# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:02 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 4UBD |
| Title | : | Crystal structure of a neutralizing human monoclonal antibody with 1968 H3 HA |
| Authors | : | Shore, D.A.; Yang, H.; Cho, M.; Donis, R.O.; Stevens, J. |
| Deposited on | : | 2014-08-12 |
| Resolution | : | 3.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

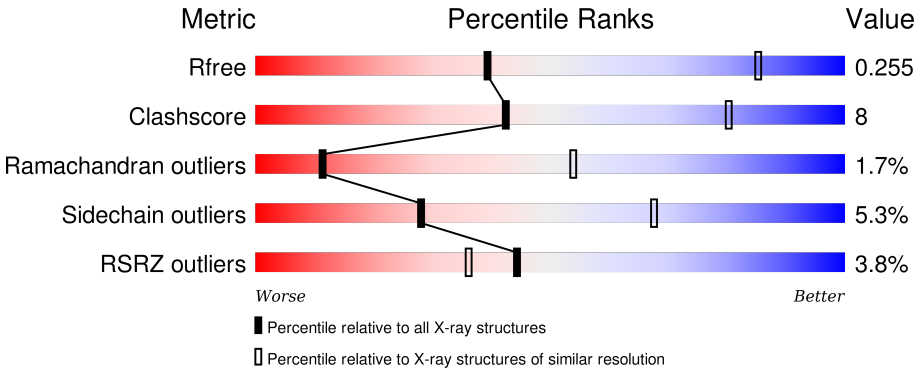
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.1 (RC1), CSD as537be (2016) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026982 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20026982 |

# 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 3.50 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 1051 (3.60-3.40) |
| Clashscore | 102246 | 1157 (3.60-3.40) |
| Ramachandran outliers | 100387 | 1120 (3.60-3.40) |
| Sidechain outliers | 100360 | 1121 (3.60-3.40) |
| RSRZ outliers | 91569 | 1058 (3.60-3.40) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 | 321 | % 83% 14% |
| 1 | E | 321 | 81% 17% |
| 1 | I | 321 | 83% 14% |
| 1 | M | 321 | 83% 15% |
| 1 | Q | 321 | 81% 16% |

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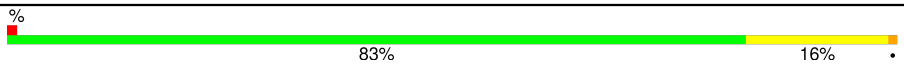
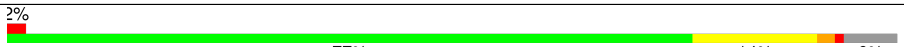
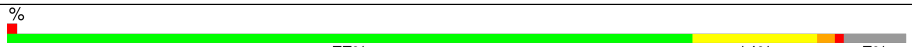
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | U | 321 |   |
| 2 | B | 175 |   |
| 2 | F | 175 |   |
| 2 | J | 175 |   |
| 2 | N | 175 |   |
| 2 | R | 175 |   |
| 2 | V | 175 |   |
| 3 | C | 226 |   |
| 3 | G | 226 |   |
| 3 | K | 226 |   |
| 3 | O | 226 |   |
| 3 | S | 226 |   |
| 3 | Y | 226 |   |
| 4 | D | 215 |   |
| 4 | H | 215 |   |
| 4 | L | 215 |   |
| 4 | P | 215 |   |
| 4 | T | 215 |   |
| 4 | X | 215 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 5 | NAG | Q | 407 | - | - | - | X |
| 5 | NAG | V | 201 | - | - | - | X |
| 7 | MAN | A | 404 | X | - | - | - |
| 7 | MAN | E | 404 | X | - | - | - |
| 7 | MAN | I | 404 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 7 | MAN | M | 404 | X | - | - | - |
| 7 | MAN | Q | 404 | X | - | - | - |
| 7 | MAN | U | 404 | X | - | - | - |

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 43086 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 Hemagglutinin HA1 chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 320 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2470 | 1546 | 434 | 477 | 13 | | | |
| 1 | U | 320 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2470 | 1546 | 434 | 477 | 13 | | | |
| 1 | I | 317 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2445 | 1531 | 429 | 472 | 13 | | | |
| 1 | M | 320 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2470 | 1546 | 434 | 477 | 13 | | | |
| 1 | Q | 320 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2470 | 1546 | 434 | 477 | 13 | | | |
| 1 | E | 320 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2470 | 1546 | 434 | 477 | 13 | | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 329 | GLN | - | expression tag | UNP Q91MA7 |
| U | 329 | GLN | - | expression tag | UNP Q91MA7 |
| I | 329 | GLN | - | expression tag | UNP Q91MA7 |
| M | 329 | GLN | - | expression tag | UNP Q91MA7 |
| Q | 329 | GLN | - | expression tag | UNP Q91MA7 |
| E | 329 | GLN | - | expression tag | UNP Q91MA7 |

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | V | 164 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1346 | 831 | 238 | 271 | 6 | | | |
| 2 | F | 163 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1338 | 825 | 237 | 270 | 6 | | | |
| 2 | B | 165 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1357 | 840 | 239 | 272 | 6 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | J | 164 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1349 | 834 | 238 | 271 | 6 | | | |
| 2 | N | 163 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1338 | 825 | 237 | 270 | 6 | | | |
| 2 | R | 166 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1359 | 839 | 241 | 273 | 6 | | | |

