.52 |
| 12:L:83:ILE:HB | 12:L:113:PHE:CE2 | 2.45 | 0.52 |
| 5:S:104:ASN:HB2 | 13:1:81:GLU:HG2 | 1.91 | 0.52 |
| 8:V:81:GLN:O | 8:V:85:GLN:HG3 | 2.10 | 0.52 |
| 6:F:127:ASN:HD22 | 6:F:127:ASN:C | 2.12 | 0.51 |
| 8:H:165:ASN:HD22 | 13:1:139:ARG:NH1 | 2.03 | 0.51 |
| 10:J:143:ARG:O | 10:J:146:MET:HG3 | 2.10 | 0.51 |
| 13:M:46:SER:OG | 13:M:98:ALA:HB3 | 2.09 | 0.51 |
| 6:T:38:ILE:HG22 | 6:T:164:ALA:CB | 2.40 | 0.51 |
| 13:1:41:THR:OG1 | 13:1:76:PRO:HG3 | 2.10 | 0.51 |
| 14:2:59:VAL:HG22 | 14:2:82:VAL:HG12 | 1.91 | 0.51 |
| 3:C:55:THR:C | 3:C:56:LEU:HD22 | 2.31 | 0.51 |
| 7:G:67:ILE:HD12 | 7:G:211:GLU:HG2 | 1.91 | 0.51 |
| 3:Q:186:VAL:O | 3:Q:190:VAL:HG23 | 2.10 | 0.51 |
| 5:S:75:GLY:HA3 | 5:S:221:PHE:CZ | 2.45 | 0.51 |
| 6:T:53:LEU:HD11 | 6:T:205:ASN:OD1 | 2.10 | 0.51 |
| 14:2:8:PHE:CE1 | 14:2:10:ASP:HB2 | 2.45 | 0.51 |
| 7:G:69:CYS:HB3 | 16:G:276:HOH:O | 2.11 | 0.51 |
| 10:J:167:PRO:CB | 10:X:168:MET:HE1 | 2.40 | 0.51 |
| 2:P:121:GLN:CG | 3:Q:83:ALA:HB1 | 2.40 | 0.51 |
| 2:P:21(A):LYS:O | 2:P:21(B):GLY:C | 2.49 | 0.51 |
| 5:S:227:GLU:N | 5:S:227:GLU:CD | 2.63 | 0.51 |
| 7:U:227:GLU:HG2 | 16:U:282:HOH:O | 2.11 | 0.51 |
| 9:W:2:ILE:HG21 | 9:W:130:ALA:HB3 | 1.92 | 0.51 |
| 2:B:71:ASN:HD22 | 2:B:72:ASP:N | 2.07 | 0.51 |
| 4:D:229:THR:O | 4:D:233:ILE:HG12 | 2.11 | 0.51 |
| 5:E:68:ILE:HB | 5:E:76:LEU:CD2 | 2.39 | 0.51 |
| 5:E:107:LEU:HD11 | 5:E:111:ARG:HG2 | 1.92 | 0.51 |
| 7:G:192:PHE:CD1 | 7:G:192:PHE:C | 2.83 | 0.51 |
| 10:J:113:ILE:HA | 10:J:118:THR:O | 2.11 | 0.51 |
| 9:W:1:GLY:HA3 | 9:W:33:LYS:HE2 | 1.92 | 0.51 |
| 9:W:48:LEU:HG | 9:W:50:THR:HG22 | 1.92 | 0.51 |
| 14:2:163:ILE:HG23 | 14:2:170:GLY:HA2 | 1.91 | 0.51 |
| 3:C:172:VAL:HG23 | 3:C:196:SER:HB2 | 1.91 | 0.51 |
| 5:E:58:LEU:N | 5:E:58:LEU:HD12 | 2.25 | 0.51 |
| 11:K:10(A):ARG:HH11 | 11:K:10(A):ARG:HG2 | 1.75 | 0.51 |
| 2:P:224:PHE:N | 2:P:224:PHE:HD2 | 2.08 | 0.51 |
| 3:Q:71:ASP:HA | 10:X:68:ILE:HD13 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:T:21(B):THR:O | 6:T:21(C):ASN:HB2 | 2.10 | 0.51 |
| 11:Y:40:PHE:HB3 | 11:Y:73:ARG:NH2 | 2.26 | 0.51 |
| 1:A:4:MET:SD | 1:A:5:THR:N | 2.68 | 0.51 |
| 9:I:14:ILE:HG13 | 9:I:34:ILE:HD12 | 1.91 | 0.51 |
| 10:J:168:MET:CE | 10:X:168:MET:HE3 | 2.40 | 0.51 |
| 4:R:90:GLU:OE2 | 11:Y:69:ARG:NH1 | 2.44 | 0.51 |
| 2:B:234:VAL:HA | 2:B:239:THR:HA | 1.93 | 0.51 |
| 4:D:112:LEU:C | 4:D:112:LEU:HD13 | 2.31 | 0.51 |
| 4:D:12(D):ALA:HB3 | 4:D:126:ARG:CD | 2.37 | 0.51 |
| 8:H:53:GLU:O | 8:H:56:THR:HG22 | 2.11 | 0.51 |
| 13:M:-6:GLN:HG3 | 13:M:-6:GLN:O | 2.10 | 0.51 |
| 1:O:33:GLN:HE21 | 1:O:33:GLN:CA | 2.24 | 0.51 |
| 4:R:97:VAL:HG21 | 11:Y:65:LEU:HD13 | 1.93 | 0.51 |
| 13:1:-6:GLN:O | 13:1:-6:GLN:HG3 | 2.11 | 0.51 |
| 3:C:79:SER:HA | 16:C:260:HOH:O | 2.09 | 0.51 |
| 3:C:175:PHE:O | 3:C:179:ASN:HB2 | 2.10 | 0.51 |
| 7:G:186:TRP:O | 7:G:190:VAL:HG23 | 2.11 | 0.51 |
| 14:N:84:LYS:HG3 | 14:N:119:VAL:CG2 | 2.40 | 0.51 |
| 5:S:194:VAL:O | 5:S:197:ILE:HG22 | 2.10 | 0.51 |
| 7:U:158:VAL:HG22 | 7:U:159:GLY:N | 2.26 | 0.51 |
| 1:A:197:LEU:CD2 | 1:A:210:ILE:HD12 | 2.41 | 0.51 |
| 2:B:224:PHE:HD2 | 2:B:224:PHE:N | 2.09 | 0.51 |
| 10:X:13:ILE:HD12 | 10:X:177:ILE:HD13 | 1.93 | 0.51 |
| 2:B:224:PHE:N | 2:B:224:PHE:CD2 | 2.79 | 0.51 |
| 7:G:77:VAL:HG12 | 7:G:137:THR:HB | 1.93 | 0.51 |
| 8:V:33:LYS:HD3 | 15:V:1001:BIQ:H253 | 1.92 | 0.51 |
| 9:W:23:GLN:HB2 | 16:W:228:HOH:O | 2.11 | 0.51 |
| 13:1:179:ASP:HB3 | 13:1:18(A):THR:OG1 | 2.11 | 0.51 |
| 2:B:27:ALA:O | 2:B:31:ILE:HG12 | 2.12 | 0.50 |
| 13:M:139:ARG:NH1 | 8:V:165:ASN:HD22 | 2.02 | 0.50 |
| 1:O:32:LYS:HE2 | 1:O:32:LYS:HA | 1.92 | 0.50 |
| 2:P:224:PHE:N | 2:P:224:PHE:CD2 | 2.79 | 0.50 |
| 7:U:18(G):GLU:HG2 | 7:U:188:LYS:HB3 | 1.93 | 0.50 |
| 2:P:6:ARG:HG2 | 3:Q:10:ARG:NH2 | 2.25 | 0.50 |
| 2:P:235:LYS:C | 2:P:237:GLY:H | 2.14 | 0.50 |
| 11:Y:10(A):ARG:HH11 | 11:Y:10(A):ARG:HG2 | 1.76 | 0.50 |
| 11:K:207:ASN:ND2 | 10:X:144:PRO:CG | 2.74 | 0.50 |
| 14:2:112:THR:CG2 | 14:2:120:HIS:HB2 | 2.42 | 0.50 |
| 7:G:77:VAL:CG1 | 7:G:137:THR:HB | 2.42 | 0.50 |
| 12:L:31:GLU:HA | 16:L:212:HOH:O | 2.11 | 0.50 |
| 2:P:27:ALA:O | 2:P:31:ILE:HG12 | 2.11 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:U:38:LEU:C | 7:U:38:LEU:HD12 | 2.31 | 0.50 |
| 12:Z:7:ALA:HB2 | 12:Z:110:VAL:HG23 | 1.93 | 0.50 |
| 5:E:86:ARG:HG3 | 5:E:86:ARG:HH11 | 1.75 | 0.50 |
| 8:H:41:ILE:HG13 | 8:H:76:VAL:HG22 | 1.93 | 0.50 |
| 8:H:200:LYS:HE3 | 9:I:140:SER:O | 2.12 | 0.50 |
| 8:V:20:SER:HB3 | 8:V:28:ASP:HB3 | 1.93 | 0.50 |
| 10:X:14:LEU:HD12 | 10:X:42:LEU:HD23 | 1.94 | 0.50 |
| 12:Z:99:THR:HG23 | 12:Z:113:PHE:HB2 | 1.92 | 0.50 |
| 8:H:20:SER:HB3 | 8:H:28:ASP:HB3 | 1.94 | 0.50 |
| 13:M:179:ASP:HB3 | 13:M:18(A):THR:OG1 | 2.11 | 0.50 |
| 1:A:85:TYR:O | 1:A:89:VAL:HG23 | 2.11 | 0.50 |
| 5:E:75:GLY:HA3 | 5:E:221:PHE:CZ | 2.47 | 0.50 |
| 8:H:172:ASN:HD22 | 8:H:193:THR:HA | 1.76 | 0.50 |
| 6:T:69:VAL:HG12 | 16:T:264:HOH:O | 2.12 | 0.50 |
| 7:U:177:GLU:O | 7:U:17(B):LYS:HG3 | 2.12 | 0.50 |
| 8:V:34:LEU:HB2 | 16:V:1019:HOH:O | 2.10 | 0.50 |
| 6:F:170:GLN:HB2 | 16:F:265:HOH:O | 2.12 | 0.50 |
| 1:O:6:ASP:OD2 | 1:O:8:TYR:HB2 | 2.12 | 0.50 |
| 1:O:197:LEU:CD2 | 1:O:210:ILE:HD12 | 2.42 | 0.50 |
| 6:T:36:THR:HG22 | 6:T:51:GLU:OE2 | 2.11 | 0.50 |
| 11:K:32:LYS:HD2 | 11:K:32:LYS:N | 2.27 | 0.50 |
| 14:2:66:TYR:CD2 | 14:2:74:PRO:HB3 | 2.47 | 0.50 |
| 2:B:185:LYS:HD2 | 2:B:187:ASP:H | 1.77 | 0.49 |
| 6:F:38:ILE:HG22 | 6:F:164:ALA:CB | 2.42 | 0.49 |
| 7:U:77:VAL:HG12 | 7:U:137:THR:HB | 1.93 | 0.49 |
| 5:E:17:PRO:HA | 6:F:26:TYR:CD2 | 2.47 | 0.49 |
| 7:G:49:ILE:HD13 | 7:G:193:ALA:HB1 | 1.92 | 0.49 |
| 12:Z:137:PHE:CE1 | 12:Z:141:GLN:HG3 | 2.47 | 0.49 |
| 13:1:152:GLU:O | 13:1:156:VAL:HG23 | 2.11 | 0.49 |
| 7:G:72:ARG:HH11 | 7:G:72:ARG:CB | 2.24 | 0.49 |
| 9:I:97:VAL:HG23 | 9:I:99:PRO:HD3 | 1.94 | 0.49 |
| 13:M:17:ASP:HA | 13:M:173:PHE:CB | 2.43 | 0.49 |
| 5:S:39:GLY:O | 5:S:162:GLY:HA2 | 2.11 | 0.49 |
| 7:U:192:PHE:CD1 | 7:U:192:PHE:C | 2.84 | 0.49 |
| 2:B:38:ILE:HD13 | 2:B:164:SER:HB3 | 1.94 | 0.49 |
| 10:J:6:ILE:CG2 | 10:J:13:ILE:HB | 2.42 | 0.49 |
| 1:O:4:MET:SD | 1:O:5:THR:N | 2.70 | 0.49 |
| 3:Q:57:LYS:NZ | 16:Q:250:HOH:O | 2.46 | 0.49 |
| 5:S:54:ASN:ND2 | 5:S:56:ASP:O | 2.43 | 0.49 |
| 5:S:221:PHE:CE1 | 5:S:223:ILE:HD11 | 2.47 | 0.49 |
| 1:A:58:LEU:HD12 | 7:G:173:THR:HG23 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:17:PRO:HD2 | 16:D:271:HOH:O | 2.11 | 0.49 |
| 9:I:137:MET:HE3 | 9:I:141:LEU:HD11 | 1.95 | 0.49 |
| 10:J:168:MET:CE | 10:X:168:MET:CE | 2.90 | 0.49 |
| 2:P:4:GLY:HA3 | 5:S:127:TYR:CE1 | 2.47 | 0.49 |
| 3:Q:71:ASP:HA | 10:X:68:ILE:CD1 | 2.43 | 0.49 |
| 6:T:127:ASN:HD22 | 6:T:127:ASN:C | 2.14 | 0.49 |
| 10:X:16:SER:HB2 | 16:X:226:HOH:O | 2.13 | 0.49 |
| 10:X:18:LYS:HG2 | 10:X:174:ILE:HG13 | 1.94 | 0.49 |
| 2:B:190:ILE:HG23 | 2:B:212:PHE:CE2 | 2.48 | 0.49 |
| 2:B:235:LYS:C | 2:B:237:GLY:H | 2.15 | 0.49 |
| 5:E:104:ASN:HB2 | 13:M:81:GLU:HG2 | 1.93 | 0.49 |
| 10:J:3:ILE:HG22 | 10:J:100:LEU:CD1 | 2.42 | 0.49 |
| 10:J:133:TYR:OH | 10:X:24:ILE:HG12 | 2.12 | 0.49 |
| 4:R:68:VAL:HG21 | 4:R:89:ILE:HD12 | 1.94 | 0.49 |
| 7:U:203:THR:HG22 | 7:U:204:GLU:N | 2.27 | 0.49 |
| 2:B:101:LYS:NZ | 10:J:85:GLN:NE2 | 2.60 | 0.49 |
| 4:D:243:ALA:O | 4:D:244:GLU:CB | 2.60 | 0.49 |
| 5:E:231:LYS:H | 5:E:231:LYS:HD2 | 1.77 | 0.49 |
| 6:F:53:LEU:HD11 | 6:F:205:ASN:OD1 | 2.12 | 0.49 |
| 8:H:172:ASN:ND2 | 8:H:193:THR:HA | 2.28 | 0.49 |
| 12:L:166:HIS:CD2 | 12:L:168:GLN:H | 2.24 | 0.49 |
| 1:O:15:PHE:H | 2:P:23:GLN:NE2 | 1.93 | 0.49 |
| 2:P:185:LYS:HD2 | 2:P:187:ASP:H | 1.77 | 0.49 |
| 6:T:192:GLN:HE21 | 6:T:195:LYS:CE | 2.23 | 0.49 |
| 4:D:97:VAL:HG21 | 11:K:65:LEU:HD13 | 1.95 | 0.49 |
| 11:K:4:LEU:CD1 | 11:K:159:ILE:HD11 | 2.42 | 0.49 |
| 13:M:41:THR:OG1 | 13:M:76:PRO:HG3 | 2.13 | 0.49 |
| 1:O:17:PRO:HA | 2:P:26:TYR:CD1 | 2.48 | 0.49 |
| 2:P:51:GLU:OE2 | 2:P:209:ARG:NH2 | 2.46 | 0.49 |
| 5:S:231:LYS:H | 5:S:231:LYS:HD2 | 1.78 | 0.49 |
| 11:Y:32:LYS:HD2 | 11:Y:32:LYS:N | 2.28 | 0.49 |
| 3:C:227:GLU:H | 3:C:227:GLU:CD | 2.16 | 0.49 |
| 5:E:15:PHE:N | 6:F:23:GLN:HE22 | 2.04 | 0.49 |
| 10:J:144:PRO:CG | 11:Y:207:ASN:HD21 | 2.25 | 0.49 |
| 3:Q:201:VAL:HG11 | 3:Q:210:ILE:HG13 | 1.94 | 0.49 |
| 4:R:12(F):GLY:O | 4:R:12(G):GLU:HB2 | 2.12 | 0.49 |
| 6:T:175:GLU:OE1 | 6:T:199:LEU:HD23 | 2.13 | 0.49 |
| 8:V:179:GLU:OE2 | 8:V:182:LYS:HE2 | 2.11 | 0.49 |
| 8:H:81:GLN:O | 8:H:85:GLN:HG3 | 2.13 | 0.49 |
| 14:N:94:ASN:ND2 | 16:N:228:HOH:O | 2.39 | 0.49 |
| 4:R:15:PHE:HB2 | 5:S:23:GLN:OE1 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:243:ALA:O | 4:R:244:GLU:CB | 2.61 | 0.49 |
| 8:V:105:ASP:HB2 | 8:V:10(A):PRO:HD2 | 1.93 | 0.49 |
| 10:X:6:ILE:CG2 | 10:X:13:ILE:HB | 2.43 | 0.49 |
| 10:X:18:LYS:HD3 | 10:X:174:ILE:HG13 | 1.95 | 0.49 |
| 2:B:21(A):LYS:O | 2:B:21(B):GLY:C | 2.50 | 0.48 |
| 12:L:7:ALA:HB2 | 12:L:110:VAL:HG23 | 1.95 | 0.48 |
| 12:L:137:PHE:CE1 | 12:L:141:GLN:HG3 | 2.47 | 0.48 |
| 2:P:194:LEU:O | 2:P:198:SER:HB2 | 2.13 | 0.48 |
| 3:Q:175:PHE:O | 3:Q:179:ASN:HB2 | 2.13 | 0.48 |
| 7:U:170:GLN:NE2 | 7:U:174:THR:HG23 | 2.28 | 0.48 |
| 11:Y:4:LEU:CD1 | 11:Y:159:ILE:HD11 | 2.43 | 0.48 |
| 3:C:201:VAL:HG11 | 3:C:210:ILE:HG13 | 1.95 | 0.48 |
| 11:K:131:GLN:HG3 | 11:K:132:THR:N | 2.28 | 0.48 |
| 14:N:59:VAL:HG22 | 14:N:82:VAL:HG12 | 1.95 | 0.48 |
| 7:U:72:ARG:HH11 | 7:U:72:ARG:CB | 2.24 | 0.48 |
| 9:W:33:LYS:O | 9:W:44:GLY:HA2 | 2.14 | 0.48 |
| 11:Y:131:GLN:HG3 | 11:Y:132:THR:N | 2.28 | 0.48 |
| 14:N:171:GLY:HA2 | 13:1:197:TRP:CH2 | 2.48 | 0.48 |
| 4:R:175:GLU:OE1 | 4:R:175:GLU:HA | 2.13 | 0.48 |
| 5:S:58:LEU:HD12 | 5:S:58:LEU:N | 2.28 | 0.48 |
| 7:U:49:ILE:HD13 | 7:U:193:ALA:HB1 | 1.94 | 0.48 |
| 7:U:77:VAL:CG1 | 7:U:137:THR:HB | 2.42 | 0.48 |
| 4:D:68:VAL:HG21 | 4:D:89:ILE:HD12 | 1.95 | 0.48 |
| 6:F:199:LEU:HD12 | 6:F:240:ILE:HD13 | 1.95 | 0.48 |
| 2:P:27:ALA:O | 2:P:30:SER:HB3 | 2.13 | 0.48 |
| 2:P:234:VAL:HA | 2:P:239:THR:HA | 1.94 | 0.48 |
| 2:B:186:VAL:O | 2:B:190:ILE:HG13 | 2.14 | 0.48 |
| 5:E:38:VAL:HG12 | 5:E:39:GLY:N | 2.29 | 0.48 |
| 7:G:8:TYR:C | 7:G:10:ARG:N | 2.67 | 0.48 |
| 1:O:85:TYR:O | 1:O:89:VAL:HG23 | 2.13 | 0.48 |
| 2:P:186:VAL:O | 2:P:190:ILE:HG13 | 2.13 | 0.48 |
| 4:R:32:LYS:O | 4:R:167:SER:HA | 2.13 | 0.48 |
| 5:E:185:ASN:C | 5:E:185:ASN:HD22 | 2.16 | 0.48 |
| 7:G:203:THR:HG22 | 7:G:204:GLU:N | 2.27 | 0.48 |
| 12:L:98:HIS:HD2 | 16:L:200:HOH:O | 1.95 | 0.48 |
| 5:S:107:LEU:HD11 | 5:S:111:ARG:HG2 | 1.94 | 0.48 |
| 6:T:158:TRP:CZ3 | 7:U:64:VAL:HA | 2.49 | 0.48 |
| 13:1:104:VAL:HG23 | 13:1:178:ILE:CG2 | 2.41 | 0.48 |
| 3:Q:15:PHE:N | 4:R:23:GLN:HE22 | 1.95 | 0.48 |
| 1:A:6:ASP:OD2 | 1:A:8:TYR:HB2 | 2.14 | 0.48 |
| 2:B:15:PHE:N | 3:C:23:GLN:HE22 | 1.99 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:216:LYS:HB2 | 3:C:220:ASP:HB3 | 1.96 | 0.48 |
| 5:E:221:PHE:CE1 | 5:E:223:ILE:HD11 | 2.49 | 0.48 |
| 12:L:48:PHE:CZ | 12:L:50:ALA:HB3 | 2.49 | 0.48 |
| 2:P:190:ILE:HG23 | 2:P:212:PHE:CE2 | 2.48 | 0.48 |
| 13:1:184:LEU:C | 13:1:184:LEU:HD23 | 2.34 | 0.48 |
| 13:1:205:GLY:HA3 | 13:1:209:GLN:HB3 | 1.96 | 0.48 |
| 6:F:192:GLN:HE21 | 6:F:195:LYS:CE | 2.26 | 0.48 |
| 14:N:112:THR:CG2 | 14:N:120:HIS:HB2 | 2.42 | 0.48 |
| 2:P:6:ARG:HD3 | 4:R:9:ASP:HB3 | 1.94 | 0.48 |
| 2:P:73:LYS:C | 2:P:74:ILE:HD12 | 2.35 | 0.48 |
| 2:P:224:PHE:HD2 | 2:P:224:PHE:H | 1.62 | 0.48 |
| 3:Q:40:VAL:HG12 | 3:Q:162:ALA:CB | 2.43 | 0.48 |
| 4:R:160:TYR:CZ | 4:R:163:LYS:HD3 | 2.49 | 0.48 |
| 5:S:86:ARG:HG3 | 5:S:86:ARG:HH11 | 1.78 | 0.48 |
| 12:L:153:LYS:HG2 | 8:V:201:GLN:HG3 | 1.95 | 0.48 |
| 3:Q:168:ASN:O | 3:Q:172:VAL:HG12 | 2.14 | 0.48 |
| 3:Q:216:LYS:HB2 | 3:Q:220:ASP:HB3 | 1.96 | 0.48 |
| 6:T:56:SER:OG | 6:T:57:LYS:N | 2.45 | 0.48 |
| 2:B:51:GLU:OE2 | 2:B:209:ARG:NH2 | 2.47 | 0.47 |
| 3:C:15:PHE:N | 4:D:23:GLN:HE22 | 2.00 | 0.47 |
| 6:F:238:LYS:HZ2 | 6:F:239:GLU:HG3 | 1.79 | 0.47 |
| 13:M:14(A):VAL:HG23 | 13:M:14(A):VAL:O | 2.13 | 0.47 |
| 1:O:118:LYS:HE2 | 1:O:122:GLU:OE1 | 2.13 | 0.47 |
| 3:Q:97:GLN:HA | 3:Q:97:GLN:NE2 | 2.29 | 0.47 |
| 5:S:15:PHE:N | 6:T:23:GLN:HE22 | 2.02 | 0.47 |
| 9:W:97:VAL:HG23 | 9:W:99:PRO:HD3 | 1.96 | 0.47 |
| 2:B:191:GLU:O | 2:B:195:LYS:HG2 | 2.14 | 0.47 |
| 4:D:122:ARG:HH11 | 4:D:122:ARG:HG2 | 1.79 | 0.47 |
| 5:E:82:ALA:HB3 | 5:E:83:PRO:HD3 | 1.96 | 0.47 |
| 6:F:36:THR:CG2 | 6:F:51:GLU:OE2 | 2.63 | 0.47 |
| 7:G:170:GLN:NE2 | 7:G:174:THR:HG23 | 2.28 | 0.47 |
| 3:Q:149:TYR:CE1 | 3:Q:159:SER:HB3 | 2.49 | 0.47 |
| 12:Z:99:THR:CG2 | 16:Z:200:HOH:O | 2.62 | 0.47 |
| 2:B:4:GLY:HA3 | 5:E:127:TYR:CE1 | 2.48 | 0.47 |
| 5:E:142:ASP:HB2 | 16:M:258:HOH:O | 2.13 | 0.47 |
| 7:G:158:VAL:HG22 | 7:G:159:GLY:H | 1.79 | 0.47 |
| 2:P:21:LEU:O | 2:P:25:GLU:HG2 | 2.14 | 0.47 |
| 5:S:70:CYS:SG | 5:S:92:LEU:HD23 | 2.54 | 0.47 |
| 8:V:41:ILE:HG13 | 8:V:76:VAL:HG22 | 1.96 | 0.47 |
| 4:D:12(F):GLY:O | 4:D:12(G):GLU:HB2 | 2.14 | 0.47 |
| 6:F:56:SER:OG | 6:F:57:LYS:N | 2.46 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:173:VAL:HB | 8:H:192:LEU:HB2 | 1.96 | 0.47 |
| 4:R:215:ILE:HD13 | 4:R:215:ILE:C | 2.34 | 0.47 |
| 7:U:17:PRO:HD3 | 16:U:263:HOH:O | 2.14 | 0.47 |
| 7:U:78:VAL:HG11 | 7:U:85:ALA:CB | 2.44 | 0.47 |
| 7:U:158:VAL:HG22 | 7:U:159:GLY:H | 1.79 | 0.47 |
| 3:C:225:SER:OG | 3:C:228:GLU:HG3 | 2.14 | 0.47 |
| 5:E:194:VAL:HG13 | 5:E:207:LEU:CD1 | 2.44 | 0.47 |
| 14:N:20:THR:OG1 | 14:N:28:ASN:HB3 | 2.14 | 0.47 |
| 4:R:159:ARG:O | 5:S:60:SER:N | 2.47 | 0.47 |
| 13:1:157:ASN:HB3 | 16:1:249:HOH:O | 2.14 | 0.47 |
| 3:C:163:GLN:HE22 | 3:C:173:ARG:NE | 2.10 | 0.47 |
| 4:D:45:GLY:HA2 | 4:D:146:TYR:CD1 | 2.50 | 0.47 |
| 8:H:152:ILE:O | 8:H:156:SER:HB2 | 2.15 | 0.47 |
| 9:I:33:LYS:O | 9:I:44:GLY:HA2 | 2.15 | 0.47 |
| 12:L:21:ILE:HD11 | 12:L:168:GLN:NE2 | 2.29 | 0.47 |
| 13:M:152:GLU:O | 13:M:156:VAL:HG23 | 2.14 | 0.47 |
| 3:Q:39:GLY:HA2 | 3:Q:47:VAL:O | 2.14 | 0.47 |
| 3:Q:112:LEU:O | 3:Q:112:LEU:HD13 | 2.14 | 0.47 |
| 4:R:65:GLU:HA | 16:R:750:HOH:O | 2.14 | 0.47 |
| 5:S:15:PHE:HB2 | 6:T:23:GLN:HE22 | 1.79 | 0.47 |
| 5:S:38:VAL:HG12 | 5:S:39:GLY:N | 2.29 | 0.47 |
| 10:X:7:ARG:HG2 | 10:X:7:ARG:NH1 | 2.30 | 0.47 |
| 13:1:104:VAL:CG2 | 13:1:178:ILE:HG22 | 2.41 | 0.47 |
| 2:B:141:TYR:CD1 | 2:B:141:TYR:C | 2.88 | 0.47 |
| 4:D:67:ILE:HG22 | 4:D:221:PHE:HZ | 1.80 | 0.47 |
| 4:D:175:GLU:OE1 | 4:D:175:GLU:HA | 2.14 | 0.47 |
| 8:H:156:SER:HB3 | 16:H:1030:HOH:O | 2.14 | 0.47 |
| 9:I:113:PHE:N | 9:I:113:PHE:CD2 | 2.82 | 0.47 |
| 10:J:18:LYS:CG | 10:J:174:ILE:HG13 | 2.44 | 0.47 |
| 11:K:208:ASN:HB3 | 16:K:236:HOH:O | 2.15 | 0.47 |
| 12:L:114:ASP:CB | 12:L:118:SER:HB3 | 2.39 | 0.47 |
| 5:S:194:VAL:HG13 | 5:S:207:LEU:CD1 | 2.45 | 0.47 |
| 6:T:238:LYS:HZ2 | 6:T:239:GLU:HG3 | 1.80 | 0.47 |
| 7:U:87:ASN:C | 7:U:87:ASN:ND2 | 2.67 | 0.47 |
| 7:U:151:THR:HG22 | 7:U:157:TYR:CB | 2.42 | 0.47 |
| 14:2:20:THR:OG1 | 14:2:28:ASN:HB3 | 2.13 | 0.47 |
| 7:G:39:ALA:CB | 7:G:48:VAL:HG12 | 2.43 | 0.47 |
| 10:J:168:MET:HE2 | 10:X:168:MET:HE2 | 1.97 | 0.47 |
| 1:O:207:ASN:HB2 | 16:O:261:HOH:O | 2.15 | 0.47 |
| 3:Q:55:THR:O | 3:Q:56:LEU:HD22 | 2.15 | 0.47 |
| 5:S:77:SER:OG | 5:S:137:LEU:HB2 | 2.15 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:S:227:GLU:CD | 5:S:227:GLU:H | 2.18 | 0.47 |
| 7:U:8:TYR:C | 7:U:10:ARG:N | 2.67 | 0.47 |
| 10:X:18:LYS:CG | 10:X:174:ILE:HG13 | 2.45 | 0.47 |
| 6:F:198:TYR:HE2 | 6:F:237:GLN:HE21 | 1.63 | 0.47 |
| 10:J:64:GLN:NE2 | 16:J:215:HOH:O | 2.39 | 0.47 |
| 13:M:184:LEU:HD23 | 13:M:184:LEU:C | 2.36 | 0.47 |
| 2:P:101:LYS:NZ | 10:X:85:GLN:HE22 | 2.06 | 0.47 |
| 2:P:186:VAL:HG21 | 2:P:216:ARG:HD3 | 1.97 | 0.47 |
| 3:Q:227:GLU:OE1 | 3:Q:227:GLU:N | 2.44 | 0.47 |
| 6:T:199:LEU:HD12 | 6:T:240:ILE:HD13 | 1.96 | 0.47 |
| 8:V:22:GLN:HE22 | 15:V:1001:BIQ:H32 | 1.80 | 0.47 |
| 13:1:175:LEU:HD23 | 13:1:176:ALA:N | 2.30 | 0.47 |
| 1:A:118:LYS:HE2 | 1:A:122:GLU:OE1 | 2.15 | 0.47 |
| 10:J:6:ILE:HG22 | 10:J:13:ILE:HB | 1.97 | 0.47 |
| 14:N:29:ARG:HG2 | 16:N:223:HOH:O | 2.15 | 0.47 |
| 5:S:185:ASN:C | 5:S:185:ASN:HD22 | 2.18 | 0.47 |
| 9:W:113:PHE:HA | 9:W:118:CYS:O | 2.15 | 0.47 |
| 3:C:55:THR:O | 3:C:56:LEU:HD22 | 2.15 | 0.46 |
| 2:P:146:TYR:OH | 2:P:21(A):LYS:HB2 | 2.14 | 0.46 |
| 12:Z:-6:PRO:O | 13:1:91:ARG:NH1 | 2.41 | 0.46 |
| 7:G:74:ILE:HD12 | 7:G:109:CYS:HA | 1.97 | 0.46 |
| 10:J:14:LEU:HD12 | 10:J:42:LEU:HD23 | 1.96 | 0.46 |
| 10:J:24:ILE:HG12 | 10:X:133:TYR:OH | 2.16 | 0.46 |
| 12:L:109:ALA:HB2 | 12:L:121:ARG:NH2 | 2.30 | 0.46 |
| 14:N:36:ARG:HG3 | 14:N:42:TRP:CZ2 | 2.51 | 0.46 |
| 2:P:191:GLU:O | 2:P:195:LYS:HG2 | 2.16 | 0.46 |
| 3:Q:206:GLY:CA | 3:Q:209:ASN:HB2 | 2.37 | 0.46 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:HE3 | 2.28 | 0.46 |
| 12:Z:-7:ASN:HD22 | 12:Z:-7:ASN:C | 2.18 | 0.46 |
| 13:1:113:VAL:HA | 13:1:118:VAL:O | 2.15 | 0.46 |
| 13:1:14(C):ARG:HH11 | 13:1:14(C):ARG:CG | 2.28 | 0.46 |
| 14:2:36:ARG:HG3 | 14:2:42:TRP:CZ2 | 2.50 | 0.46 |
| 3:C:35:THR:HB | 3:C:51:GLU:HG3 | 1.97 | 0.46 |
| 3:C:40:VAL:HG12 | 3:C:162:ALA:CB | 2.43 | 0.46 |
| 5:E:2(C):VAL:HG13 | 5:E:2(D):ASP:N | 2.30 | 0.46 |
| 6:F:175:GLU:OE1 | 6:F:199:LEU:HD23 | 2.16 | 0.46 |
| 7:G:151:THR:HG22 | 7:G:157:TYR:CB | 2.44 | 0.46 |
| 3:Q:227:GLU:H | 3:Q:227:GLU:CD | 2.18 | 0.46 |
| 5:S:82:ALA:HB3 | 5:S:83:PRO:HD3 | 1.97 | 0.46 |
| 5:S:2(C):VAL:HG13 | 5:S:2(D):ASP:N | 2.30 | 0.46 |
| 6:T:192:GLN:NE2 | 6:T:195:LYS:CE | 2.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 7:U:39:ALA:CB | 7:U:48:VAL:HG12 | 2.44 | 0.46 |
| 9:W:159:LEU:CD2 | 9:W:173:ALA:HB1 | 2.46 | 0.46 |
| 16:X:220:HOH:O | 11:Y:132:THR:HG22 | 2.16 | 0.46 |
| 12:Z:21:ILE:HD11 | 12:Z:168:GLN:NE2 | 2.31 | 0.46 |
| 3:C:39:GLY:HA2 | 3:C:47:VAL:O | 2.15 | 0.46 |
| 4:D:32:LYS:O | 4:D:167:SER:HA | 2.15 | 0.46 |