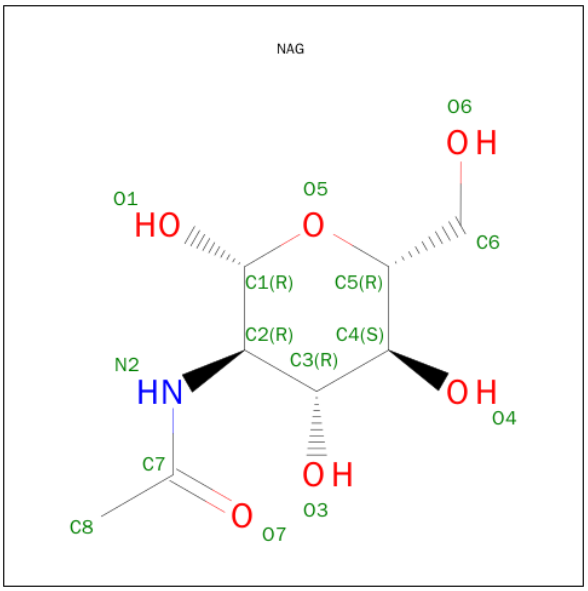
- Molecule 3 is a protein called monoclonal antibody H chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |
| 3 | Y | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |
| 3 | G | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |
| 3 | S | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |
| 3 | O | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |
| 3 | K | 219 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1637 | 1036 | 278 | 319 | 4 | | | |

- Molecule 4 is a protein called monoclonal antibody L chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |
| 4 | X | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |
| 4 | H | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |
| 4 | T | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |
| 4 | P | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |
| 4 | L | 213 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1650 | 1029 | 290 | 327 | 4 | | | |

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | A | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | U | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | U | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | U | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | V | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | I | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | I | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | I | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |

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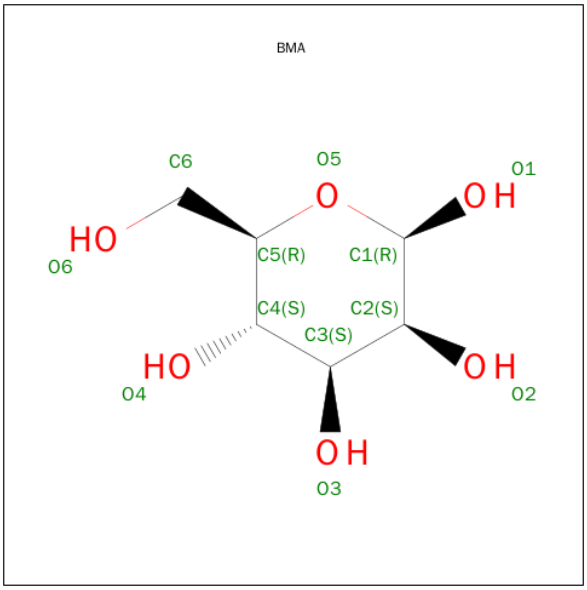
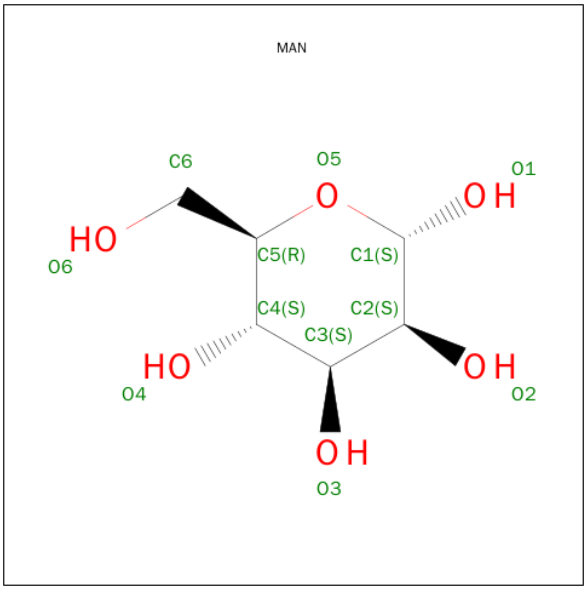
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | M | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | Q | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | Q | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | Q | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | Q | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | Q | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | E | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |
| 5 | F | 1 | Total | C | N | O | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | A | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 6 | U | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 6 | I | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 6 | M | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 6 | Q | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 6 | E | 1 | Total C O<br>11 6 5 | 0 | 0 |

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



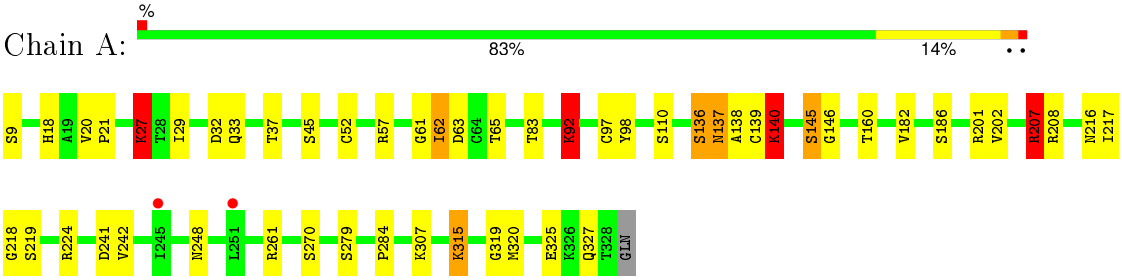

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 7 | A | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 7 | U | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 7 | I | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 7 | M | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 7 | Q | 1 | Total C O<br>11 6 5 | 0 | 0 |
| 7 | E | 1 | Total C O<br>11 6 5 | 0 | 0 |