| 6:F:195:LYS:O | 6:F:199:LEU:HD13 | 2.16 | 0.46 |
| 8:H:175:VAL:HG12 | 8:H:176:CYS:N | 2.31 | 0.46 |
| 9:I:29:ASN:HD22 | 9:I:29:ASN:N | 2.11 | 0.46 |
| 10:J:18:LYS:HD3 | 10:J:174:ILE:HG13 | 1.98 | 0.46 |
| 5:S:194:VAL:HG13 | 5:S:207:LEU:HD11 | 1.98 | 0.46 |
| 1:A:4:MET:HG2 | 6:F:126:TYR:CE2 | 2.51 | 0.46 |
| 5:E:194:VAL:CG1 | 5:E:207:LEU:HD11 | 2.45 | 0.46 |
| 9:I:122:ALA:HB3 | 9:I:125:ILE:CD1 | 2.46 | 0.46 |
| 12:L:34:VAL:HB | 16:L:232:HOH:O | 2.15 | 0.46 |
| 2:P:235:LYS:N | 2:P:235:LYS:HD3 | 2.31 | 0.46 |
| 3:Q:100:ARG:NH1 | 3:Q:106:PRO:HB3 | 2.30 | 0.46 |
| 6:T:36:THR:CG2 | 6:T:51:GLU:OE2 | 2.64 | 0.46 |
| 12:Z:166:HIS:CD2 | 12:Z:168:GLN:H | 2.27 | 0.46 |
| 14:2:3:ILE:HG22 | 14:2:16:ALA:CB | 2.46 | 0.46 |
| 4:D:160:TYR:CZ | 4:D:163:LYS:HD3 | 2.51 | 0.46 |
| 5:E:4:PHE:CG | 5:E:5:ARG:N | 2.83 | 0.46 |
| 5:E:70:CYS:SG | 5:E:92:LEU:HD23 | 2.56 | 0.46 |
| 6:F:127:ASN:C | 6:F:127:ASN:ND2 | 2.68 | 0.46 |
| 3:Q:197:LEU:O | 3:Q:201:VAL:HG23 | 2.15 | 0.46 |
| 5:S:179:THR:O | 5:S:179:THR:HG22 | 2.14 | 0.46 |
| 10:X:35:ARG:HA | 10:X:35:ARG:HD3 | 1.72 | 0.46 |
| 13:1:17:ASP:HA | 13:1:173:PHE:CB | 2.45 | 0.46 |
| 13:1:14(A):VAL:HG23 | 13:1:14(A):VAL:O | 2.15 | 0.46 |
| 5:E:2(C):VAL:O | 5:E:226:GLY:HA2 | 2.16 | 0.46 |
| 13:M:205:GLY:HA3 | 13:M:209:GLN:HB3 | 1.97 | 0.46 |
| 9:W:44:GLY:O | 9:W:45:ILE:HD13 | 2.15 | 0.46 |
| 1:A:97:HIS:CD2 | 8:H:61:SER:OG | 2.67 | 0.46 |
| 2:B:27:ALA:O | 2:B:30:SER:HB3 | 2.15 | 0.46 |
| 2:B:186:VAL:HG21 | 2:B:216:ARG:HD3 | 1.98 | 0.46 |
| 5:E:39:GLY:O | 5:E:162:GLY:HA2 | 2.16 | 0.46 |
| 8:H:113:ILE:HG12 | 8:H:119:THR:HG22 | 1.98 | 0.46 |
| 13:M:129:PHE:HE2 | 14:2:24:ALA:HB3 | 1.79 | 0.46 |
| 2:P:181:LYS:HE2 | 2:P:183:ASP:OD1 | 2.15 | 0.46 |
| 5:S:136:LEU:HD12 | 5:S:151:PHE:CD2 | 2.51 | 0.46 |
| 8:V:173:VAL:HB | 8:V:192:LEU:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:W:122:ALA:HB3 | 9:W:125:ILE:CD1 | 2.46 | 0.46 |
| 10:X:6:ILE:HG22 | 10:X:13:ILE:HB | 1.97 | 0.46 |
| 8:H:29:LYS:HE2 | 12:Z:165:ARG:CZ | 2.46 | 0.46 |
| 10:J:48:GLU:OE1 | 10:J:48:GLU:HA | 2.16 | 0.46 |
| 13:M:104:VAL:CG2 | 13:M:178:ILE:HG22 | 2.43 | 0.46 |
| 3:Q:225:SER:OG | 3:Q:228:GLU:HG3 | 2.15 | 0.46 |
| 5:S:194:VAL:CG1 | 5:S:207:LEU:HD11 | 2.46 | 0.46 |
| 9:W:101:VAL:O | 9:W:110:ILE:HA | 2.16 | 0.46 |
| 11:Y:46:ALA:HB3 | 11:Y:98:GLY:O | 2.15 | 0.46 |
| 13:1:83:LEU:O | 13:1:87:MET:HG2 | 2.15 | 0.46 |
| 1:A:207:ASN:HA | 1:A:233:LEU:CD1 | 2.45 | 0.46 |
| 2:B:161:LYS:HG3 | 3:C:59:GLN:O | 2.15 | 0.46 |
| 2:B:181:LYS:HE2 | 2:B:183:ASP:OD1 | 2.15 | 0.46 |
| 3:C:112:LEU:HD13 | 3:C:112:LEU:O | 2.15 | 0.46 |
| 2:P:141:TYR:CD1 | 2:P:141:TYR:C | 2.89 | 0.46 |
| 3:Q:31:VAL:HG11 | 3:Q:135:SER:HB2 | 1.98 | 0.46 |
| 4:R:59:LEU:C | 4:R:59:LEU:HD13 | 2.37 | 0.46 |
| 10:X:166:MET:CE | 10:X:168:MET:HB2 | 2.46 | 0.46 |
| 11:Y:5:ALA:HA | 11:Y:13:ILE:O | 2.16 | 0.46 |
| 2:B:52:ARG:HH22 | 2:B:63(A):SER:HB3 | 1.80 | 0.45 |
| 5:E:214:ILE:HG13 | 5:E:215:VAL:H | 1.79 | 0.45 |
| 6:F:28:VAL:O | 6:F:32:GLU:HG3 | 2.17 | 0.45 |
| 14:N:104:TYR:OH | 14:N:180:ALA:HB2 | 2.16 | 0.45 |
| 2:P:52:ARG:HH22 | 2:P:63(A):SER:HB3 | 1.81 | 0.45 |
| 5:S:15:PHE:HB2 | 6:T:23:GLN:NE2 | 2.31 | 0.45 |
| 6:T:31:VAL:HG22 | 6:T:134:VAL:HA | 1.98 | 0.45 |
| 7:U:191:GLU:HG3 | 7:U:232:ARG:HG3 | 1.98 | 0.45 |
| 1:A:33:GLN:HE21 | 1:A:33:GLN:CA | 2.26 | 0.45 |
| 5:E:54:ASN:ND2 | 5:E:56:ASP:O | 2.42 | 0.45 |
| 5:E:227:GLU:CD | 5:E:227:GLU:H | 2.18 | 0.45 |
| 6:F:31:VAL:HG22 | 6:F:134:VAL:HA | 1.99 | 0.45 |
| 8:H:139:GLU:OE2 | 8:H:139:GLU:HA | 2.16 | 0.45 |
| 13:M:40:ASN:N | 13:M:40:ASN:ND2 | 2.64 | 0.45 |
| 14:N:85:GLU:O | 14:N:89:GLU:HB2 | 2.15 | 0.45 |
| 14:N:89:GLU:OE1 | 14:N:89:GLU:HA | 2.16 | 0.45 |
| 1:O:40:ILE:HD12 | 1:O:193:ALA:HB2 | 1.99 | 0.45 |
| 2:P:74:ILE:CD1 | 2:P:74:ILE:N | 2.78 | 0.45 |
| 4:R:86:ARG:HD3 | 4:R:86:ARG:HA | 1.69 | 0.45 |
| 4:R:122:ARG:HG2 | 4:R:122:ARG:HH11 | 1.81 | 0.45 |
| 6:T:40:ILE:HD12 | 6:T:193:ALA:HB2 | 1.99 | 0.45 |
| 12:Z:99:THR:HG22 | 16:Z:200:HOH:O | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:146:TYR:OH | 2:B:21(A):LYS:HB2 | 2.17 | 0.45 |
| 3:C:158:SER:HB2 | 4:D:59:LEU:HD21 | 1.98 | 0.45 |
| 10:J:144:PRO:CG | 11:Y:207:ASN:ND2 | 2.79 | 0.45 |
| 1:O:62:GLU:C | 1:O:64:LEU:H | 2.19 | 0.45 |
| 1:O:161:LYS:HD2 | 2:P:58:LEU:HA | 1.98 | 0.45 |
| 3:Q:62(A):ILE:HG13 | 3:Q:63:THR:N | 2.31 | 0.45 |
| 4:R:67:ILE:HG22 | 4:R:221:PHE:HZ | 1.80 | 0.45 |
| 8:V:18:THR:HB | 8:V:30:ASN:HD22 | 1.81 | 0.45 |
| 8:H:18:THR:HB | 8:H:30:ASN:HD22 | 1.81 | 0.45 |
| 10:J:168:MET:CE | 10:X:168:MET:HG2 | 2.46 | 0.45 |
| 12:L:90:LYS:HD3 | 12:L:95:TYR:CZ | 2.52 | 0.45 |
| 1:O:207:ASN:HA | 1:O:233:LEU:CD1 | 2.46 | 0.45 |
| 3:Q:35:THR:HB | 3:Q:51:GLU:HG3 | 1.98 | 0.45 |
| 4:R:21:LEU:HD21 | 5:S:130:ARG:HD2 | 1.99 | 0.45 |
| 5:S:214:ILE:HG13 | 5:S:215:VAL:H | 1.80 | 0.45 |
| 10:X:44:SER:HG | 10:X:100:LEU:HB2 | 1.81 | 0.45 |
| 10:X:90(B):ARG:NH1 | 16:X:204:HOH:O | 2.41 | 0.45 |
| 14:2:89:GLU:HA | 14:2:89:GLU:OE1 | 2.15 | 0.45 |
| 1:A:177:GLU:HG2 | 2:B:58:LEU:HD21 | 1.96 | 0.45 |
| 5:E:194:VAL:HG13 | 5:E:207:LEU:HD11 | 1.98 | 0.45 |
| 6:F:103:TYR:O | 6:F:104:LYS:HB3 | 2.17 | 0.45 |
| 8:H:8:PHE:HB3 | 8:H:151:ALA:HB2 | 1.99 | 0.45 |
| 10:J:166:MET:CE | 10:J:168:MET:HB2 | 2.46 | 0.45 |
| 1:O:198:LYS:HE3 | 1:O:236:LEU:HD11 | 1.98 | 0.45 |
| 14:2:85:GLU:O | 14:2:89:GLU:HB2 | 2.16 | 0.45 |
| 3:C:97:GLN:HA | 3:C:97:GLN:NE2 | 2.32 | 0.45 |
| 4:D:59:LEU:HD13 | 4:D:59:LEU:C | 2.36 | 0.45 |
| 9:I:159:LEU:CD2 | 9:I:173:ALA:HB1 | 2.47 | 0.45 |
| 3:Q:46:VAL:HG22 | 3:Q:146:PRO:HB2 | 1.99 | 0.45 |
| 5:S:134:VAL:O | 5:S:153:PRO:HG3 | 2.16 | 0.45 |
| 6:T:70:VAL:HG11 | 6:T:112:PHE:CE1 | 2.51 | 0.45 |
| 6:T:103:TYR:O | 6:T:104:LYS:HB3 | 2.17 | 0.45 |
| 8:V:139:GLU:HA | 8:V:139:GLU:OE2 | 2.17 | 0.45 |
| 15:V:1001:BIQ:H122 | 9:W:114:ASP:OD1 | 2.17 | 0.45 |
| 14:2:3:ILE:HG22 | 14:2:16:ALA:HB2 | 1.97 | 0.45 |
| 14:2:15:GLY:HA2 | 14:2:174:ARG:O | 2.17 | 0.45 |
| 5:E:136:LEU:HD12 | 5:E:151:PHE:CD2 | 2.52 | 0.45 |
| 5:E:179:THR:HG22 | 5:E:179:THR:O | 2.17 | 0.45 |
| 3:Q:55:THR:O | 3:Q:56:LEU:HD13 | 2.17 | 0.45 |
| 8:V:200:LYS:HE3 | 9:W:140:SER:O | 2.17 | 0.45 |
| 10:X:143:ARG:HG2 | 10:X:143:ARG:HH11 | 1.82 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 11:Y:4:LEU:C | 11:Y:4:LEU:HD22 | 2.37 | 0.45 |
| 1:A:169:SER:O | 1:A:173:LYS:HG3 | 2.16 | 0.45 |
| 3:C:168:ASN:O | 3:C:172:VAL:HG12 | 2.17 | 0.45 |
| 8:H:147:THR:HG23 | 8:H:150:GLU:OE1 | 2.17 | 0.45 |
| 8:H:201:GLN:HG3 | 12:Z:153:LYS:HG2 | 1.98 | 0.45 |
| 13:M:70:ASN:ND2 | 13:M:70(A):ALA:HA | 2.32 | 0.45 |
| 12:Z:-7:ASN:ND2 | 12:Z:-7:ASN:C | 2.70 | 0.45 |
| 1:A:198:LYS:HE3 | 1:A:236:LEU:HD11 | 1.98 | 0.45 |
| 2:B:224:PHE:HD2 | 2:B:224:PHE:H | 1.62 | 0.45 |
| 7:G:52:LYS:HA | 16:G:257:HOH:O | 2.16 | 0.45 |
| 7:G:78:VAL:HG11 | 7:G:85:ALA:CB | 2.47 | 0.45 |
| 10:J:123:PRO:HB2 | 10:J:124:TYR:CD1 | 2.52 | 0.45 |
| 11:K:75:SER:HB2 | 11:K:106:GLU:OE2 | 2.17 | 0.45 |
| 4:R:45:GLY:HA2 | 4:R:146:TYR:CD1 | 2.51 | 0.45 |
| 5:S:4:PHE:CG | 5:S:5:ARG:N | 2.84 | 0.45 |
| 13:1:1:THR:OG1 | 13:1:2:SER:N | 2.50 | 0.45 |
| 6:F:18:ASP:OD1 | 6:F:20:ARG:HD3 | 2.17 | 0.45 |
| 4:R:161:ASN:HB3 | 4:R:180:TRP:CE2 | 2.52 | 0.45 |
| 6:T:136:THR:O | 6:T:150:MET:HA | 2.17 | 0.45 |
| 6:T:176:LEU:HB3 | 7:U:58:LEU:HD21 | 1.99 | 0.45 |
| 7:U:188:LYS:HD3 | 7:U:188:LYS:HA | 1.82 | 0.45 |
| 12:Z:90:LYS:HD3 | 12:Z:95:TYR:CZ | 2.52 | 0.45 |
| 2:B:20:ARG:HG2 | 2:B:20:ARG:HH11 | 1.83 | 0.44 |
| 12:L:165:ARG:CZ | 8:V:29:LYS:HE2 | 2.47 | 0.44 |
| 13:M:14(C):ARG:HH11 | 13:M:14(C):ARG:CG | 2.29 | 0.44 |
| 1:O:26:TYR:CD1 | 7:U:17:PRO:HA | 2.52 | 0.44 |
| 3:Q:105:ASP:OD2 | 3:Q:106:PRO:HD2 | 2.17 | 0.44 |
| 6:T:175:GLU:CB | 6:T:196:ILE:HD12 | 2.47 | 0.44 |
| 1:A:62:GLU:C | 1:A:64:LEU:H | 2.20 | 0.44 |
| 1:A:62:GLU:CD | 1:A:62:GLU:H | 2.21 | 0.44 |
| 2:B:49:ALA:HB2 | 2:B:212:PHE:CE1 | 2.51 | 0.44 |
| 9:I:101:VAL:O | 9:I:110:ILE:HA | 2.17 | 0.44 |
| 13:M:113:VAL:HA | 13:M:118:VAL:O | 2.16 | 0.44 |
| 13:M:14(G):ILE:N | 13:M:144:PRO:HD2 | 2.33 | 0.44 |
| 14:N:18(G):TYR:HA | 14:N:18(J):LEU:HG | 1.99 | 0.44 |
| 1:O:159:PRO:HB2 | 2:P:60:GLU:HB3 | 1.99 | 0.44 |
| 3:Q:241:GLN:C | 3:Q:243:GLN:N | 2.70 | 0.44 |
| 4:R:112:LEU:HD13 | 4:R:112:LEU:C | 2.37 | 0.44 |
| 5:S:18(F):ILE:O | 5:S:18(F):ILE:HG22 | 2.17 | 0.44 |
| 10:X:10(B):LYS:HB2 | 10:X:10(B):LYS:NZ | 2.32 | 0.44 |
| 11:Y:20:ALA:HB2 | 11:Y:31:VAL:HG21 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:2:104:TYR:OH | 14:2:180:ALA:HB2 | 2.16 | 0.44 |
| 12:L:-7:ASN:HD22 | 12:L:-7:ASN:C | 2.21 | 0.44 |
| 14:N:67:THR:HA | 14:N:72:GLY:O | 2.17 | 0.44 |
| 2:P:209:ARG:HG2 | 2:P:209:ARG:HH11 | 1.83 | 0.44 |
| 8:V:8:PHE:HB3 | 8:V:151:ALA:HB2 | 1.99 | 0.44 |
| 9:W:19:ARG:HB2 | 9:W:171:TRP:HB2 | 2.00 | 0.44 |
| 13:1:140:LYS:HG3 | 16:1:219:HOH:O | 2.17 | 0.44 |
| 1:A:150:GLN:O | 1:A:157:TYR:HA | 2.17 | 0.44 |
| 3:C:195:ARG:HD3 | 16:C:270:HOH:O | 2.17 | 0.44 |
| 4:D:215:ILE:C | 4:D:215:ILE:HD13 | 2.37 | 0.44 |
| 6:F:176:LEU:O | 6:F:180:VAL:HG23 | 2.17 | 0.44 |
| 7:G:87:ASN:C | 7:G:87:ASN:ND2 | 2.71 | 0.44 |
| 10:J:10(B):LYS:HB2 | 10:J:10(B):LYS:NZ | 2.32 | 0.44 |
| 1:O:150:GLN:O | 1:O:157:TYR:HA | 2.17 | 0.44 |
| 2:P:122:GLY:C | 2:P:124:THR:H | 2.21 | 0.44 |
| 6:T:127:ASN:C | 6:T:127:ASN:ND2 | 2.70 | 0.44 |
| 12:Z:48:PHE:CZ | 12:Z:50:ALA:HB3 | 2.53 | 0.44 |
| 13:1:8:TYR:CZ | 13:1:148:VAL:HG13 | 2.52 | 0.44 |
| 1:A:40:ILE:HD12 | 1:A:193:ALA:HB2 | 1.99 | 0.44 |
| 6:F:40:ILE:HD12 | 6:F:193:ALA:HB2 | 2.00 | 0.44 |
| 1:O:232:ARG:HG3 | 1:O:232:ARG:NH1 | 2.33 | 0.44 |
| 4:R:160:TYR:CE2 | 4:R:163:LYS:HD3 | 2.53 | 0.44 |
| 6:T:18:ASP:OD1 | 6:T:20:ARG:HD3 | 2.16 | 0.44 |
| 7:U:49:ILE:N | 7:U:49:ILE:HD12 | 2.33 | 0.44 |
| 5:E:221:PHE:HE1 | 5:E:223:ILE:HD11 | 1.83 | 0.44 |
| 12:L:84:GLN:HG3 | 12:L:117:GLY:O | 2.18 | 0.44 |
| 2:P:38:ILE:HD13 | 2:P:164:SER:HB3 | 1.98 | 0.44 |
| 3:Q:45:CYS:HA | 3:Q:141:PHE:HZ | 1.82 | 0.44 |
| 4:R:81:LEU:HD12 | 4:R:133:GLY:HA3 | 2.00 | 0.44 |
| 5:S:41:ARG:NH1 | 5:S:42:SER:O | 2.51 | 0.44 |
| 13:1:133:MET:C | 13:1:136:PRO:HD2 | 2.38 | 0.44 |
| 1:A:141:HIS:HA | 1:A:146:GLY:O | 2.17 | 0.44 |
| 3:C:120:GLN:O | 3:C:124:THR:HG23 | 2.18 | 0.44 |
| 5:E:97:ASN:HD22 | 5:E:97:ASN:HA | 1.67 | 0.44 |
| 7:G:191:GLU:HG3 | 7:G:232:ARG:HG3 | 2.00 | 0.44 |
| 11:K:86:LEU:C | 11:K:86:LEU:HD13 | 2.38 | 0.44 |
| 11:K:10(A):ARG:HG2 | 11:K:10(A):ARG:NH1 | 2.32 | 0.44 |
| 2:P:229:ILE:O | 2:P:233:LEU:HB2 | 2.18 | 0.44 |
| 6:T:198:TYR:HE2 | 6:T:237:GLN:HE21 | 1.63 | 0.44 |
| 11:Y:172:SER:HA | 11:Y:192:VAL:HG23 | 2.00 | 0.44 |
| 3:C:57:LYS:CG | 3:C:208:LYS:HZ1 | 2.30 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:241:GLN:C | 3:C:243:GLN:N | 2.70 | 0.44 |
| 4:D:177:LEU:CD1 | 5:E:58:LEU:HD11 | 2.46 | 0.44 |
| 6:F:136:THR:O | 6:F:150:MET:HA | 2.18 | 0.44 |
| 6:F:203:GLU:HA | 6:F:203:GLU:OE1 | 2.17 | 0.44 |
| 1:O:27:ALA:O | 1:O:31:VAL:HG23 | 2.18 | 0.44 |
| 5:S:52:LYS:HD3 | 5:S:211:SER:HB2 | 2.00 | 0.44 |
| 6:T:63:LYS:O | 6:T:65:VAL:HG23 | 2.18 | 0.44 |
| 6:T:176:LEU:O | 6:T:180:VAL:HG23 | 2.17 | 0.44 |
| 8:V:152:ILE:O | 8:V:156:SER:HB2 | 2.18 | 0.44 |
| 10:X:185:ARG:HG2 | 10:X:185:ARG:HH11 | 1.82 | 0.44 |
| 5:E:18(F):ILE:HG22 | 5:E:18(F):ILE:O | 2.18 | 0.44 |
| 7:G:17(C):LYS:HB2 | 7:G:17(C):LYS:HE3 | 1.78 | 0.44 |
| 10:J:7:ARG:HG2 | 10:J:7:ARG:NH1 | 2.33 | 0.44 |
| 10:J:168:MET:HG2 | 10:X:168:MET:CE | 2.47 | 0.44 |
| 11:K:174:ASN:HD21 | 11:K:189:ASN:HB2 | 1.83 | 0.44 |
| 12:L:42:VAL:HG23 | 12:L:102:ALA:HB3 | 2.00 | 0.44 |
| 12:L:109:ALA:HA | 16:L:227:HOH:O | 2.18 | 0.44 |
| 13:M:8:TYR:CZ | 13:M:148:VAL:HG13 | 2.53 | 0.44 |
| 1:O:130:ARG:NH2 | 7:U:124:THR:HG22 | 2.22 | 0.44 |
| 2:P:136:PHE:O | 2:P:150:THR:HA | 2.18 | 0.44 |
| 7:U:78:VAL:HG11 | 7:U:85:ALA:HB2 | 2.00 | 0.44 |
| 7:U:204:GLU:HG3 | 16:U:283:HOH:O | 2.18 | 0.44 |
| 8:V:84:LYS:HE2 | 8:V:119:THR:HG23 | 2.00 | 0.44 |
| 10:X:123:PRO:HB2 | 10:X:124:TYR:CD1 | 2.53 | 0.44 |
| 11:Y:6:PHE:HA | 11:Y:123:ASP:O | 2.17 | 0.44 |
| 11:Y:174:ASN:HD21 | 11:Y:189:ASN:HB2 | 1.83 | 0.44 |
| 1:A:117:ALA:HB1 | 1:A:155:GLY:O | 2.18 | 0.43 |
| 4:D:177:LEU:HD22 | 5:E:58:LEU:CD1 | 2.47 | 0.43 |
| 11:K:5:ALA:HA | 11:K:13:ILE:O | 2.18 | 0.43 |
| 1:O:141:HIS:HA | 1:O:146:GLY:O | 2.18 | 0.43 |
| 13:1:70:ASN:ND2 | 13:1:70(A):ALA:HA | 2.32 | 0.43 |
| 2:B:161:LYS:HE3 | 3:C:59:GLN:O | 2.18 | 0.43 |
| 2:B:209:ARG:HG2 | 2:B:209:ARG:HH11 | 1.81 | 0.43 |
| 3:C:45:CYS:HA | 3:C:141:PHE:HZ | 1.82 | 0.43 |
| 5:E:134:VAL:O | 5:E:153:PRO:HG3 | 2.18 | 0.43 |
| 6:F:63:LYS:O | 6:F:65:VAL:HG23 | 2.18 | 0.43 |
| 7:G:49:ILE:HD12 | 7:G:49:ILE:N | 2.33 | 0.43 |
| 8:H:72:ARG:HG3 | 8:H:72:ARG:NH1 | 2.32 | 0.43 |
| 8:H:128:GLY:O | 8:H:131:SER:CB | 2.65 | 0.43 |
| 10:J:34:THR:HG21 | 10:J:176:LYS:NZ | 2.33 | 0.43 |
| 10:J:76:PRO:HD2 | 16:J:210:HOH:O | 2.16 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 13:M:11:GLY:HA3 | 13:M:178:ILE:O | 2.17 | 0.43 |
| 1:O:62:GLU:H | 1:O:62:GLU:CD | 2.21 | 0.43 |
| 4:R:159:ARG:HB3 | 5:S:60:SER:HB3 | 1.99 | 0.43 |
| 6:T:203:GLU:OE1 | 6:T:203:GLU:HA | 2.18 | 0.43 |
| 7:U:56:ASP:HB3 | 7:U:59:LEU:HG | 2.00 | 0.43 |
| 11:Y:10(A):ARG:HG2 | 11:Y:10(A):ARG:NH1 | 2.33 | 0.43 |
| 12:Z:42:VAL:HG23 | 12:Z:102:ALA:HB3 | 2.01 | 0.43 |
| 4:D:81:LEU:HD12 | 4:D:133:GLY:HA3 | 2.00 | 0.43 |
| 6:F:70:VAL:HG11 | 6:F:112:PHE:CE1 | 2.52 | 0.43 |
| 6:F:90:ASN:O | 6:F:94:GLU:HG3 | 2.17 | 0.43 |
| 6:F:180:VAL:HG21 | 7:G:58:LEU:HD23 | 1.99 | 0.43 |
| 8:H:112:SER:OG | 8:H:120:ASP:HB2 | 2.18 | 0.43 |
| 2:P:66:LYS:O | 2:P:77:ALA:HA | 2.18 | 0.43 |
| 9:W:113:PHE:CD2 | 9:W:113:PHE:N | 2.85 | 0.43 |
| 13:1:14(G):ILE:N | 13:1:144:PRO:HD2 | 2.32 | 0.43 |
| 14:2:18(G):TYR:HA | 14:2:18(J):LEU:HG | 2.00 | 0.43 |
| 3:C:62(A):ILE:HG13 | 3:C:63:THR:N | 2.32 | 0.43 |
| 5:E:58:LEU:N | 5:E:58:LEU:CD1 | 2.81 | 0.43 |
| 6:F:240:ILE:HD12 | 6:F:240:ILE:HA | 1.91 | 0.43 |
| 7:G:56:ASP:HB3 | 7:G:59:LEU:HG | 2.00 | 0.43 |
| 7:G:105:TYR:OH | 8:H:66:HIS:HE1 | 2.02 | 0.43 |
| 9:I:29:ASN:ND2 | 9:I:29:ASN:N | 2.65 | 0.43 |
| 10:J:185:ARG:HG2 | 10:J:185:ARG:HH11 | 1.84 | 0.43 |
| 11:K:172:SER:HA | 11:K:192:VAL:HG23 | 2.00 | 0.43 |
| 6:T:195:LYS:O | 6:T:199:LEU:HD13 | 2.19 | 0.43 |
| 9:W:143:GLU:HG3 | 9:W:146:LEU:HD21 | 2.01 | 0.43 |
| 13:1:40:ASN:N | 13:1:40:ASN:ND2 | 2.64 | 0.43 |
| 2:B:39:GLY:O | 2:B:162:ALA:HA | 2.18 | 0.43 |
| 5:E:77:SER:OG | 5:E:137:LEU:HB2 | 2.18 | 0.43 |
| 6:F:176:LEU:HB3 | 7:G:58:LEU:HD21 | 2.00 | 0.43 |
| 9:I:124:PHE:O | 9:I:125:ILE:HD12 | 2.19 | 0.43 |
| 11:K:4:LEU:HD22 | 11:K:4:LEU:C | 2.39 | 0.43 |
| 2:P:49:ALA:HB2 | 2:P:212:PHE:CE1 | 2.54 | 0.43 |
| 2:P:141:TYR:CE2 | 2:P:145:GLY:HA2 | 2.54 | 0.43 |
| 5:S:2(C):VAL:O | 5:S:226:GLY:HA2 | 2.18 | 0.43 |
| 7:U:171:GLU:OE1 | 7:U:171:GLU:N | 2.52 | 0.43 |
| 7:U:18(H):GLU:H | 7:U:18(H):GLU:CD | 2.22 | 0.43 |
| 13:1:137:LEU:O | 13:1:140:LYS:HB2 | 2.19 | 0.43 |
| 2:B:143:ASP:OD2 | 10:J:10(B):LYS:HE2 | 2.19 | 0.43 |
| 3:C:71:ASP:OD1 | 3:C:100:ARG:NH1 | 2.51 | 0.43 |
| 4:D:207:LEU:HD21 | 4:D:233:ILE:CD1 | 2.48 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:19:ARG:NE | 12:L:171:ASP:OD2 | 2.44 | 0.43 |
| 5:S:160:LEU:HD22 | 6:T:59:LEU:HD12 | 2.01 | 0.43 |
| 7:U:143:GLU:HA | 7:U:217:LYS:NZ | 2.34 | 0.43 |
| 13:1:11:GLY:HA3 | 13:1:178:ILE:O | 2.18 | 0.43 |
| 1:A:13:THR:O | 2:B:130:ARG:HD3 | 2.19 | 0.43 |
| 2:B:74:ILE:CD1 | 2:B:74:ILE:N | 2.81 | 0.43 |
| 5:E:41:ARG:NH1 | 5:E:42:SER:O | 2.51 | 0.43 |
| 5:E:18(C):PHE:HA | 5:E:18(F):ILE:CG1 | 2.47 | 0.43 |
| 6:F:175:GLU:CB | 6:F:196:ILE:HD12 | 2.49 | 0.43 |
| 9:I:29:ASN:HD22 | 9:I:30:LYS:HG3 | 1.84 | 0.43 |
| 9:I:113:PHE:HA | 9:I:118:CYS:O | 2.18 | 0.43 |
| 10:J:19:ALA:HB2 | 10:J:171:LYS:HG2 | 1.99 | 0.43 |
| 13:M:175:LEU:HD23 | 13:M:176:ALA:N | 2.33 | 0.43 |
| 14:N:3:ILE:HG22 | 14:N:16:ALA:CB | 2.48 | 0.43 |
| 14:N:126:ILE:HD13 | 14:N:126:ILE:N | 2.34 | 0.43 |
| 14:N:133:PHE:HA | 14:2:132:THR:O | 2.19 | 0.43 |
| 7:U:139:VAL:HA | 7:U:147:SER:O | 2.19 | 0.43 |
| 8:V:3:ILE:HD11 | 8:V:127:LEU:HB2 | 2.01 | 0.43 |
| 10:X:40:HIS:CD2 | 10:X:10(A):LYS:HD3 | 2.54 | 0.43 |
| 10:X:166:MET:HA | 10:X:167:PRO:HD3 | 1.81 | 0.43 |
| 12:Z:-7:ASN:HD22 | 12:Z:-6:PRO:N | 2.17 | 0.43 |
| 3:C:31:VAL:HG11 | 3:C:135:SER:HB2 | 2.00 | 0.43 |
| 3:C:100:ARG:NH1 | 3:C:106:PRO:HB3 | 2.34 | 0.43 |
| 4:D:160:TYR:CE2 | 4:D:163:LYS:HD3 | 2.54 | 0.43 |
| 4:D:161:ASN:HB3 | 4:D:180:TRP:CE2 | 2.53 | 0.43 |
| 8:H:189:ARG:O | 8:H:190:ASN:HB2 | 2.19 | 0.43 |
| 2:P:39:GLY:O | 2:P:162:ALA:HA | 2.19 | 0.43 |
| 5:S:4:PHE:O | 5:S:6:ASN:N | 2.52 | 0.43 |
| 7:U:46:THR:HG21 | 7:U:139:VAL:HB | 2.00 | 0.43 |
| 7:U:172:ILE:HD11 | 7:U:201:LEU:HD21 | 2.01 | 0.43 |
| 8:V:84:LYS:HG3 | 8:V:85:GLN:N | 2.34 | 0.43 |
| 8:V:113:ILE:HG12 | 8:V:119:THR:HG22 | 2.01 | 0.43 |
| 10:X:19:ALA:HB2 | 10:X:171:LYS:HG2 | 2.00 | 0.43 |
| 10:X:32:ASP:CG | 10:X:34:THR:HG22 | 2.39 | 0.43 |
| 12:Z:109:ALA:HB2 | 12:Z:121:ARG:NH2 | 2.34 | 0.43 |
| 12:Z:113:PHE:CD1 | 12:Z:113:PHE:N | 2.86 | 0.43 |
| 2:B:17:PRO:HA | 3:C:26:TYR:CZ | 2.53 | 0.43 |
| 5:E:2(B):THR:H | 5:E:2(E):ASN:HB3 | 1.84 | 0.43 |
| 7:G:82:ILE:CG2 | 7:G:83:PRO:HD3 | 2.48 | 0.43 |
| 7:G:152:ASP:HB2 | 7:G:153:PRO:HD2 | 2.01 | 0.43 |
| 7:G:172:ILE:HD11 | 7:G:201:LEU:HD21 | 1.99 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:I:66:TYR:CZ | 9:I:70:GLU:HG3 | 2.54 | 0.43 |
| 14:N:15:GLY:HA2 | 14:N:174:ARG:O | 2.18 | 0.43 |
| 1:O:35:VAL:HG11 | 1:O:51:GLU:HB3 | 2.01 | 0.43 |
| 5:E:179:THR:O | 5:E:18(B):THR:HB | 2.19 | 0.43 |
| 12:L:-7:ASN:HD22 | 12:L:-6:PRO:N | 2.17 | 0.43 |
| 12:L:113:PHE:N | 12:L:113:PHE:CD1 | 2.86 | 0.43 |
| 12:L:177:ILE:N | 12:L:177:ILE:HD12 | 2.34 | 0.43 |
| 13:M:133:MET:C | 13:M:136:PRO:HD2 | 2.39 | 0.43 |
| 3:Q:136:THR:O | 3:Q:150:GLN:HA | 2.19 | 0.43 |
| 4:R:207:LEU:HD21 | 4:R:233:ILE:CD1 | 2.49 | 0.43 |
| 5:S:97:ASN:ND2 | 12:Z:61:ASN:HD21 | 2.10 | 0.43 |
| 5:S:179:THR:O | 5:S:18(B):THR:HB | 2.18 | 0.43 |
| 7:U:152:ASP:HB2 | 7:U:153:PRO:HD2 | 2.00 | 0.43 |
| 7:U:18(D):ILE:HD12 | 7:U:18(D):ILE:N | 2.34 | 0.43 |
| 8:V:147:THR:HG23 | 8:V:150:GLU:OE1 | 2.19 | 0.43 |
| 9:W:183:GLU:HA | 16:W:229:HOH:O | 2.19 | 0.43 |
| 10:X:12:VAL:CG2 | 10:X:108:PRO:HB2 | 2.49 | 0.43 |
| 10:X:124:TYR:CD2 | 10:X:138:LEU:HD13 | 2.54 | 0.43 |
| 11:Y:25:TRP:CH2 | 12:Z:132:SER:HA | 2.54 | 0.43 |
| 2:B:20:ARG:HG2 | 2:B:20:ARG:NH1 | 2.34 | 0.42 |
| 2:B:71:ASN:HB3 | 2:B:74:ILE:H | 1.84 | 0.42 |
| 2:B:235:LYS:N | 2:B:235:LYS:HD3 | 2.33 | 0.42 |
| 5:E:11:ASP:OD1 | 5:E:13:VAL:HG12 | 2.20 | 0.42 |
| 15:H:1000:BIQ:H122 | 9:I:114:ASP:OD1 | 2.18 | 0.42 |
| 6:T:18:ASP:OD2 | 6:T:18:ASP:N | 2.44 | 0.42 |
| 7:U:82:ILE:N | 7:U:83:PRO:HD2 | 2.34 | 0.42 |
| 8:V:175:VAL:HG12 | 8:V:176:CYS:N | 2.33 | 0.42 |
| 10:X:52:THR:HG22 | 10:X:53:VAL:H | 1.84 | 0.42 |
| 1:A:110:LYS:HG2 | 16:A:246:HOH:O | 2.18 | 0.42 |
| 3:C:186:VAL:HG21 | 3:C:216:LYS:HE2 | 2.00 | 0.42 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:CE | 2.82 | 0.42 |
| 7:G:143:GLU:HA | 7:G:217:LYS:NZ | 2.34 | 0.42 |
| 13:M:175:LEU:HD23 | 13:M:175:LEU:C | 2.39 | 0.42 |
| 14:N:3:ILE:HG22 | 14:N:16:ALA:HB2 | 2.00 | 0.42 |
| 1:O:13:THR:O | 2:P:130:ARG:HD3 | 2.19 | 0.42 |
| 2:P:202:THR:HG22 | 2:P:203:ASP:N | 2.34 | 0.42 |
| 3:Q:55:THR:HG22 | 3:Q:56:LEU:CD2 | 2.44 | 0.42 |
| 14:2:116:GLY:HA3 | 16:2:190:HOH:O | 2.18 | 0.42 |
| 1:A:232:ARG:HG3 | 1:A:232:ARG:NH1 | 2.34 | 0.42 |
| 2:B:63:THR:HG22 | 2:B:63:THR:O | 2.19 | 0.42 |
| 2:B:194:LEU:O | 2:B:198:SER:HB2 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:65:SER:HB2 | 16:C:252:HOH:O | 2.19 | 0.42 |
| 10:J:12:VAL:CG2 | 10:J:108:PRO:HB2 | 2.50 | 0.42 |
| 1:O:169:SER:O | 1:O:173:LYS:HG3 | 2.20 | 0.42 |
| 2:P:71:ASN:HB3 | 2:P:74:ILE:H | 1.84 | 0.42 |
| 3:Q:134:VAL:HG12 | 3:Q:135:SER:N | 2.33 | 0.42 |
| 5:S:160:LEU:CD2 | 6:T:59:LEU:HD12 | 2.49 | 0.42 |
| 6:T:240:ILE:HD12 | 6:T:240:ILE:HA | 1.91 | 0.42 |
| 12:Z:134:ILE:HD11 | 12:Z:162:ALA:HB2 | 2.01 | 0.42 |
| 1:A:27:ALA:O | 1:A:31:VAL:HG23 | 2.19 | 0.42 |
| 2:B:6:ARG:HG2 | 3:C:10:ARG:NH2 | 2.34 | 0.42 |
| 3:C:52:ARG:HH21 | 3:C:211:GLU:HB3 | 1.84 | 0.42 |
| 3:C:149:TYR:CE1 | 3:C:159:SER:HB3 | 2.54 | 0.42 |
| 3:C:197:LEU:O | 3:C:201:VAL:HG23 | 2.19 | 0.42 |
| 5:E:2(C):VAL:CG1 | 5:E:2(D):ASP:N | 2.83 | 0.42 |
| 8:H:3:ILE:HD11 | 8:H:127:LEU:HB2 | 2.01 | 0.42 |
| 8:H:50:ALA:CB | 9:I:116:ILE:HG13 | 2.50 | 0.42 |
| 13:M:83:LEU:O | 13:M:87:MET:HG2 | 2.20 | 0.42 |
| 13:M:191:GLN:HE21 | 13:M:191:GLN:HB3 | 1.57 | 0.42 |
| 3:Q:120:GLN:O | 3:Q:124:THR:HG23 | 2.20 | 0.42 |
| 5:S:2(C):VAL:CG1 | 5:S:2(D):ASP:N | 2.82 | 0.42 |
| 12:Z:-8:PHE:CB | 13:1:-8:THR:HG23 | 2.49 | 0.42 |
| 2:B:229:ILE:O | 2:B:233:LEU:HB2 | 2.19 | 0.42 |
| 4:D:185:THR:HG23 | 4:D:188:GLU:OE1 | 2.19 | 0.42 |
| 5:E:4:PHE:O | 5:E:6:ASN:N | 2.53 | 0.42 |
| 6:F:50:VAL:HG22 | 6:F:51:GLU:N | 2.35 | 0.42 |
| 6:F:158:TRP:CZ3 | 7:G:64:VAL:HA | 2.54 | 0.42 |
| 7:G:18(D):ILE:N | 7:G:18(D):ILE:HD12 | 2.34 | 0.42 |
| 11:K:6:PHE:HA | 11:K:123:ASP:O | 2.19 | 0.42 |
| 2:P:63:THR:HG22 | 2:P:63:THR:O | 2.18 | 0.42 |
| 3:Q:52:ARG:HH21 | 3:Q:211:GLU:HB3 | 1.84 | 0.42 |
| 7:U:47:VAL:HG12 | 7:U:49:ILE:CD1 | 2.50 | 0.42 |
| 8:V:18:THR:CB | 8:V:30:ASN:HD22 | 2.33 | 0.42 |
| 10:X:48:GLU:HA | 10:X:48:GLU:OE1 | 2.19 | 0.42 |
| 12:Z:93:PHE:N | 12:Z:94:PRO:CD | 2.81 | 0.42 |
| 2:B:202:THR:HG22 | 2:B:203:ASP:N | 2.34 | 0.42 |
| 3:C:57:LYS:HD2 | 3:C:58:LEU:N | 2.35 | 0.42 |
| 3:C:105:ASP:OD2 | 3:C:106:PRO:HD2 | 2.20 | 0.42 |
| 3:C:134:VAL:HG12 | 3:C:135:SER:N | 2.34 | 0.42 |
| 3:C:136:THR:O | 3:C:150:GLN:HA | 2.19 | 0.42 |
| 7:G:82:ILE:HG22 | 7:G:83:PRO:HD3 | 2.01 | 0.42 |
| 8:H:18:THR:CB | 8:H:30:ASN:HD22 | 2.33 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:148:LYS:HE3 | 8:H:177:VAL:HG11 | 2.01 | 0.42 |
| 9:I:19:ARG:HB2 | 9:I:171:TRP:HB2 | 2.01 | 0.42 |
| 10:J:13:ILE:HD12 | 10:J:177:ILE:HD13 | 2.01 | 0.42 |
| 11:K:20:ALA:HB2 | 11:K:31:VAL:HG21 | 2.00 | 0.42 |
| 11:K:70:GLU:O | 11:K:71:LYS:C | 2.57 | 0.42 |
| 5:S:11:ASP:OD1 | 5:S:13:VAL:HG12 | 2.19 | 0.42 |
| 5:S:52:LYS:CB | 5:S:63:TYR:HB3 | 2.50 | 0.42 |
| 6:T:28:VAL:O | 6:T:32:GLU:HG3 | 2.19 | 0.42 |
| 9:W:29:ASN:HD22 | 9:W:29:ASN:N | 2.12 | 0.42 |
| 10:X:129:TYR:O | 10:X:132:PHE:HB2 | 2.20 | 0.42 |
| 6:F:192:GLN:NE2 | 6:F:195:LYS:HE3 | 2.31 | 0.42 |
| 7:G:78:VAL:HG11 | 7:G:85:ALA:HB2 | 2.02 | 0.42 |
| 10:J:40:HIS:CD2 | 10:J:10(A):LYS:HD3 | 2.54 | 0.42 |
| 11:K:40:PHE:CD1 | 11:K:73:ARG:CZ | 3.02 | 0.42 |
| 1:O:122:GLU:C | 1:O:124:THR:H | 2.23 | 0.42 |
| 4:R:160:TYR:HA | 5:S:58:LEU:O | 2.20 | 0.42 |
| 5:S:97:ASN:HD22 | 5:S:97:ASN:HA | 1.66 | 0.42 |
| 9:W:66:TYR:CZ | 9:W:70:GLU:HG3 | 2.54 | 0.42 |
| 14:2:67:THR:HA | 14:2:72:GLY:O | 2.19 | 0.42 |
| 9:I:14:ILE:HG12 | 9:I:34:ILE:HD12 | 2.01 | 0.42 |
| 13:M:1:THR:OG1 | 13:M:2:SER:N | 2.51 | 0.42 |
| 14:N:114:PRO:HD2 | 14:N:118:SER:O | 2.20 | 0.42 |
| 5:S:52:LYS:O | 5:S:63:TYR:HD2 | 2.03 | 0.42 |
| 6:T:20(B):GLU:HG3 | 6:T:20(C):LYS:N | 2.34 | 0.42 |
| 6:T:212:ILE:HG22 | 6:T:213:SER:N | 2.35 | 0.42 |
| 7:U:82:ILE:CG2 | 7:U:83:PRO:HD3 | 2.49 | 0.42 |
| 9:W:29:ASN:ND2 | 9:W:29:ASN:N | 2.65 | 0.42 |
| 10:X:35:ARG:NH1 | 10:X:57:GLU:HG2 | 2.34 | 0.42 |
| 13:1:80:PHE:CE1 | 13:1:111:ARG:HD3 | 2.54 | 0.42 |
| 4:D:31:ILE:HD13 | 4:D:135:ALA:HB2 | 2.01 | 0.42 |
| 5:E:172:ALA:HB2 | 5:E:196:ALA:O | 2.20 | 0.42 |
| 9:I:22:SER:O | 9:I:23:GLN:HB2 | 2.19 | 0.42 |
| 10:J:143:ARG:HG2 | 10:J:143:ARG:HH11 | 1.85 | 0.42 |
| 14:N:132:THR:O | 14:2:133:PHE:HA | 2.20 | 0.42 |
| 6:T:90:ASN:O | 6:T:94:GLU:HG3 | 2.20 | 0.42 |
| 7:U:74:ILE:HD12 | 7:U:109:CYS:HA | 2.00 | 0.42 |
| 7:U:234:VAL:O | 7:U:237:ALA:HB3 | 2.19 | 0.42 |
| 11:Y:86:LEU:C | 11:Y:86:LEU:HD13 | 2.40 | 0.42 |
| 7:G:171:GLU:OE1 | 7:G:171:GLU:N | 2.52 | 0.42 |
| 9:I:28:SER:CB | 10:J:120:VAL:HG21 | 2.49 | 0.42 |
| 10:J:22:ARG:HD3 | 10:J:22:ARG:HA | 1.95 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 10:J:35:ARG:HA | 10:J:35:ARG:HD3 | 1.71 | 0.42 |
| 10:J:166:MET:HA | 10:J:167:PRO:HD3 | 1.81 | 0.42 |
| 2:P:24:VAL:HG11 | 2:P:154:SER:HB3 | 2.02 | 0.42 |
| 3:Q:186:VAL:HG21 | 3:Q:216:LYS:HE2 | 2.02 | 0.42 |
| 5:S:162:GLY:O | 5:S:163:THR:HB | 2.20 | 0.42 |
| 14:2:126:ILE:HD13 | 14:2:126:ILE:N | 2.34 | 0.42 |
| 14:2:184:VAL:HG21 | 16:2:194:HOH:O | 2.20 | 0.42 |
| 2:B:160:TRP:CZ3 | 3:C:59:GLN:HG2 | 2.55 | 0.41 |
| 3:C:46:VAL:HG22 | 3:C:146:PRO:HB2 | 2.02 | 0.41 |
| 8:H:24:PRO:HG2 | 8:H:25:ILE:HD12 | 2.01 | 0.41 |
| 10:J:32:ASP:CG | 10:J:34:THR:HG22 | 2.40 | 0.41 |
| 4:R:117:CYS:SG | 4:R:157:PHE:HB3 | 2.60 | 0.41 |
| 2:B:66:LYS:O | 2:B:77:ALA:HA | 2.20 | 0.41 |
| 3:C:55:THR:O | 3:C:56:LEU:HD13 | 2.20 | 0.41 |
| 5:E:52:LYS:HD3 | 5:E:211:SER:HB2 | 2.02 | 0.41 |
| 14:N:107:LYS:CG | 14:N:108:GLY:N | 2.79 | 0.41 |
| 1:O:117:ALA:HB1 | 1:O:155:GLY:O | 2.20 | 0.41 |
| 5:S:221:PHE:HE1 | 5:S:223:ILE:HD11 | 1.82 | 0.41 |
| 6:T:107:ILE:HA | 6:T:108:PRO:HD3 | 1.83 | 0.41 |
| 6:T:186:ALA:HB3 | 6:T:21(A):GLU:HG3 | 2.01 | 0.41 |
| 7:U:236:ILE:HD12 | 7:U:236:ILE:C | 2.41 | 0.41 |
| 8:V:148:LYS:HE3 | 8:V:177:VAL:HG11 | 2.02 | 0.41 |
| 9:W:20:LEU:HD13 | 9:W:20:LEU:C | 2.40 | 0.41 |
| 9:W:99:PRO:HB2 | 9:W:113:PHE:CD2 | 2.55 | 0.41 |
| 13:1:112:TYR:HE1 | 13:1:127:THR:HG22 | 1.85 | 0.41 |
| 2:B:136:PHE:O | 2:B:150:THR:HA | 2.19 | 0.41 |
| 6:F:186:ALA:HB3 | 6:F:21(A):GLU:HG3 | 2.02 | 0.41 |
| 7:G:47:VAL:HG12 | 7:G:49:ILE:CD1 | 2.51 | 0.41 |
| 11:K:97:MET:O | 11:K:114:ASP:HA | 2.20 | 0.41 |
| 13:M:1:THR:HG22 | 16:M:213:HOH:O | 2.20 | 0.41 |
| 3:Q:57:LYS:HD2 | 3:Q:58:LEU:N | 2.34 | 0.41 |
| 5:S:64:GLN:HA | 16:S:242:HOH:O | 2.19 | 0.41 |
| 5:S:172:ALA:HB2 | 5:S:196:ALA:O | 2.20 | 0.41 |
| 7:U:18(H):GLU:CD | 7:U:18(H):GLU:N | 2.74 | 0.41 |
| 9:W:16:CYS:SG | 9:W:34:ILE:HG12 | 2.60 | 0.41 |
| 10:X:34:THR:HG21 | 10:X:176:LYS:NZ | 2.35 | 0.41 |
| 10:X:90(A):ILE:HD13 | 10:X:90(A):ILE:HA | 1.89 | 0.41 |
| 9:I:143:GLU:HG3 | 9:I:146:LEU:HD21 | 2.02 | 0.41 |
| 9:I:159:LEU:HD21 | 9:I:173:ALA:HB1 | 2.02 | 0.41 |
| 13:M:112:TYR:HE1 | 13:M:127:THR:HG22 | 1.84 | 0.41 |
| 2:P:233:LEU:HD12 | 2:P:233:LEU:HA | 1.92 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:31:ILE:HD13 | 4:R:135:ALA:HB2 | 2.02 | 0.41 |
| 5:S:58:LEU:CD1 | 5:S:58:LEU:N | 2.83 | 0.41 |
| 7:U:82:ILE:HG22 | 7:U:83:PRO:HD3 | 2.01 | 0.41 |
| 9:W:14:ILE:CG2 | 9:W:176:TYR:HB2 | 2.51 | 0.41 |
| 9:W:55:LEU:CD1 | 9:W:97:VAL:HG21 | 2.50 | 0.41 |
| 11:Y:75:SER:HB2 | 11:Y:106:GLU:OE2 | 2.20 | 0.41 |
| 1:A:4:MET:HG2 | 6:F:126:TYR:CZ | 2.55 | 0.41 |
| 1:A:21(B):ASN:CB | 1:A:21(F):LEU:HD12 | 2.51 | 0.41 |
| 3:C:57:LYS:HG3 | 3:C:208:LYS:HZ1 | 1.86 | 0.41 |
| 4:D:12:VAL:CG2 | 4:D:12(A):GLY:HA2 | 2.50 | 0.41 |
| 7:G:188:LYS:HD3 | 7:G:191:GLU:OE2 | 2.20 | 0.41 |
| 11:K:46:ALA:HB3 | 11:K:98:GLY:O | 2.20 | 0.41 |
| 13:M:57:ARG:CD | 16:M:247:HOH:O | 2.68 | 0.41 |
| 4:R:12:VAL:CG2 | 4:R:12(A):GLY:HA2 | 2.51 | 0.41 |
| 11:Y:70:GLU:O | 11:Y:71:LYS:C | 2.59 | 0.41 |
| 13:1:191:GLN:HE21 | 13:1:191:GLN:HB3 | 1.58 | 0.41 |
| 3:C:20:HIS:HB3 | 3:C:25:GLU:OE1 | 2.21 | 0.41 |
| 5:E:57:GLU:C | 5:E:58:LEU:HD12 | 2.41 | 0.41 |
| 5:E:150:GLU:O | 5:E:157:VAL:HA | 2.21 | 0.41 |
| 6:F:49:ALA:HA | 6:F:211:GLU:O | 2.20 | 0.41 |
| 10:J:168:MET:HE3 | 10:X:168:MET:CE | 2.48 | 0.41 |
| 12:L:-8:PHE:CB | 13:M:-8:THR:HG23 | 2.51 | 0.41 |
| 13:M:80:PHE:CE1 | 13:M:111:ARG:HD3 | 2.56 | 0.41 |
| 5:S:198:SER:HA | 5:S:201:LEU:CG | 2.43 | 0.41 |
| 9:W:36:HIS:HB3 | 9:W:42:PHE:CD2 | 2.55 | 0.41 |
| 11:Y:138:LEU:HD13 | 11:Y:158:SER:OG | 2.21 | 0.41 |
| 13:1:-5:PRO:HD3 | 13:1:96:TRP:CE2 | 2.56 | 0.41 |
| 13:1:175:LEU:HD23 | 13:1:175:LEU:C | 2.41 | 0.41 |
| 3:C:57:LYS:O | 3:C:58:LEU:HB2 | 2.20 | 0.41 |
| 4:D:91:HIS:CG | 4:D:119:LEU:HD11 | 2.56 | 0.41 |
| 9:I:16:CYS:SG | 9:I:34:ILE:HG12 | 2.61 | 0.41 |
| 2:P:143:ASP:OD2 | 10:X:10(B):LYS:HE2 | 2.21 | 0.41 |
| 3:Q:33:ARG:NH1 | 3:Q:33:ARG:CB | 2.71 | 0.41 |
| 5:S:52:LYS:HB3 | 5:S:63:TYR:O | 2.21 | 0.41 |
| 5:S:67:ILE:HG21 | 5:S:223:ILE:HD12 | 2.01 | 0.41 |
| 6:T:50:VAL:HG22 | 6:T:51:GLU:N | 2.35 | 0.41 |
| 12:Z:177:ILE:HD12 | 12:Z:177:ILE:N | 2.35 | 0.41 |
| 3:C:241:GLN:O | 3:C:243:GLN:N | 2.50 | 0.41 |
| 7:G:82:ILE:N | 7:G:83:PRO:HD2 | 2.35 | 0.41 |
| 7:G:139:VAL:HA | 7:G:147:SER:O | 2.20 | 0.41 |
| 8:H:53:GLU:O | 8:H:57:GLN:HG3 | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:L:-2:ASN:HA | 12:L:21:ILE:O | 2.20 | 0.41 |
| 3:Q:241:GLN:O | 3:Q:243:GLN:N | 2.50 | 0.41 |
| 6:T:13:SER:HB2 | 7:U:130:ARG:HD3 | 2.02 | 0.41 |
| 9:W:22:SER:O | 9:W:23:GLN:HB2 | 2.21 | 0.41 |
| 1:A:7:ARG:NH1 | 5:E:127:TYR:HD2 | 2.19 | 0.41 |
| 5:E:139:ILE:HD12 | 5:E:215:VAL:HG12 | 2.02 | 0.41 |
| 6:F:20(B):GLU:HG3 | 6:F:20(C):LYS:N | 2.36 | 0.41 |
| 8:H:84:LYS:HG3 | 8:H:85:GLN:N | 2.35 | 0.41 |
| 10:J:52:THR:HG22 | 10:J:53:VAL:H | 1.86 | 0.41 |
| 12:L:8:GLY:HA3 | 12:L:11:PHE:CZ | 2.56 | 0.41 |
| 13:M:-5:PRO:HD3 | 13:M:96:TRP:CE2 | 2.56 | 0.41 |
| 14:N:24:ALA:HB3 | 13:1:129:PHE:HE2 | 1.85 | 0.41 |
| 14:N:144:GLU:O | 14:N:145:ASN:HB2 | 2.21 | 0.41 |
| 2:P:4:GLY:HA3 | 5:S:127:TYR:CZ | 2.56 | 0.41 |
| 3:Q:38:VAL:HG22 | 3:Q:39:GLY:N | 2.36 | 0.41 |
| 3:Q:44:ASN:O | 3:Q:45:CYS:HB3 | 2.21 | 0.41 |
| 3:Q:18(A):ASP:OD2 | 3:Q:18(C):LYS:HG2 | 2.20 | 0.41 |
| 5:S:4:PHE:O | 5:S:5:ARG:C | 2.59 | 0.41 |
| 8:V:189:ARG:O | 8:V:190:ASN:HB2 | 2.21 | 0.41 |
| 9:W:124:PHE:O | 9:W:125:ILE:HD12 | 2.21 | 0.41 |
| 9:W:130:ALA:HB2 | 9:W:166:ASP:CB | 2.51 | 0.41 |
| 10:X:7:ARG:HD3 | 16:X:195:HOH:O | 2.21 | 0.41 |
| 2:B:73:LYS:C | 2:B:74:ILE:HD12 | 2.41 | 0.41 |
| 3:C:44:ASN:O | 3:C:45:CYS:HB3 | 2.20 | 0.41 |
| 3:C:224:LEU:HD12 | 3:C:224:LEU:N | 2.36 | 0.41 |
| 5:E:52:LYS:CB | 5:E:63:TYR:HB3 | 2.51 | 0.41 |
| 5:E:67:ILE:HG21 | 5:E:223:ILE:HD12 | 2.03 | 0.41 |
| 6:F:212:ILE:HG22 | 6:F:213:SER:N | 2.36 | 0.41 |
| 7:G:29:LYS:HD2 | 7:G:29:LYS:HA | 1.75 | 0.41 |
| 11:K:12:ILE:HG13 | 11:K:108:PRO:HB3 | 2.03 | 0.41 |
| 13:M:14(G):ILE:HB | 13:M:144:PRO:CD | 2.51 | 0.41 |
| 3:Q:57:LYS:CG | 3:Q:208:LYS:HZ1 | 2.34 | 0.41 |
| 3:Q:224:LEU:HD12 | 3:Q:224:LEU:N | 2.36 | 0.41 |
| 8:V:18:THR:HG21 | 8:V:30:ASN:ND2 | 2.35 | 0.41 |
| 9:W:29:ASN:HD22 | 9:W:29:ASN:C | 2.24 | 0.41 |
| 2:B:21(C):ASP:OD2 | 2:B:219:GLU:HB3 | 2.21 | 0.40 |
| 8:H:84:LYS:HE2 | 8:H:119:THR:HG23 | 2.02 | 0.40 |
| 9:I:93:GLY:N | 9:I:94:PRO:CD | 2.83 | 0.40 |
| 9:I:149:GLU:H | 9:I:149:GLU:CD | 2.24 | 0.40 |
| 12:L:-7:ASN:ND2 | 12:L:-7:ASN:C | 2.73 | 0.40 |
| 12:L:42:VAL:CG2 | 12:L:102:ALA:HB3 | 2.51 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:P:21(C):ASP:OD2 | 2:P:219:GLU:HB3 | 2.21 | 0.40 |
| 3:Q:106:PRO:HG2 | 3:Q:143:PRO:HG2 | 1.99 | 0.40 |
| 4:R:101:LEU:CD1 | 11:Y:57:THR:HG22 | 2.51 | 0.40 |
| 4:R:105:GLU:OE1 | 12:Z:66:TYR:OH | 2.33 | 0.40 |
| 5:S:2(B):THR:H | 5:S:2(E):ASN:HB3 | 1.85 | 0.40 |
| 8:V:72:ARG:HG3 | 8:V:72:ARG:NH1 | 2.34 | 0.40 |
| 8:V:128:GLY:O | 8:V:131:SER:CB | 2.66 | 0.40 |
| 9:W:23:GLN:CB | 16:W:228:HOH:O | 2.67 | 0.40 |
| 10:X:22:ARG:HD3 | 10:X:22:ARG:HA | 1.94 | 0.40 |
| 2:B:147:GLN:HG2 | 3:C:62(A):ILE:HG21 | 2.02 | 0.40 |
| 3:C:106:PRO:HG2 | 3:C:143:PRO:HG2 | 2.00 | 0.40 |
| 6:F:18:ASP:OD2 | 6:F:18:ASP:N | 2.44 | 0.40 |
| 7:G:234:VAL:O | 7:G:237:ALA:HB3 | 2.21 | 0.40 |
| 10:J:129:TYR:O | 10:J:132:PHE:HB2 | 2.21 | 0.40 |
| 10:J:147:THR:HG23 | 10:J:150:GLU:OE2 | 2.21 | 0.40 |
| 2:P:101:LYS:HZ2 | 10:X:85:GLN:HE21 | 1.68 | 0.40 |
| 3:Q:185:THR:HG22 | 3:Q:186:VAL:N | 2.35 | 0.40 |
| 4:R:97:VAL:HG13 | 16:Y:226:HOH:O | 2.21 | 0.40 |
| 4:R:185:THR:HG23 | 4:R:188:GLU:OE1 | 2.21 | 0.40 |
| 5:S:139:ILE:HD12 | 5:S:215:VAL:HG12 | 2.03 | 0.40 |
| 9:W:93:GLY:N | 9:W:94:PRO:CD | 2.84 | 0.40 |
| 12:Z:42:VAL:CG2 | 12:Z:102:ALA:HB3 | 2.51 | 0.40 |
| 12:Z:114:ASP:OD2 | 12:Z:115:PRO:HD2 | 2.21 | 0.40 |
| 14:2:144:GLU:O | 14:2:145:ASN:HB2 | 2.21 | 0.40 |
| 1:A:111:LEU:HD23 | 1:A:111:LEU:HA | 1.89 | 0.40 |
| 5:E:162:GLY:O | 5:E:163:THR:HB | 2.21 | 0.40 |
| 6:F:179:LEU:HD11 | 6:F:192:GLN:HG3 | 2.03 | 0.40 |
| 11:K:76:VAL:N | 11:K:106:GLU:OE2 | 2.49 | 0.40 |
| 13:M:137:LEU:O | 13:M:140:LYS:HB2 | 2.20 | 0.40 |
| 6:T:175:GLU:HB2 | 6:T:196:ILE:HD12 | 2.03 | 0.40 |
| 9:W:28:SER:CB | 10:X:120:VAL:HG21 | 2.51 | 0.40 |
| 3:C:62(A):ILE:O | 3:C:63:THR:C | 2.60 | 0.40 |
| 5:E:17:PRO:HA | 6:F:26:TYR:CE2 | 2.56 | 0.40 |
| 6:F:175:GLU:HB2 | 6:F:196:ILE:HD12 | 2.04 | 0.40 |
| 9:I:137:MET:CE | 9:I:141:LEU:HD11 | 2.51 | 0.40 |
| 10:J:12:VAL:HG23 | 10:J:108:PRO:HB2 | 2.03 | 0.40 |
| 11:K:25:TRP:HH2 | 12:L:135:MET:HB2 | 1.86 | 0.40 |
| 11:K:138:LEU:HD13 | 11:K:158:SER:OG | 2.22 | 0.40 |
| 1:O:21(B):ASN:CB | 1:O:21(F):LEU:HD12 | 2.51 | 0.40 |
| 3:Q:15:PHE:H | 4:R:23:GLN:NE2 | 1.95 | 0.40 |
| 3:Q:108:THR:HG23 | 16:Q:255:HOH:O | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:S:7:ASN:HD22 | 5:S:7:ASN:HA | 1.76 | 0.40 |
| 5:S:230:ALA:C | 5:S:232:TYR:H | 2.25 | 0.40 |
| 7:U:17(C):LYS:HE3 | 7:U:17(C):LYS:HB2 | 1.76 | 0.40 |
| 13:1:19:LEU:HD12 | 13:1:20:GLY:H | 1.87 | 0.40 |
| 3:C:134:VAL:CG1 | 3:C:135:SER:N | 2.84 | 0.40 |
| 7:G:46:THR:HG21 | 7:G:139:VAL:HB | 2.03 | 0.40 |
| 8:H:18:THR:HG21 | 8:H:30:ASN:ND2 | 2.37 | 0.40 |
| 8:H:41:ILE:HD12 | 8:H:41:ILE:N | 2.37 | 0.40 |
| 9:I:99:PRO:HB2 | 9:I:113:PHE:CD2 | 2.57 | 0.40 |
| 12:L:1:GLY:N | 16:L:220:HOH:O | 2.55 | 0.40 |
| 3:Q:134:VAL:CG1 | 3:Q:135:SER:N | 2.84 | 0.40 |
| 5:S:152:GLN:HA | 5:S:153:PRO:HD3 | 1.96 | 0.40 |
| 9:W:55:LEU:HD23 | 9:W:55:LEU:HA | 1.94 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 248/250 (99%) | 232 (94%) | 13 (5%) | 3 (1%) | 13 | 37 |
| 1 | O | 248/250 (99%) | 231 (93%) | 13 (5%) | 4 (2%) | 9 | 29 |
| 2 | B | 242/244 (99%) | 224 (93%) | 12 (5%) | 6 (2%) | 5 | 18 |
| 2 | P | 242/244 (99%) | 222 (92%) | 14 (6%) | 6 (2%) | 5 | 18 |
| 3 | C | 239/241 (99%) | 216 (90%) | 18 (8%) | 5 (2%) | 7 | 22 |
| 3 | Q | 239/241 (99%) | 216 (90%) | 18 (8%) | 5 (2%) | 7 | 22 |
| 4 | D | 240/242 (99%) | 226 (94%) | 10 (4%) | 4 (2%) | 9 | 27 |
| 4 | R | 240/242 (99%) | 224 (93%) | 12 (5%) | 4 (2%) | 9 | 27 |
| 5 | E | 231/233 (99%) | 209 (90%) | 15 (6%) | 7 (3%) | 4 | 14 |
| 5 | S | 231/233 (99%) | 208 (90%) | 16 (7%) | 7 (3%) | 4 | 14 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 6 | F | 242/244 (99%) | 227 (94%) | 13 (5%) | 2 (1%) | 19 | 47 |
| 6 | T | 242/244 (99%) | 226 (93%) | 13 (5%) | 3 (1%) | 13 | 37 |
| 7 | G | 241/243 (99%) | 226 (94%) | 13 (5%) | 2 (1%) | 19 | 47 |
| 7 | U | 241/243 (99%) | 227 (94%) | 11 (5%) | 3 (1%) | 13 | 37 |
| 8 | H | 220/222 (99%) | 207 (94%) | 12 (6%) | 1 (0%) | 29 | 59 |
| 8 | V | 220/222 (99%) | 209 (95%) | 10 (4%) | 1 (0%) | 29 | 59 |
| 9 | I | 202/204 (99%) | 192 (95%) | 10 (5%) | 0 | 100 | 100 |
| 9 | W | 202/204 (99%) | 192 (95%) | 10 (5%) | 0 | 100 | 100 |
| 10 | J | 196/198 (99%) | 189 (96%) | 5 (3%) | 2 (1%) | 15 | 42 |
| 10 | X | 196/198 (99%) | 187 (95%) | 7 (4%) | 2 (1%) | 15 | 42 |
| 11 | K | 210/212 (99%) | 203 (97%) | 7 (3%) | 0 | 100 | 100 |
| 11 | Y | 210/212 (99%) | 204 (97%) | 6 (3%) | 0 | 100 | 100 |
| 12 | L | 220/222 (99%) | 210 (96%) | 9 (4%) | 1 (0%) | 29 | 59 |
| 12 | Z | 220/222 (99%) | 209 (95%) | 10 (4%) | 1 (0%) | 29 | 59 |
| 13 | 1 | 231/233 (99%) | 218 (94%) | 13 (6%) | 0 | 100 | 100 |
| 13 | M | 231/233 (99%) | 217 (94%) | 14 (6%) | 0 | 100 | 100 |
| 14 | 2 | 194/196 (99%) | 185 (95%) | 9 (5%) | 0 | 100 | 100 |
| 14 | N | 194/196 (99%) | 185 (95%) | 9 (5%) | 0 | 100 | 100 |
| All | All | 6312/6368 (99%) | 5921 (94%) | 322 (5%) | 69 (1%) | 14 | 39 |