# 3 Residue-property plots (i)

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

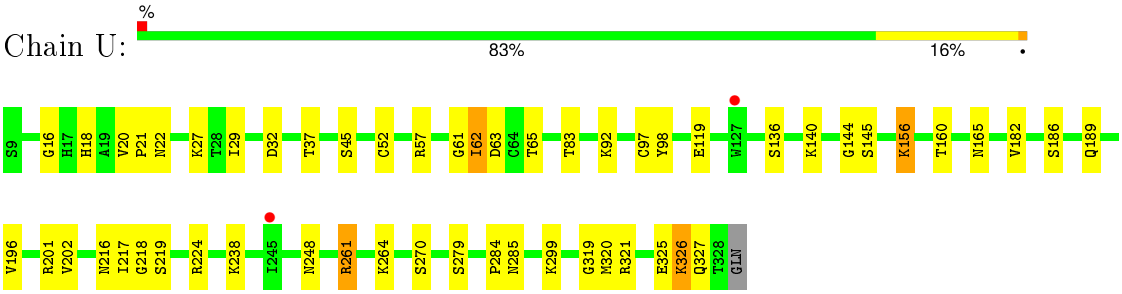
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



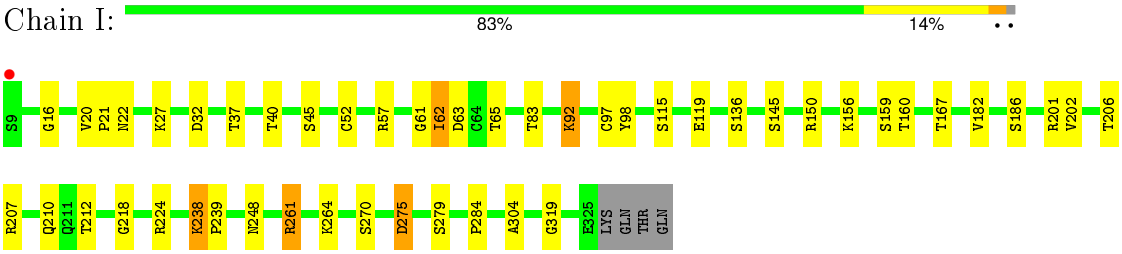

- Molecule 1: Hemagglutinin HA1 chain

Chain U:



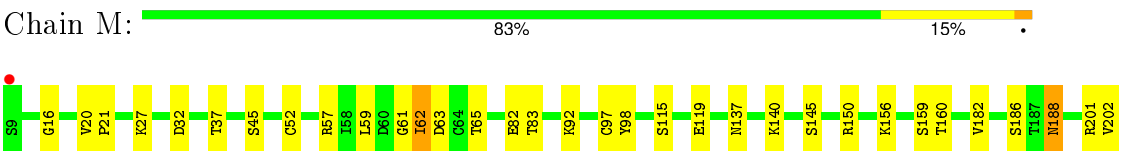

- Molecule 1: Hemagglutinin HA1 chain

Chain I:

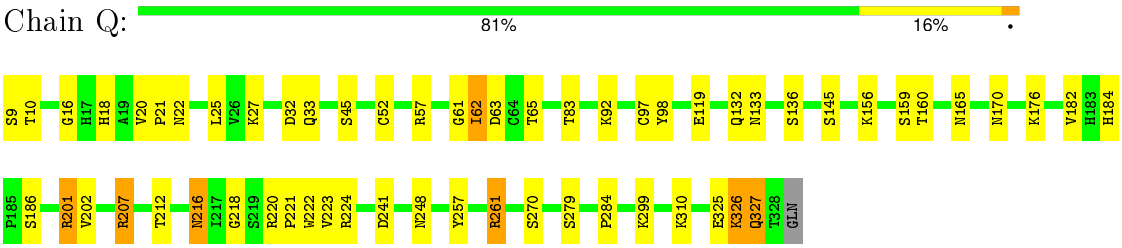



- Molecule 1: Hemagglutinin HA1 chain

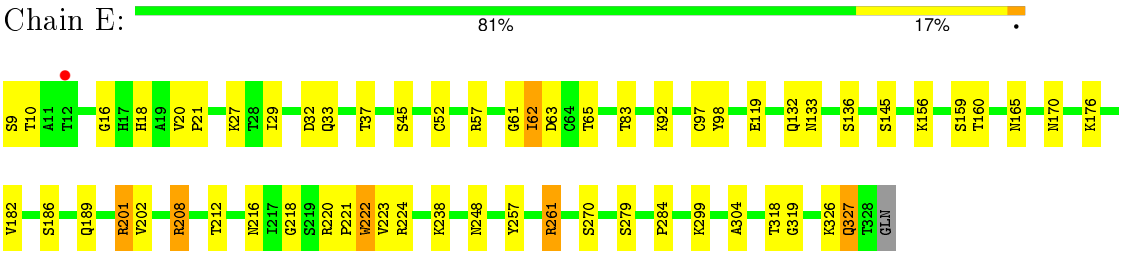
Chain M:



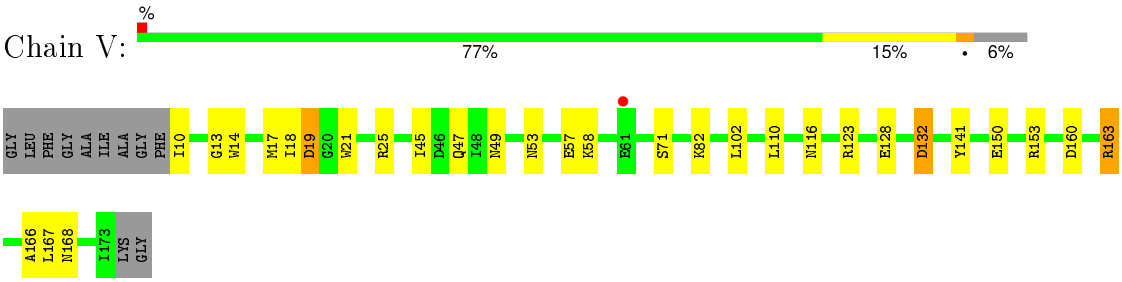

• Molecule 1: Hemagglutinin HA1 chain



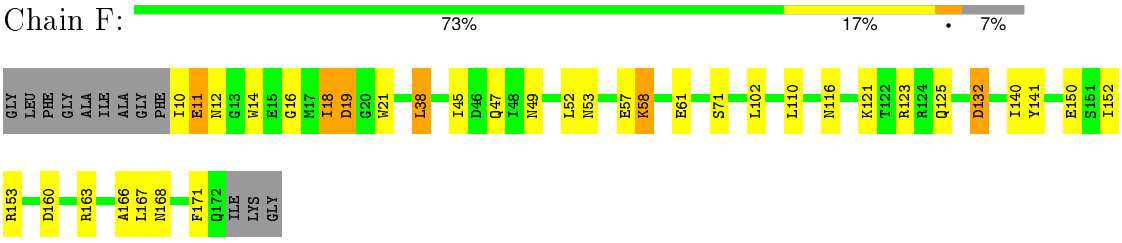

• Molecule 1: Hemagglutinin HA1 chain



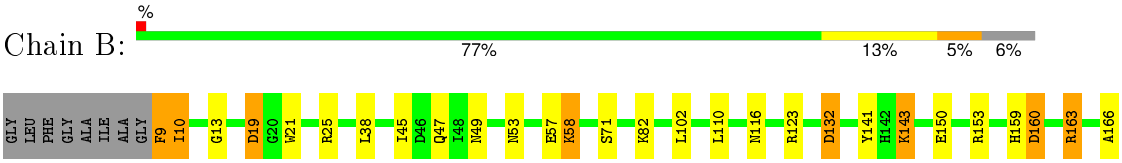

• Molecule 2: Hemagglutinin HA2 chain

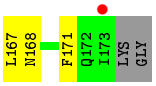



• Molecule 2: Hemagglutinin HA2 chain



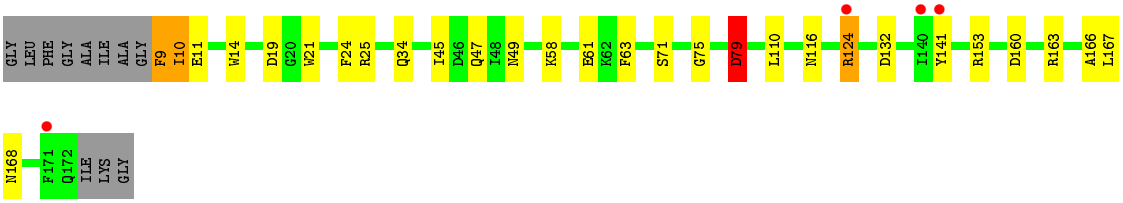

• Molecule 2: Hemagglutinin HA2 chain






• Molecule 2: Hemagglutinin HA2 chain

Chain J:

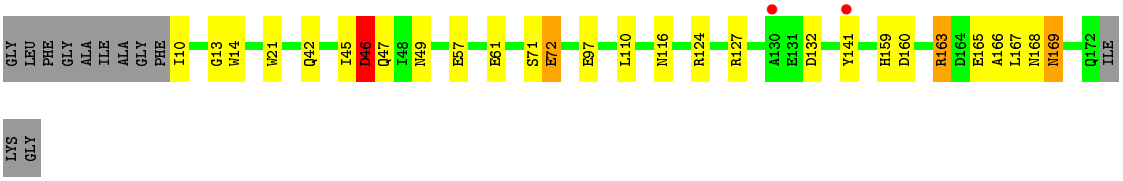







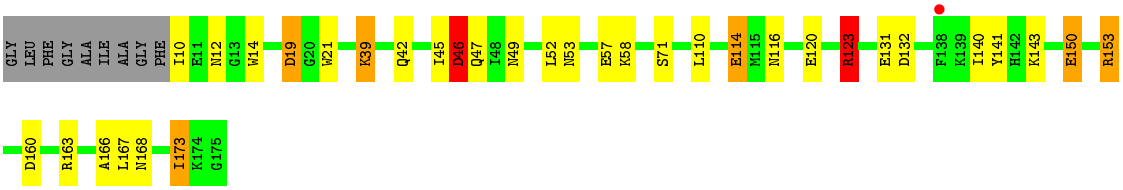
• Molecule 2: Hemagglutinin HA2 chain

Chain N:

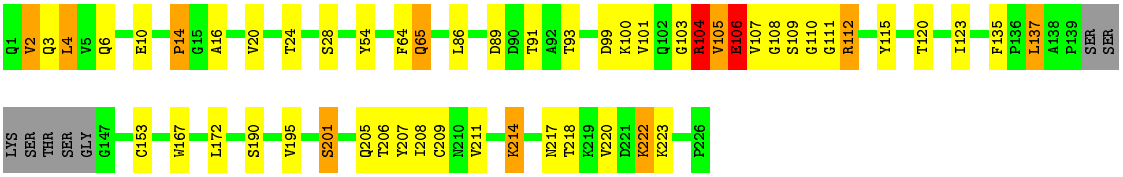

• Molecule 2: Hemagglutinin HA2 chain

Chain R:

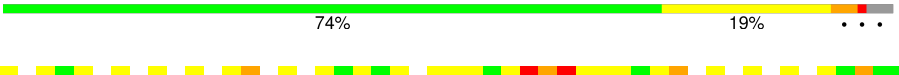

• Molecule 3: monoclonal antibody H chain

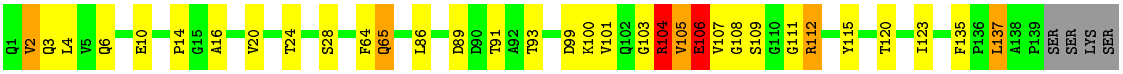
Chain C:

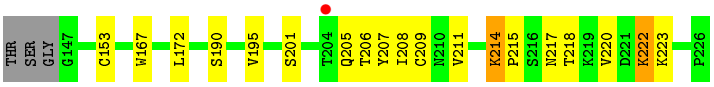




• Molecule 3: monoclonal antibody H chain

Chain Y:

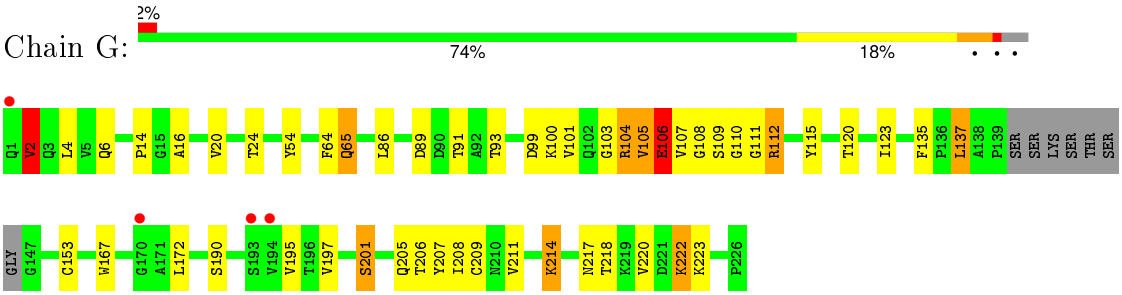




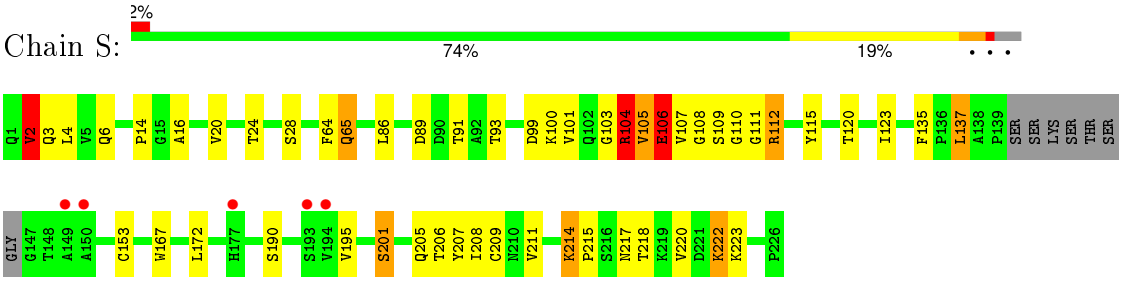
- Molecule 3: monoclonal antibody H chain

Chain G:



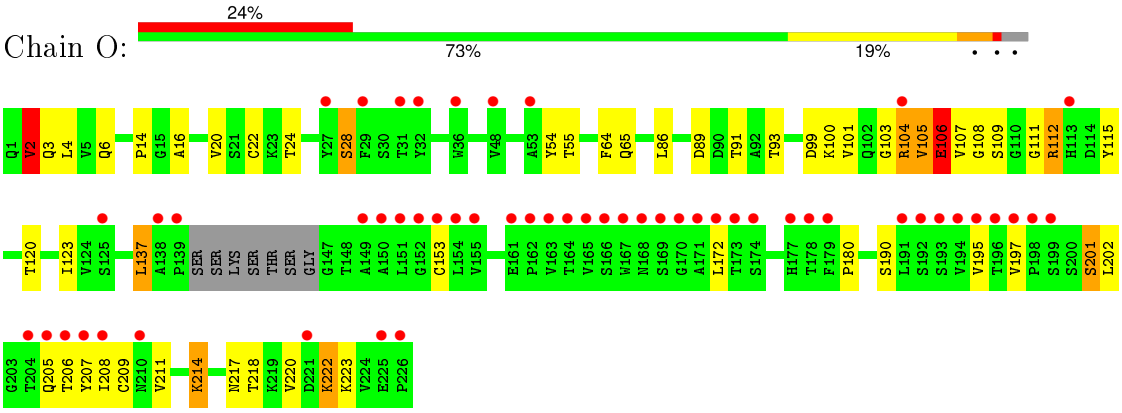
- Molecule 3: monoclonal antibody H chain

Chain S:



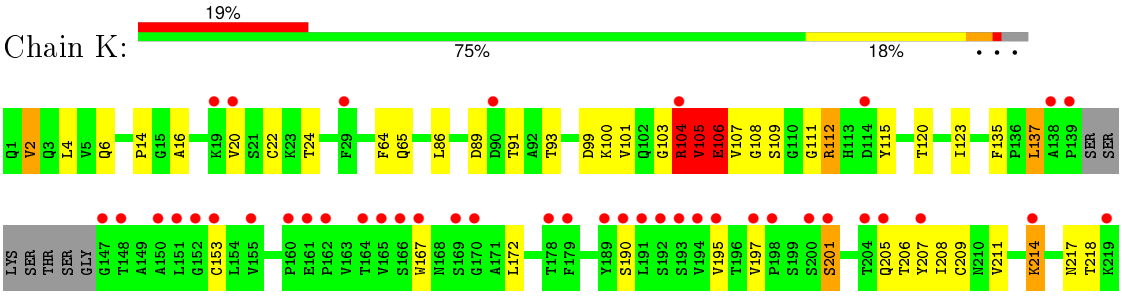
- Molecule 3: monoclonal antibody H chain

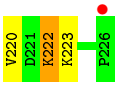
Chain O:



- Molecule 3: monoclonal antibody H chain

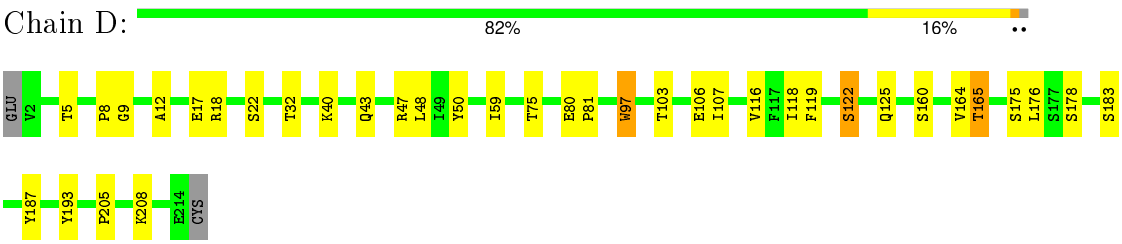
Chain K:





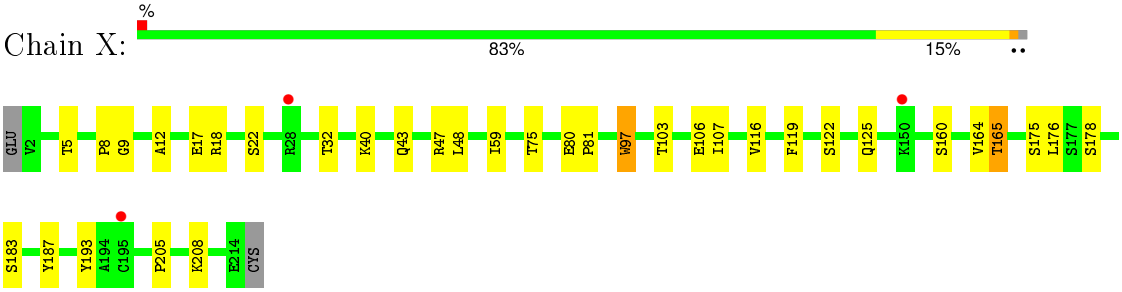

• Molecule 4: monoclonal antibody L chain

Chain D:



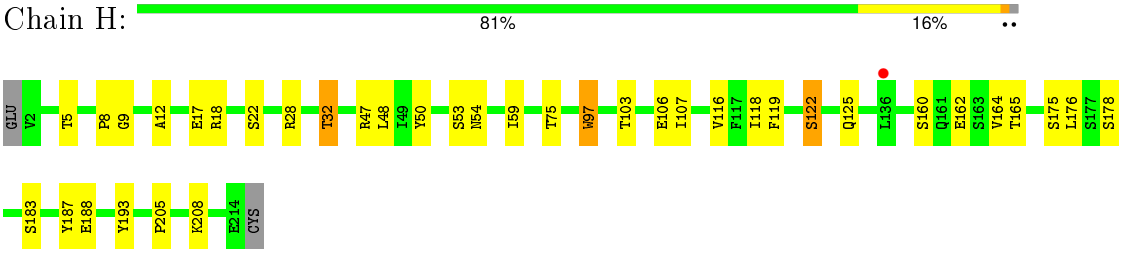

• Molecule 4: monoclonal antibody L chain

Chain X:



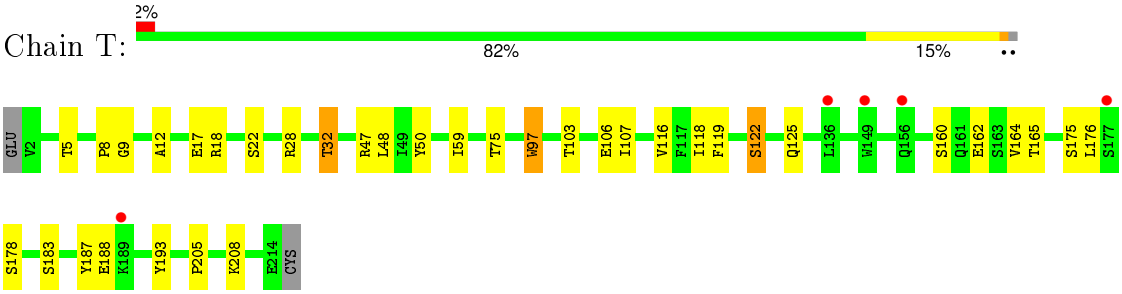

• Molecule 4: monoclonal antibody L chain

Chain H:



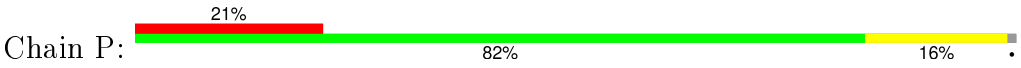

• Molecule 4: monoclonal antibody L chain

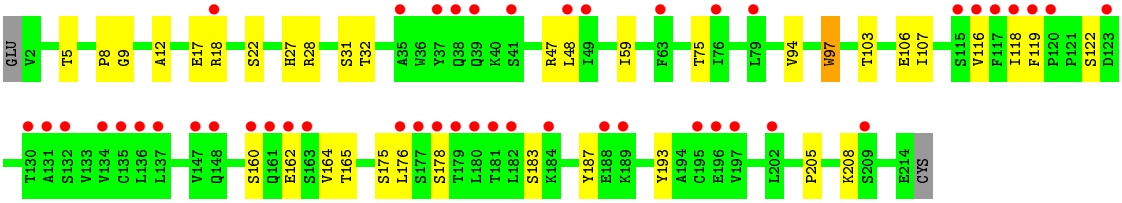
Chain T:




• Molecule 4: monoclonal antibody L chain

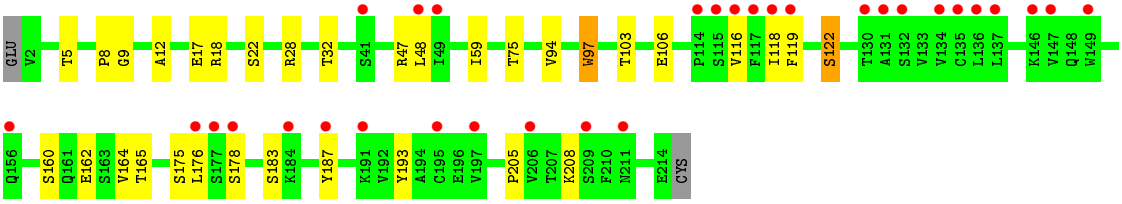
Chain P:






- Molecule 4: monoclonal antibody L chain

Chain L:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 128.70Å 128.70Å 428.32Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 50.00 – 3.50<br>48.26 – 3.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.3 (50.00-3.50)<br>99.4 (48.26-3.50) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.06 (at 3.48Å) | Xtriage |
| Refinement program | REFMAC 5.8.0049 | Depositor |
| R, $R_{free}$ | 0.212 , 0.258<br>0.216 , 0.255 | Depositor<br>DCC |
| $R_{free}$ test set | 4962 reflections (5.25%) | DCC |
| Wilson B-factor (Å$^2$) | 97.5 | Xtriage |
| Anisotropy | 0.212 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 63.4 | EDS |
| Estimated twinning fraction | 0.006 for -h,-k,l<br>0.410 for h,-h-k,-l<br>0.018 for -k,-h,-l | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Outliers | 0 of 99485 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 43086 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 117.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, NAG, MAN