All (69) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 58 | LEU |
| 4 | D | 12(G) | GLU |
| 5 | E | 5 | ARG |
| 5 | E | 202 | ARG |
| 3 | Q | 58 | LEU |
| 4 | R | 12(G) | GLU |
| 5 | S | 5 | ARG |
| 5 | S | 202 | ARG |
| 1 | A | 5 | THR |
| 2 | B | 54 | VAL |
| 2 | B | 20(A) | SER |
| 2 | B | 21(B) | GLY |
| 2 | B | 21(C) | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 183 | PRO |
| 3 | C | 203 | THR |
| 5 | E | 64 | GLN |
| 5 | E | 217 | LYS |
| 7 | G | 239 | GLN |
| 10 | J | 192 | ALA |
| 1 | O | 5 | THR |
| 2 | P | 54 | VAL |
| 2 | P | 20(A) | SER |
| 2 | P | 21(B) | GLY |
| 2 | P | 21(C) | ASP |
| 3 | Q | 183 | PRO |
| 3 | Q | 203 | THR |
| 5 | S | 64 | GLN |
| 5 | S | 217 | LYS |
| 7 | U | 239 | GLN |
| 8 | V | 91 | GLN |
| 10 | X | 192 | ALA |
| 3 | C | 184 | ALA |
| 5 | E | 203 | ASP |
| 8 | H | 91 | GLN |
| 3 | Q | 184 | ALA |
| 5 | S | 203 | ASP |
| 6 | T | 206 | LYS |
| 1 | A | 56 | SER |
| 1 | A | 167 | LYS |
| 2 | B | 184 | MET |
| 4 | D | 12(C) | GLY |
| 4 | D | 12(F) | GLY |
| 5 | E | 180 | LEU |
| 5 | E | 231 | LYS |
| 6 | F | 64 | ASN |
| 6 | F | 206 | LYS |
| 10 | J | 49 | ALA |
| 1 | O | 56 | SER |
| 1 | O | 167 | LYS |
| 2 | P | 6 | ARG |
| 2 | P | 184 | MET |
| 4 | R | 12(C) | GLY |
| 4 | R | 12(F) | GLY |
| 5 | S | 180 | LEU |
| 5 | S | 231 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | T | 64 | ASN |
| 3 | C | 242 | GLU |
| 4 | D | 120 | ALA |
| 12 | L | 93 | PHE |
| 1 | O | 53 | LYS |
| 3 | Q | 242 | GLU |
| 4 | R | 120 | ALA |
| 6 | T | 143 | LYS |
| 10 | X | 49 | ALA |
| 12 | Z | 93 | PHE |
| 2 | B | 6 | ARG |
| 7 | U | 61 | PRO |
| 7 | U | 55 | PRO |
| 7 | G | 61 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 209/209 (100%) | 203 (97%) | 6 (3%) | 42 | 74 |
| 1 | O | 209/209 (100%) | 203 (97%) | 6 (3%) | 42 | 74 |
| 2 | B | 203/203 (100%) | 190 (94%) | 13 (6%) | 17 | 44 |
| 2 | P | 203/203 (100%) | 190 (94%) | 13 (6%) | 17 | 44 |
| 3 | C | 213/213 (100%) | 203 (95%) | 10 (5%) | 26 | 57 |
| 3 | Q | 213/213 (100%) | 203 (95%) | 10 (5%) | 26 | 57 |
| 4 | D | 198/198 (100%) | 188 (95%) | 10 (5%) | 24 | 54 |
| 4 | R | 198/198 (100%) | 188 (95%) | 10 (5%) | 24 | 54 |
| 5 | E | 192/192 (100%) | 175 (91%) | 17 (9%) | 9 | 27 |
| 5 | S | 192/192 (100%) | 175 (91%) | 17 (9%) | 9 | 27 |
| 6 | F | 201/201 (100%) | 185 (92%) | 16 (8%) | 12 | 32 |
| 6 | T | 201/201 (100%) | 185 (92%) | 16 (8%) | 12 | 32 |
| 7 | G | 207/207 (100%) | 197 (95%) | 10 (5%) | 25 | 56 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 7 | U | 207/207 (100%) | 196 (95%) | 11 (5%) | 22 52 |
| 8 | H | 181/181 (100%) | 174 (96%) | 7 (4%) | 32 64 |
| 8 | V | 181/181 (100%) | 174 (96%) | 7 (4%) | 32 64 |
| 9 | I | 172/172 (100%) | 167 (97%) | 5 (3%) | 42 74 |
| 9 | W | 172/172 (100%) | 167 (97%) | 5 (3%) | 42 74 |
| 10 | J | 175/175 (100%) | 169 (97%) | 6 (3%) | 37 69 |
| 10 | X | 175/175 (100%) | 169 (97%) | 6 (3%) | 37 69 |
| 11 | K | 169/169 (100%) | 162 (96%) | 7 (4%) | 30 63 |
| 11 | Y | 169/169 (100%) | 162 (96%) | 7 (4%) | 30 63 |
| 12 | L | 185/185 (100%) | 175 (95%) | 10 (5%) | 22 51 |
| 12 | Z | 185/185 (100%) | 175 (95%) | 10 (5%) | 22 51 |
| 13 | 1 | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 64 |
| 13 | M | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 64 |
| 14 | 2 | 162/162 (100%) | 155 (96%) | 7 (4%) | 29 60 |
| 14 | N | 162/162 (100%) | 155 (96%) | 7 (4%) | 29 60 |
| All | All | 5332/5332 (100%) | 5067 (95%) | 265 (5%) | 24 55 |

All (265) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 33 | GLN |
| 1 | A | 64 | LEU |
| 1 | A | 124 | THR |
| 1 | A | 158 | PHE |
| 1 | A | 179 | ARG |
| 1 | A | 229 | ILE |
| 2 | B | 58 | LEU |
| 2 | B | 71 | ASN |
| 2 | B | 74 | ILE |
| 2 | B | 121 | GLN |
| 2 | B | 135 | SER |
| 2 | B | 150 | THR |
| 2 | B | 163 | ILE |
| 2 | B | 185 | LYS |
| 2 | B | 187 | ASP |
| 2 | B | 192 | LEU |
| 2 | B | 212 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 218 | ASN |
| 2 | B | 224 | PHE |
| 3 | C | 10 | ARG |
| 3 | C | 25 | GLU |
| 3 | C | 57 | LYS |
| 3 | C | 121 | GLN |
| 3 | C | 135 | SER |
| 3 | C | 150 | GLN |
| 3 | C | 172 | VAL |
| 3 | C | 174 | GLU |
| 3 | C | 208 | LYS |
| 3 | C | 227 | GLU |
| 4 | D | 28 | LEU |
| 4 | D | 76 | CYS |
| 4 | D | 110 | GLU |
| 4 | D | 126 | ARG |
| 4 | D | 170 | GLU |
| 4 | D | 177 | LEU |
| 4 | D | 191 | LEU |
| 4 | D | 194 | LEU |
| 4 | D | 215 | ILE |
| 4 | D | 244 | GLU |
| 5 | E | 11 | ASP |
| 5 | E | 12 | THR |
| 5 | E | 32 | LYS |
| 5 | E | 56 | ASP |
| 5 | E | 57 | GLU |
| 5 | E | 76 | LEU |
| 5 | E | 97 | ASN |
| 5 | E | 104 | ASN |
| 5 | E | 121 | GLN |
| 5 | E | 185 | ASN |
| 5 | E | 189 | LEU |
| 5 | E | 199 | GLN |
| 5 | E | 207 | LEU |
| 5 | E | 214 | ILE |
| 5 | E | 227 | GLU |
| 5 | E | 231 | LYS |
| 5 | E | 233 | ILE |
| 6 | F | 11 | SER |
| 6 | F | 35 | THR |
| 6 | F | 36 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | F | 43 | ASN |
| 6 | F | 105 | THR |
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |
| 6 | F | 169 | ARG |
| 6 | F | 176 | LEU |
| 6 | F | 18(E) | GLU |
| 6 | F | 187 | ARG |
| 6 | F | 203 | GLU |
| 6 | F | 204 | ASP |
| 6 | F | 205 | ASN |
| 6 | F | 214 | TRP |
| 6 | F | 21(C) | ASN |
| 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 | 184 | ASN |
| 7 | G | 197 | MET |
| 7 | G | 232 | ARG |
| 7 | G | 233 | LEU |
| 8 | H | 30 | ASN |
| 8 | H | 34 | LEU |
| 8 | H | 43 | CYS |
| 8 | H | 56 | THR |
| 8 | H | 68 | LEU |
| 8 | H | 144 | GLN |
| 8 | H | 197 | ARG |
| 9 | I | 29 | ASN |
| 9 | I | 61 | TYR |
| 9 | I | 113 | PHE |
| 9 | I | 116 | ILE |
| 9 | I | 160 | LEU |
| 10 | J | 52 | THR |
| 10 | J | 70 | GLU |
| 10 | J | 77 | GLN |
| 10 | J | 90(A) | ILE |
| 10 | J | 121 | GLU |
| 10 | J | 177 | ILE |
| 11 | K | 4 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 11 | K | 9 | GLN |
| 11 | K | 65 | LEU |
| 11 | K | 87 | VAL |
| 11 | K | 104 | TYR |
| 11 | K | 10(B) | LYS |
| 11 | K | 138 | LEU |
| 12 | L | -7 | ASN |
| 12 | L | 14 | LEU |
| 12 | L | 40 | ASN |
| 12 | L | 58 | ARG |
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 98 | HIS |
| 12 | L | 99 | THR |
| 12 | L | 120 | GLU |
| 12 | L | 145 | TYR |
| 13 | M | 40 | ASN |
| 13 | M | 62 | LEU |
| 13 | M | 91 | ARG |
| 13 | M | 129 | PHE |
| 13 | M | 14(C) | ARG |
| 13 | M | 148 | VAL |
| 13 | M | 149 | GLN |
| 13 | M | 204 | LYS |
| 14 | N | 36 | ARG |
| 14 | N | 89 | GLU |
| 14 | N | 10(B) | LYS |
| 14 | N | 119 | VAL |
| 14 | N | 126 | ILE |
| 14 | N | 18(A) | ILE |
| 14 | N | 18(I) | GLN |
| 1 | O | 33 | GLN |
| 1 | O | 64 | LEU |
| 1 | O | 124 | THR |
| 1 | O | 158 | PHE |
| 1 | O | 179 | ARG |
| 1 | O | 229 | ILE |
| 2 | P | 58 | LEU |
| 2 | P | 71 | ASN |
| 2 | P | 74 | ILE |
| 2 | P | 121 | GLN |
| 2 | P | 135 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | P | 150 | THR |
| 2 | P | 163 | ILE |
| 2 | P | 185 | LYS |
| 2 | P | 187 | ASP |
| 2 | P | 192 | LEU |
| 2 | P | 212 | PHE |
| 2 | P | 218 | ASN |
| 2 | P | 224 | PHE |
| 3 | Q | 10 | ARG |
| 3 | Q | 25 | GLU |
| 3 | Q | 57 | LYS |
| 3 | Q | 121 | GLN |
| 3 | Q | 135 | SER |
| 3 | Q | 150 | GLN |
| 3 | Q | 172 | VAL |
| 3 | Q | 174 | GLU |
| 3 | Q | 208 | LYS |
| 3 | Q | 227 | GLU |
| 4 | R | 28 | LEU |
| 4 | R | 76 | CYS |
| 4 | R | 110 | GLU |
| 4 | R | 126 | ARG |
| 4 | R | 170 | GLU |
| 4 | R | 177 | LEU |
| 4 | R | 191 | LEU |
| 4 | R | 194 | LEU |
| 4 | R | 215 | ILE |
| 4 | R | 244 | GLU |
| 5 | S | 11 | ASP |
| 5 | S | 12 | THR |
| 5 | S | 32 | LYS |
| 5 | S | 56 | ASP |
| 5 | S | 57 | GLU |
| 5 | S | 76 | LEU |
| 5 | S | 97 | ASN |
| 5 | S | 104 | ASN |
| 5 | S | 121 | GLN |
| 5 | S | 185 | ASN |
| 5 | S | 189 | LEU |
| 5 | S | 199 | GLN |
| 5 | S | 207 | LEU |
| 5 | S | 214 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | S | 227 | GLU |
| 5 | S | 231 | LYS |
| 5 | S | 233 | ILE |
| 6 | T | 11 | SER |
| 6 | T | 35 | THR |
| 6 | T | 36 | THR |
| 6 | T | 43 | ASN |
| 6 | T | 105 | THR |
| 6 | T | 121 | GLN |
| 6 | T | 127 | ASN |
| 6 | T | 169 | ARG |
| 6 | T | 176 | LEU |
| 6 | T | 18(E) | GLU |
| 6 | T | 187 | ARG |
| 6 | T | 203 | GLU |
| 6 | T | 204 | ASP |
| 6 | T | 205 | ASN |
| 6 | T | 214 | TRP |
| 6 | T | 21(C) | ASN |
| 7 | U | 38 | LEU |
| 7 | U | 72 | ARG |
| 7 | U | 87 | ASN |
| 7 | U | 119 | LEU |
| 7 | U | 121 | GLN |
| 7 | U | 124 | THR |
| 7 | U | 169 | GLN |
| 7 | U | 184 | ASN |
| 7 | U | 197 | MET |
| 7 | U | 232 | ARG |
| 7 | U | 233 | LEU |
| 8 | V | 30 | ASN |
| 8 | V | 34 | LEU |
| 8 | V | 43 | CYS |
| 8 | V | 56 | THR |
| 8 | V | 68 | LEU |
| 8 | V | 144 | GLN |
| 8 | V | 197 | ARG |
| 9 | W | 29 | ASN |
| 9 | W | 61 | TYR |
| 9 | W | 113 | PHE |
| 9 | W | 116 | ILE |
| 9 | W | 160 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | X | 52 | THR |
| 10 | X | 70 | GLU |
| 10 | X | 77 | GLN |
| 10 | X | 90(A) | ILE |
| 10 | X | 121 | GLU |
| 10 | X | 177 | ILE |
| 11 | Y | 4 | LEU |
| 11 | Y | 9 | GLN |
| 11 | Y | 65 | LEU |
| 11 | Y | 87 | VAL |
| 11 | Y | 104 | TYR |
| 11 | Y | 10(B) | LYS |
| 11 | Y | 138 | LEU |
| 12 | Z | -7 | ASN |
| 12 | Z | 14 | LEU |
| 12 | Z | 40 | ASN |
| 12 | Z | 58 | ARG |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 98 | HIS |
| 12 | Z | 99 | THR |
| 12 | Z | 120 | GLU |
| 12 | Z | 145 | TYR |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 62 | LEU |
| 13 | 1 | 91 | ARG |
| 13 | 1 | 129 | PHE |
| 13 | 1 | 14(C) | ARG |
| 13 | 1 | 148 | VAL |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 204 | LYS |
| 14 | 2 | 36 | ARG |
| 14 | 2 | 89 | GLU |
| 14 | 2 | 10(B) | LYS |
| 14 | 2 | 119 | VAL |
| 14 | 2 | 126 | ILE |
| 14 | 2 | 18(A) | ILE |
| 14 | 2 | 18(I) | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 33 | GLN |
| 1 | A | 97 | HIS |
| 2 | B | 23 | GLN |
| 2 | B | 71 | ASN |
| 2 | B | 95 | HIS |
| 2 | B | 97 | GLN |
| 2 | B | 121 | GLN |
| 2 | B | 125 | GLN |
| 2 | B | 156 | ASN |
| 2 | B | 177 | GLN |
| 2 | B | 218 | ASN |
| 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 | 238 | GLN |
| 3 | C | 243 | GLN |
| 4 | D | 23 | GLN |
| 4 | D | 108 | ASN |
| 4 | D | 147 | GLN |
| 4 | D | 161 | ASN |
| 4 | D | 211 | GLN |
| 4 | D | 218 | GLN |
| 4 | D | 226 | ASN |
| 5 | E | 7 | ASN |
| 5 | E | 33 | GLN |
| 5 | E | 64 | GLN |
| 5 | E | 73 | HIS |
| 5 | E | 104 | ASN |
| 5 | E | 121 | GLN |
| 5 | E | 123 | ASN |
| 5 | E | 125 | GLN |
| 5 | E | 185 | ASN |
| 5 | E | 199 | GLN |
| 5 | E | 2(E) | ASN |
| 6 | F | 23 | GLN |
| 6 | F | 43 | ASN |
| 6 | F | 90 | ASN |
| 6 | F | 121 | GLN |
| 6 | F | 127 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | F | 192 | GLN |
| 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 |
| 7 | G | 228 | ASN |
| 8 | H | 30 | ASN |
| 8 | H | 66 | HIS |
| 8 | H | 144 | GLN |
| 8 | H | 165 | ASN |
| 8 | H | 172 | ASN |
| 8 | H | 190 | ASN |
| 9 | I | 29 | ASN |
| 9 | I | 81 | GLN |
| 9 | I | 161 | ASN |
| 10 | J | 54 | GLN |
| 10 | J | 77 | GLN |
| 10 | J | 85 | GLN |
| 10 | J | 112 | GLN |
| 10 | J | 140 | HIS |
| 10 | J | 141 | HIS |
| 10 | J | 186 | GLN |
| 10 | J | 193 | GLN |
| 11 | K | 9 | GLN |
| 11 | K | 85 | ASN |
| 11 | K | 174 | ASN |
| 11 | K | 207 | ASN |
| 12 | L | -9 | GLN |
| 12 | L | -7 | ASN |
| 12 | L | 40 | ASN |
| 12 | L | 46 | ASN |
| 12 | L | 61 | ASN |
| 12 | L | 70(A) | ASN |
| 12 | L | 82 | ASN |
| 12 | L | 85 | HIS |
| 12 | L | 98 | HIS |
| 12 | L | 123 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 12 | L | 1(I) | ASN |
| 12 | L | 166 | HIS |
| 12 | L | 168 | GLN |
| 13 | M | -7 | GLN |
| 13 | M | 10 | ASN |
| 13 | M | 18 | ASN |
| 13 | M | 40 | ASN |
| 13 | M | 89 | GLN |
| 13 | M | 93 | ASN |
| 13 | M | 149 | GLN |
| 13 | M | 157 | ASN |
| 13 | M | 172 | ASN |
| 13 | M | 191 | GLN |
| 14 | N | 69 | GLN |
| 14 | N | 145 | ASN |
| 14 | N | 157 | HIS |
| 14 | N | 161 | GLN |
| 1 | O | 33 | GLN |
| 1 | O | 97 | HIS |
| 2 | P | 23 | GLN |
| 2 | P | 33 | HIS |
| 2 | P | 71 | ASN |
| 2 | P | 95 | HIS |
| 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 | 97 | GLN |
| 3 | Q | 121 | GLN |
| 3 | Q | 125 | GLN |
| 3 | Q | 150 | GLN |
| 3 | Q | 163 | GLN |
| 3 | Q | 238 | GLN |
| 3 | Q | 243 | GLN |
| 4 | R | 23 | GLN |
| 4 | R | 108 | ASN |
| 4 | R | 114 | GLN |
| 4 | R | 147 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | R | 161 | ASN |
| 4 | R | 211 | GLN |
| 4 | R | 218 | GLN |
| 4 | R | 226 | ASN |
| 5 | S | 7 | ASN |
| 5 | S | 64 | GLN |
| 5 | S | 73 | HIS |
| 5 | S | 104 | ASN |
| 5 | S | 121 | GLN |
| 5 | S | 123 | ASN |
| 5 | S | 125 | GLN |
| 5 | S | 185 | ASN |
| 5 | S | 199 | GLN |
| 5 | S | 2(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 |
| 7 | U | 34(A) | ASN |
| 7 | U | 87 | ASN |
| 7 | U | 118 | ASN |
| 7 | U | 121 | GLN |
| 7 | U | 125 | GLN |
| 7 | U | 169 | GLN |
| 7 | U | 170 | GLN |
| 7 | U | 178 | ASN |
| 7 | U | 184 | ASN |
| 7 | U | 228 | ASN |
| 8 | V | 30 | ASN |
| 8 | V | 66 | HIS |
| 8 | V | 144 | GLN |
| 8 | V | 165 | ASN |
| 8 | V | 172 | ASN |
| 8 | V | 190 | ASN |
| 9 | W | 29 | ASN |
| 9 | W | 64 | ASN |
| 9 | W | 81 | GLN |
| 9 | W | 161 | ASN |
| 10 | X | 54 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | X | 62 | ASN |
| 10 | X | 77 | GLN |
| 10 | X | 85 | GLN |
| 10 | X | 112 | GLN |
| 10 | X | 140 | HIS |
| 10 | X | 141 | HIS |
| 10 | X | 186 | GLN |
| 10 | X | 193 | GLN |
| 11 | Y | 9 | GLN |
| 11 | Y | 85 | ASN |
| 11 | Y | 131 | GLN |
| 11 | Y | 174 | ASN |
| 11 | Y | 207 | ASN |
| 12 | Z | -9 | GLN |
| 12 | Z | -7 | ASN |
| 12 | Z | 40 | ASN |
| 12 | Z | 46 | ASN |
| 12 | Z | 61 | ASN |
| 12 | Z | 70(A) | ASN |
| 12 | Z | 82 | ASN |
| 12 | Z | 123 | GLN |
| 12 | Z | 1(I) | ASN |
| 12 | Z | 166 | HIS |
| 12 | Z | 168 | GLN |
| 13 | 1 | 10 | ASN |
| 13 | 1 | 18 | ASN |
| 13 | 1 | 40 | ASN |
| 13 | 1 | 89 | GLN |
| 13 | 1 | 93 | ASN |
| 13 | 1 | 149 | GLN |
| 13 | 1 | 157 | ASN |
| 13 | 1 | 172 | ASN |
| 13 | 1 | 191 | GLN |
| 14 | 2 | 69 | GLN |
| 14 | 2 | 145 | ASN |
| 14 | 2 | 157 | HIS |
| 14 | 2 | 161 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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 | $\#\|Z\| > 2$ |
| 15 | BIQ | V | 1001 | - | 50,51,51 | 1.79 | 14 (28%) | 66,69,69 | 2.10 | 14 (21%) |
| 15 | BIQ | H | 1000 | - | 50,51,51 | 1.75 | 13 (26%) | 66,69,69 | 2.08 | 15 (22%) |

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 |
|---|---|---|---|---|---|---|---|
| 15 | BIQ | V | 1001 | - | - | 13/51/53/53 | 0/3/4/4 |
| 15 | BIQ | H | 1000 | - | - | 14/51/53/53 | 0/3/4/4 |

All (27) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | V | 1001 | BIQ | C37-C32 | 3.89 | 1.47 | 1.40 |
| 15 | V | 1001 | BIQ | C37-N38 | -3.72 | 1.38 | 1.45 |
| 15 | H | 1000 | BIQ | C37-C32 | 3.53 | 1.46 | 1.40 |
| 15 | H | 1000 | BIQ | C37-N38 | -3.42 | 1.39 | 1.45 |
| 15 | V | 1001 | BIQ | C5-N6 | 3.37 | 1.43 | 1.34 |
| 15 | H | 1000 | BIQ | C42-C30 | 3.35 | 1.45 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 15 | V | 1001 | BIQ | C42-C30 | 3.33 | 1.45 | 1.38 |
| 15 | H | 1000 | BIQ | O31-C32 | 3.25 | 1.46 | 1.39 |
| 15 | V | 1001 | BIQ | O31-C32 | 3.17 | 1.46 | 1.39 |
| 15 | H | 1000 | BIQ | C5-N6 | 3.06 | 1.42 | 1.34 |
| 15 | V | 1001 | BIQ | C43-C42 | 2.65 | 1.43 | 1.38 |
| 15 | H | 1000 | BIQ | O4-C5 | 2.60 | 1.40 | 1.35 |
| 15 | V | 1001 | BIQ | C36-C37 | 2.56 | 1.44 | 1.39 |
| 15 | V | 1001 | BIQ | O4-C5 | 2.56 | 1.40 | 1.35 |
| 15 | H | 1000 | BIQ | C43-C42 | 2.51 | 1.43 | 1.38 |
| 15 | H | 1000 | BIQ | C7-N6 | 2.44 | 1.51 | 1.45 |
| 15 | V | 1001 | BIQ | C33-C32 | 2.20 | 1.42 | 1.38 |
| 15 | H | 1000 | BIQ | C45-C2 | 2.19 | 1.43 | 1.38 |
| 15 | V | 1001 | BIQ | C7-N6 | 2.15 | 1.50 | 1.45 |
| 15 | V | 1001 | BIQ | C1-C2 | 2.13 | 1.43 | 1.38 |
| 15 | V | 1001 | BIQ | C28-C27 | 2.10 | 1.43 | 1.38 |
| 15 | H | 1000 | BIQ | C46-C45 | 2.10 | 1.43 | 1.38 |
| 15 | V | 1001 | BIQ | O31-C30 | 2.06 | 1.44 | 1.39 |
| 15 | H | 1000 | BIQ | O31-C30 | 2.05 | 1.44 | 1.39 |
| 15 | H | 1000 | BIQ | O39-N38 | 2.04 | 1.26 | 1.22 |
| 15 | V | 1001 | BIQ | C36-C35 | 2.01 | 1.42 | 1.38 |
| 15 | H | 1000 | BIQ | C8-N10 | 2.01 | 1.38 | 1.34 |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | H | 1000 | BIQ | C12-C11-N10 | 9.54 | 129.28 | 110.60 |
| 15 | V | 1001 | BIQ | C12-C11-N10 | 9.38 | 128.96 | 110.60 |
| 15 | V | 1001 | BIQ | C7-C8-N10 | 5.10 | 127.88 | 116.70 |
| 15 | H | 1000 | BIQ | C11-N10-C8 | 4.86 | 132.09 | 121.67 |
| 15 | V | 1001 | BIQ | C11-N10-C8 | 4.82 | 132.00 | 121.67 |
| 15 | H | 1000 | BIQ | C41-C7-N6 | -4.78 | 100.72 | 110.79 |
| 15 | H | 1000 | BIQ | C7-C8-N10 | 4.73 | 127.07 | 116.70 |
| 15 | V | 1001 | BIQ | O9-C8-N10 | -4.08 | 115.38 | 122.93 |
| 15 | V | 1001 | BIQ | C41-C7-N6 | -4.03 | 102.29 | 110.79 |
| 15 | H | 1000 | BIQ | O9-C8-N10 | -3.93 | 115.66 | 122.93 |
| 15 | V | 1001 | BIQ | C26-C19-N18 | 3.50 | 118.16 | 110.79 |
| 15 | H | 1000 | BIQ | C26-C19-N18 | 3.32 | 117.79 | 110.79 |
| 15 | H | 1000 | BIQ | C23-N22-C20 | 3.15 | 128.20 | 122.59 |
| 15 | H | 1000 | BIQ | C41-C7-C8 | 3.09 | 118.27 | 110.25 |
| 15 | V | 1001 | BIQ | C41-C7-C8 | 3.08 | 118.25 | 110.25 |
| 15 | V | 1001 | BIQ | C34-C41-C7 | 3.06 | 121.84 | 113.39 |
| 15 | H | 1000 | BIQ | C34-C41-C7 | 3.06 | 121.82 | 113.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | V | 1001 | BIQ | C32-O31-C30 | -2.82 | 110.96 | 118.00 |
| 15 | V | 1001 | BIQ | C23-N22-C20 | 2.76 | 127.51 | 122.59 |
| 15 | V | 1001 | BIQ | O31-C32-C37 | 2.66 | 122.70 | 117.49 |
| 15 | H | 1000 | BIQ | C24-C23-N22 | -2.56 | 104.22 | 112.32 |
| 15 | V | 1001 | BIQ | O4-C3-C2 | 2.53 | 115.48 | 109.39 |
| 15 | H | 1000 | BIQ | C32-O31-C30 | -2.53 | 111.70 | 118.00 |
| 15 | H | 1000 | BIQ | O31-C32-C37 | 2.49 | 122.38 | 117.49 |
| 15 | V | 1001 | BIQ | C36-C37-N38 | 2.40 | 119.04 | 116.47 |
| 15 | V | 1001 | BIQ | C24-C23-N22 | -2.39 | 104.76 | 112.32 |
| 15 | H | 1000 | BIQ | C11-C12-C13 | 2.26 | 116.73 | 112.24 |
| 15 | H | 1000 | BIQ | C20-C19-N18 | -2.20 | 105.17 | 111.16 |
| 15 | H | 1000 | BIQ | O4-C3-C2 | 2.00 | 114.21 | 109.39 |

There are no chirality outliers.

All (27) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | V | 1001 | BIQ | C16-C11-C12-C13 |
| 15 | H | 1000 | BIQ | O9-C8-N10-C11 |
| 15 | V | 1001 | BIQ | O9-C8-N10-C11 |
| 15 | V | 1001 | BIQ | C7-C8-N10-C11 |
| 15 | H | 1000 | BIQ | C7-C8-N10-C11 |
| 15 | H | 1000 | BIQ | C11-C12-C13-N14 |
| 15 | V | 1001 | BIQ | C11-C12-C13-N14 |
| 15 | H | 1000 | BIQ | C16-C11-C12-C13 |
| 15 | V | 1001 | BIQ | C12-C11-N10-C8 |
| 15 | H | 1000 | BIQ | C11-C12-C13-O15 |
| 15 | V | 1001 | BIQ | C11-C12-C13-O15 |
| 15 | H | 1000 | BIQ | N10-C11-C16-N18 |
| 15 | V | 1001 | BIQ | N10-C11-C16-N18 |
| 15 | V | 1001 | BIQ | C41-C7-N6-C5 |
| 15 | H | 1000 | BIQ | C12-C11-N10-C8 |
| 15 | H | 1000 | BIQ | C36-C37-N38-O39 |
| 15 | V | 1001 | BIQ | C36-C37-N38-O39 |
| 15 | H | 1000 | BIQ | N6-C7-C8-N10 |
| 15 | V | 1001 | BIQ | N6-C7-C8-N10 |
| 15 | H | 1000 | BIQ | C41-C7-N6-C5 |
| 15 | V | 1001 | BIQ | N6-C7-C8-O9 |
| 15 | V | 1001 | BIQ | N10-C11-C16-O17 |
| 15 | H | 1000 | BIQ | N6-C7-C8-O9 |
| 15 | H | 1000 | BIQ | N10-C11-C16-O17 |
| 15 | H | 1000 | BIQ | C35-C34-C41-C7 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | H | 1000 | BIQ | C33-C34-C41-C7 |
| 15 | V | 1001 | BIQ | C35-C34-C41-C7 |

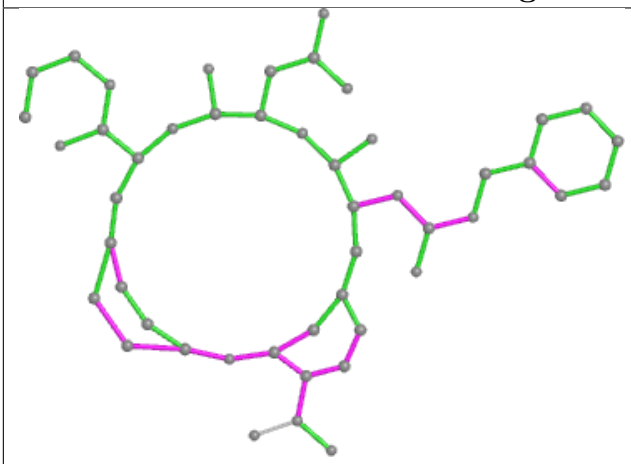
There are no ring outliers.

2 monomers are involved in 9 short contacts:

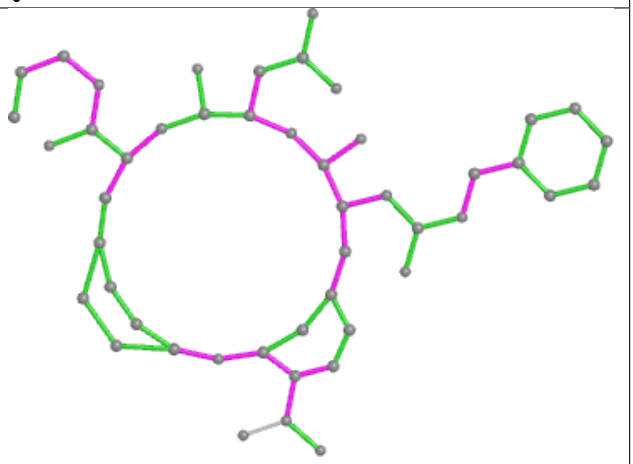
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 15 | V | 1001 | BIQ | 5 | 0 |
| 15 | H | 1000 | BIQ | 4 | 0 |

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

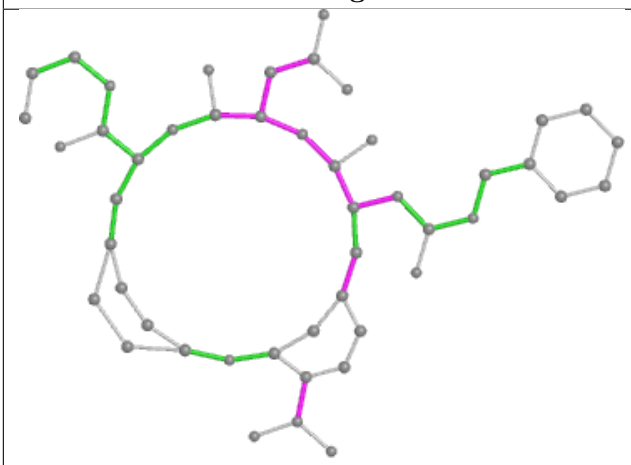
**Ligand BIQ V 1001**



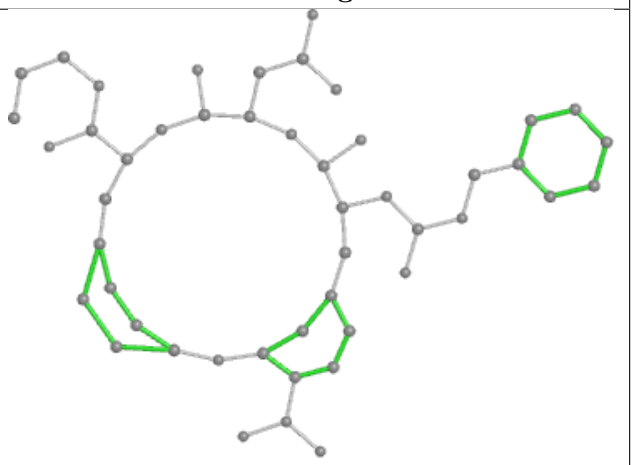
**Bond lengths**



**Bond angles**

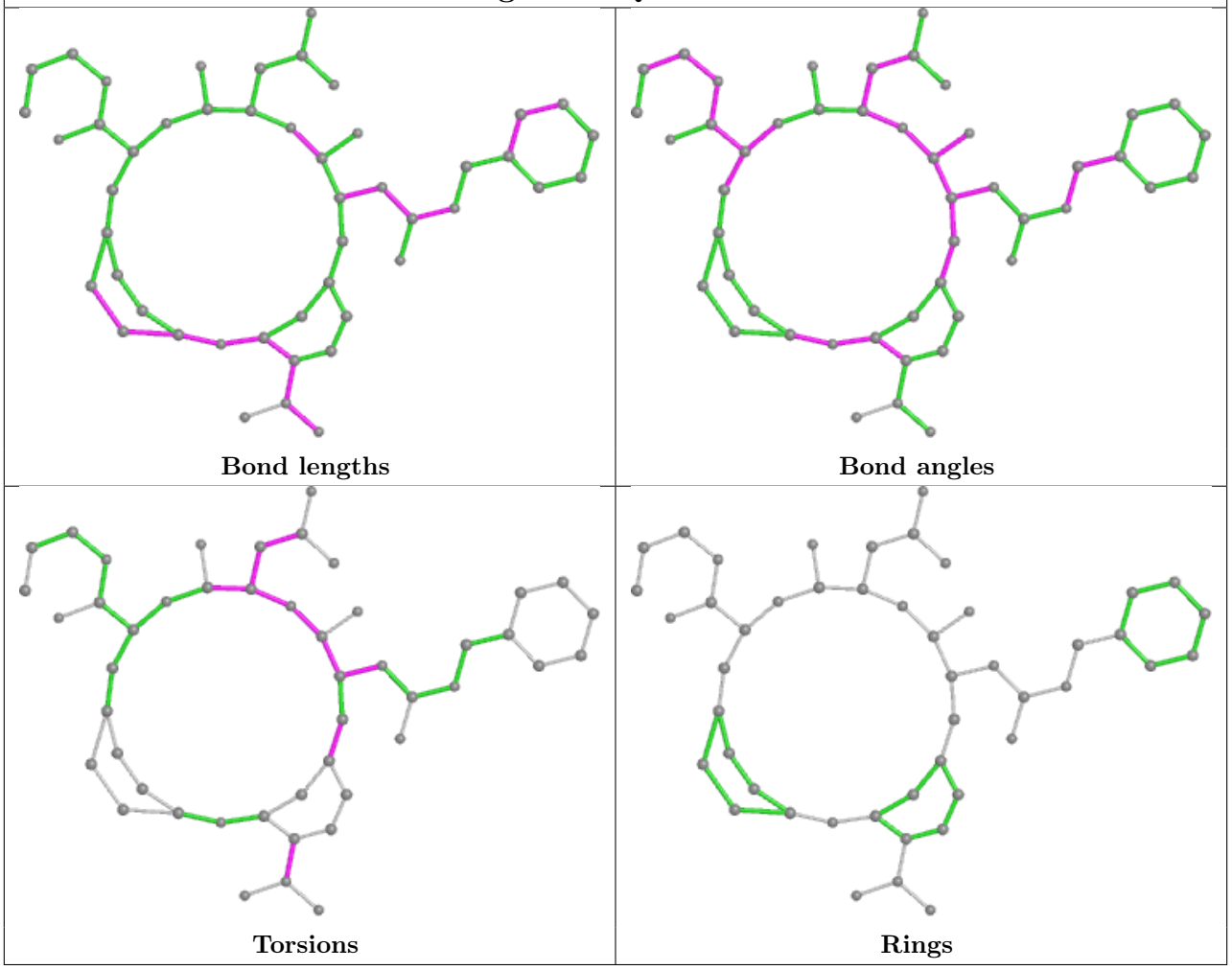


**Torsions**



**Rings**

**Ligand BIQ H 1000**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 250/250 (100%) | -0.39 | 2 (0%) | 86 | 82 | 33, 45, 76, 103 | 0 |
| 1 | O | 250/250 (100%) | -0.31 | 5 (2%) | 65 | 56 | 33, 52, 81, 106 | 0 |
| 2 | B | 244/244 (100%) | -0.19 | 9 (3%) | 41 | 31 | 31, 52, 87, 116 | 0 |
| 2 | P | 244/244 (100%) | -0.11 | 14 (5%) | 23 | 15 | 35, 55, 91, 118 | 0 |
| 3 | C | 241/241 (100%) | -0.10 | 10 (4%) | 37 | 27 | 33, 57, 109, 123 | 0 |
| 3 | Q | 241/241 (100%) | 0.04 | 12 (4%) | 28 | 20 | 37, 60, 110, 122 | 0 |
| 4 | D | 242/242 (100%) | -0.11 | 8 (3%) | 46 | 36 | 35, 56, 89, 121 | 0 |
| 4 | R | 242/242 (100%) | -0.01 | 12 (4%) | 28 | 20 | 36, 60, 91, 121 | 0 |
| 5 | E | 233/233 (100%) | -0.17 | 5 (2%) | 63 | 54 | 39, 59, 85, 110 | 0 |
| 5 | S | 233/233 (100%) | 0.07 | 17 (7%) | 15 | 8 | 38, 63, 89, 108 | 0 |
| 6 | F | 244/244 (100%) | -0.33 | 4 (1%) | 72 | 65 | 34, 54, 88, 105 | 0 |
| 6 | T | 244/244 (100%) | -0.21 | 6 (2%) | 57 | 47 | 34, 55, 90, 107 | 0 |
| 7 | G | 243/243 (100%) | -0.40 | 3 (1%) | 79 | 73 | 29, 47, 75, 114 | 0 |
| 7 | U | 243/243 (100%) | -0.36 | 2 (0%) | 86 | 82 | 30, 49, 74, 114 | 0 |
| 8 | H | 222/222 (100%) | -0.57 | 3 (1%) | 75 | 69 | 26, 43, 61, 92 | 0 |
| 8 | V | 222/222 (100%) | -0.57 | 3 (1%) | 75 | 69 | 30, 44, 63, 96 | 0 |
| 9 | I | 204/204 (100%) | -0.64 | 1 (0%) | 91 | 88 | 28, 44, 61, 80 | 0 |
| 9 | W | 204/204 (100%) | -0.62 | 1 (0%) | 91 | 88 | 31, 45, 64, 79 | 0 |
| 10 | J | 198/198 (100%) | -0.45 | 3 (1%) | 73 | 67 | 29, 45, 62, 120 | 0 |
| 10 | X | 198/198 (100%) | -0.39 | 5 (2%) | 57 | 47 | 33, 48, 63, 122 | 0 |
| 11 | K | 212/212 (100%) | -0.49 | 0 | 100 | 100 | 27, 47, 63, 74 | 0 |
| 11 | Y | 212/212 (100%) | -0.50 | 1 (0%) | 91 | 88 | 29, 48, 67, 74 | 0 |
| 12 | L | 222/222 (100%) | -0.55 | 2 (0%) | 84 | 80 | 27, 45, 69, 88 | 0 |
| 12 | Z | 222/222 (100%) | -0.53 | 1 (0%) | 91 | 88 | 30, 45, 69, 88 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 13 | 1 | 233/233 (100%) | -0.59 | 1 (0%) 92 91 | 28, 43, 57, 64 | 0 |
| 13 | M | 233/233 (100%) | -0.58 | 1 (0%) 92 91 | 29, 45, 60, 67 | 0 |
| 14 | 2 | 196/196 (100%) | -0.52 | 1 (0%) 91 88 | 24, 43, 66, 78 | 0 |
| 14 | N | 196/196 (100%) | -0.58 | 0 100 100 | 28, 42, 66, 76 | 0 |
| All | All | 6368/6368 (100%) | -0.35 | 132 (2%) 63 54 | 24, 49, 83, 123 | 0 |

All (132) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 7 | U | 240 | ASP | 9.8 |
| 3 | C | 55 | THR | 9.7 |
| 4 | D | 12(D) | ALA | 9.3 |
| 4 | R | 12(D) | ALA | 9.2 |
| 4 | R | 12(F) | GLY | 8.9 |
| 3 | C | 56 | LEU | 8.0 |
| 4 | R | 12(E) | SER | 7.8 |
| 4 | D | 12(F) | GLY | 7.6 |
| 10 | X | 193 | GLN | 7.4 |
| 2 | P | 217 | ALA | 7.3 |
| 4 | D | 12(E) | SER | 7.3 |
| 2 | B | 217 | ALA | 7.2 |
| 10 | J | 193 | GLN | 6.8 |
| 2 | B | 218 | ASN | 6.7 |
| 1 | A | 4 | MET | 6.7 |
| 7 | U | 6 | ALA | 6.5 |
| 10 | X | 192 | ALA | 6.5 |
| 7 | G | 240 | ASP | 6.4 |
| 2 | P | 218 | ASN | 6.0 |
| 4 | D | 12(C) | GLY | 6.0 |
| 4 | R | 12(C) | GLY | 5.9 |
| 10 | J | 192 | ALA | 5.8 |
| 7 | G | 6 | ALA | 5.8 |
| 3 | Q | 54 | SER | 5.7 |
| 4 | D | 126 | ARG | 5.7 |
| 5 | E | 203 | ASP | 5.2 |
| 3 | Q | 63 | THR | 5.1 |
| 5 | S | 203 | ASP | 5.0 |
| 3 | Q | 55 | THR | 4.8 |
| 6 | F | 5 | GLY | 4.8 |
| 4 | D | 12(G) | GLU | 4.8 |
| 4 | R | 126 | ARG | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | B | 54 | VAL | 4.6 |
| 2 | P | 219 | GLU | 4.5 |
| 2 | P | 21(C) | ASP | 4.4 |
| 1 | O | 4 | MET | 4.3 |
| 3 | Q | 56 | LEU | 4.2 |
| 8 | V | 223 | ASP | 4.2 |
| 2 | B | 21(B) | GLY | 4.0 |
| 9 | I | -8 | SER | 4.0 |
| 8 | H | 222 | CYS | 4.0 |
| 5 | E | 4 | PHE | 4.0 |
| 1 | O | 236 | LEU | 4.0 |
| 5 | S | 5 | ARG | 3.9 |
| 10 | X | 191 | GLN | 3.8 |
| 3 | Q | 242 | GLU | 3.8 |
| 5 | S | 206 | SER | 3.8 |
| 1 | O | 235 | ALA | 3.6 |
| 2 | B | 239 | THR | 3.6 |
| 8 | H | 223 | ASP | 3.6 |
| 10 | X | 189 | ASP | 3.6 |
| 1 | O | 5 | THR | 3.5 |
| 5 | S | 4 | PHE | 3.5 |
| 5 | S | 58 | LEU | 3.5 |
| 6 | T | 241 | ASN | 3.5 |
| 5 | E | 5 | ARG | 3.5 |
| 5 | S | 178 | ARG | 3.5 |
| 2 | P | 21(B) | GLY | 3.5 |
| 12 | Z | 14(W) | LYS | 3.4 |
| 3 | Q | 203 | THR | 3.4 |
| 3 | Q | 241 | GLN | 3.4 |
| 5 | S | 55 | ALA | 3.4 |
| 5 | S | 60 | SER | 3.4 |
| 1 | A | 5 | THR | 3.3 |
| 4 | D | 125 | GLU | 3.3 |
| 3 | C | 54 | SER | 3.3 |
| 4 | R | 125 | GLU | 3.3 |
| 10 | J | 191 | GLN | 3.3 |
| 3 | Q | 64 | PRO | 3.2 |
| 8 | V | 222 | CYS | 3.2 |
| 6 | F | 204 | ASP | 3.2 |
| 10 | X | -1 | MET | 3.2 |
| 2 | P | 63 | THR | 3.2 |
| 5 | S | 54 | ASN | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 9 | W | -8 | SER | 3.1 |
| 4 | R | 12(G) | GLU | 3.1 |
| 13 | 1 | -8 | THR | 3.1 |
| 4 | R | 127 | LEU | 3.1 |
| 5 | S | 63 | TYR | 3.1 |
| 2 | P | 54 | VAL | 3.0 |
| 3 | Q | 243 | GLN | 3.0 |
| 4 | R | 9 | ASP | 3.0 |
| 6 | T | 5 | GLY | 3.0 |
| 4 | R | 12(B) | GLU | 2.9 |
| 2 | P | 239 | THR | 2.9 |
| 2 | P | 62 | ASP | 2.9 |
| 13 | M | -8 | THR | 2.9 |
| 3 | C | 203 | THR | 2.9 |
| 2 | B | 21(C) | ASP | 2.8 |
| 3 | Q | 61 | THR | 2.7 |
| 3 | C | 242 | GLU | 2.7 |
| 5 | S | 57 | GLU | 2.7 |
| 6 | T | 240 | ILE | 2.7 |
| 3 | C | 237 | GLU | 2.7 |
| 5 | S | 56 | ASP | 2.6 |
| 6 | F | 205 | ASN | 2.6 |
| 12 | L | 145 | TYR | 2.6 |
| 11 | Y | 211 | GLY | 2.5 |
| 5 | S | 64 | GLN | 2.5 |
| 1 | O | 55 | SER | 2.5 |
| 14 | 2 | 18(I) | GLN | 2.5 |
| 3 | C | 59 | GLN | 2.5 |
| 2 | B | 21(A) | LYS | 2.4 |
| 8 | V | 220 | ASN | 2.4 |
| 4 | D | 9 | ASP | 2.4 |
| 12 | L | 14(W) | LYS | 2.4 |
| 3 | C | 53 | ARG | 2.3 |
| 2 | P | 220 | TYR | 2.3 |
| 2 | P | 20(A) | SER | 2.3 |
| 3 | Q | 62(A) | ILE | 2.2 |
| 5 | S | 59 | SER | 2.2 |
| 5 | S | 195 | GLU | 2.2 |
| 2 | P | 183 | ASP | 2.2 |
| 6 | T | 57 | LYS | 2.2 |
| 3 | C | 243 | GLN | 2.2 |
| 2 | P | 21(A) | LYS | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 5 | S | 2(E) | ASN | 2.1 |
| 8 | H | 220 | ASN | 2.1 |
| 5 | E | 57 | GLU | 2.1 |
| 3 | C | 240 | LYS | 2.1 |
| 2 | B | 219 | GLU | 2.1 |
| 2 | B | 20(A) | SER | 2.1 |
| 3 | Q | 58 | LEU | 2.1 |
| 2 | P | 53 | LYS | 2.1 |
| 7 | G | 239 | GLN | 2.1 |
| 5 | E | 6 | ASN | 2.1 |
| 4 | R | 243 | ALA | 2.0 |
| 5 | S | 6 | ASN | 2.0 |
| 6 | F | 20(B) | GLU | 2.0 |
| 6 | T | 170 | GLN | 2.0 |
| 6 | T | 238 | LYS | 2.0 |
| 4 | R | 178 | ASN | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

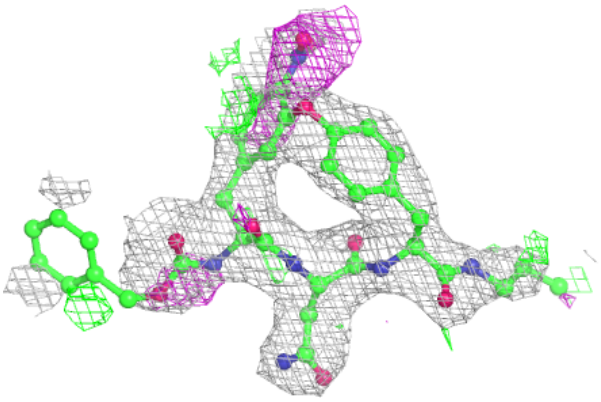
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

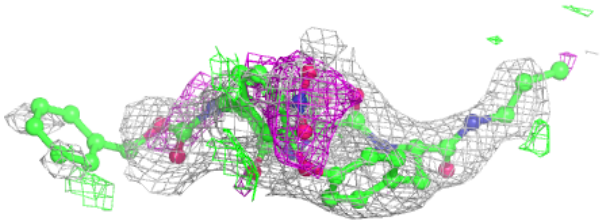
| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 15 | BIQ | V | 1001 | 48/48 | 0.81 | 0.31 | 36,57,68,71 | 6 |
| 15 | BIQ | H | 1000 | 48/48 | 0.84 | 0.29 | 28,54,64,67 | 7 |

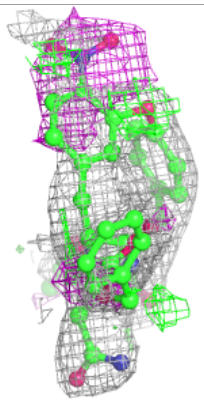
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BIQ V 1001:**

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

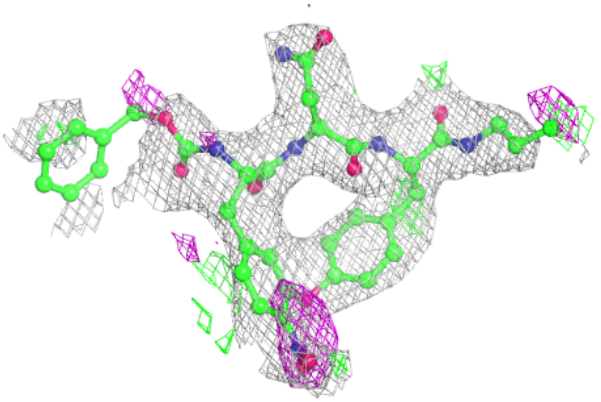


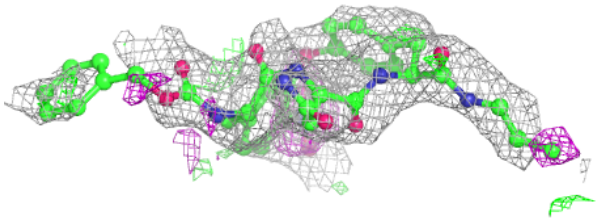


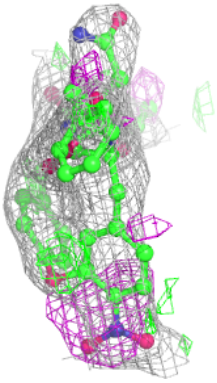


**Electron density around BIQ H 1000:**

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







## 6.5 Other polymers (i)

There are no such residues in this entry.