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 | 0.60 | 0/2526 | 0.80 | 5/3442 (0.1%) |
| 1 | E | 0.61 | 0/2526 | 0.76 | 1/3442 (0.0%) |
| 1 | I | 0.64 | 1/2501 (0.0%) | 0.77 | 2/3409 (0.1%) |
| 1 | M | 0.62 | 1/2526 (0.0%) | 0.77 | 2/3442 (0.1%) |
| 1 | Q | 0.61 | 0/2526 | 0.78 | 2/3442 (0.1%) |
| 1 | U | 0.61 | 0/2526 | 0.78 | 1/3442 (0.0%) |
| 2 | B | 0.77 | 3/1380 (0.2%) | 0.92 | 6/1855 (0.3%) |
| 2 | F | 0.74 | 3/1360 (0.2%) | 0.92 | 4/1828 (0.2%) |
| 2 | J | 0.72 | 1/1372 (0.1%) | 0.89 | 5/1844 (0.3%) |
| 2 | N | 0.74 | 1/1360 (0.1%) | 0.95 | 5/1828 (0.3%) |
| 2 | R | 0.74 | 2/1381 (0.1%) | 1.05 | 10/1855 (0.5%) |
| 2 | V | 0.78 | 4/1368 (0.3%) | 0.92 | 6/1839 (0.3%) |
| 3 | C | 0.62 | 0/1677 | 0.79 | 3/2289 (0.1%) |
| 3 | G | 0.59 | 0/1677 | 0.78 | 1/2289 (0.0%) |
| 3 | K | 0.53 | 0/1677 | 0.75 | 2/2289 (0.1%) |
| 3 | O | 0.53 | 0/1677 | 0.75 | 1/2289 (0.0%) |
| 3 | S | 0.59 | 0/1677 | 0.78 | 2/2289 (0.1%) |
| 3 | Y | 0.62 | 0/1677 | 0.79 | 3/2289 (0.1%) |
| 4 | D | 0.61 | 1/1687 (0.1%) | 0.76 | 1/2292 (0.0%) |
| 4 | H | 0.62 | 1/1687 (0.1%) | 0.76 | 1/2292 (0.0%) |
| 4 | L | 0.49 | 1/1687 (0.1%) | 0.71 | 1/2292 (0.0%) |
| 4 | P | 0.50 | 1/1687 (0.1%) | 0.72 | 1/2292 (0.0%) |
| 4 | T | 0.62 | 1/1687 (0.1%) | 0.76 | 1/2292 (0.0%) |
| 4 | X | 0.62 | 1/1687 (0.1%) | 0.76 | 1/2292 (0.0%) |
| All | All | 0.63 | 22/43536 (0.1%) | 0.80 | 67/59154 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 3 | C | 0 | 1 |
| 3 | G | 0 | 1 |
| 3 | K | 0 | 1 |
| 3 | O | 0 | 1 |
| 3 | S | 0 | 1 |
| 3 | Y | 0 | 1 |
| All | All | 0 | 6 |

All (22) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | I | 275 | ASP | CB-CG | 7.09 | 1.66 | 1.51 |
| 4 | L | 97 | TRP | CB-CG | 6.63 | 1.62 | 1.50 |
| 1 | M | 275 | ASP | CB-CG | 6.58 | 1.65 | 1.51 |
| 2 | V | 10 | ILE | CA-CB | 6.55 | 1.70 | 1.54 |
| 2 | V | 19 | ASP | CB-CG | 6.29 | 1.65 | 1.51 |
| 2 | J | 160 | ASP | CB-CG | 6.16 | 1.64 | 1.51 |
| 4 | P | 97 | TRP | CB-CG | 6.14 | 1.61 | 1.50 |
| 2 | N | 160 | ASP | CB-CG | 6.13 | 1.64 | 1.51 |
| 4 | T | 97 | TRP | CB-CG | 6.13 | 1.61 | 1.50 |
| 2 | B | 160 | ASP | CB-CG | 6.04 | 1.64 | 1.51 |
| 4 | H | 97 | TRP | CB-CG | 5.99 | 1.61 | 1.50 |
| 2 | B | 19 | ASP | CB-CG | 5.94 | 1.64 | 1.51 |
| 2 | V | 160 | ASP | CB-CG | 5.87 | 1.64 | 1.51 |
| 2 | R | 160 | ASP | CB-CG | 5.79 | 1.64 | 1.51 |
| 2 | R | 19 | ASP | CB-CG | 5.78 | 1.63 | 1.51 |
| 2 | F | 160 | ASP | CB-CG | 5.76 | 1.63 | 1.51 |
| 2 | V | 150 | GLU | CG-CD | 5.73 | 1.60 | 1.51 |
| 2 | B | 150 | GLU | CG-CD | 5.61 | 1.60 | 1.51 |
| 2 | F | 19 | ASP | CB-CG | 5.47 | 1.63 | 1.51 |
| 4 | D | 97 | TRP | CB-CG | 5.24 | 1.59 | 1.50 |
| 4 | X | 97 | TRP | CB-CG | 5.23 | 1.59 | 1.50 |
| 2 | F | 150 | GLU | CG-CD | 5.01 | 1.59 | 1.51 |

All (67) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | R | 19 | ASP | CB-CG-OD2 | 16.74 | 133.37 | 118.30 |
| 1 | U | 156 | LYS | CB-CA-C | -8.49 | 93.43 | 110.40 |
| 2 | V | 82 | LYS | CD-CE-NZ | 8.34 | 130.89 | 111.70 |
| 2 | R | 123 | ARG | NE-CZ-NH1 | 8.32 | 124.46 | 120.30 |
| 2 | R | 46 | ASP | N-CA-CB | 8.28 | 125.51 | 110.60 |
| 2 | N | 46 | ASP | N-CA-CB | 8.13 | 125.23 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | N | 163 | ARG | NE-CZ-NH1 | 7.68 | 124.14 | 120.30 |
| 2 | J | 124 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | Q | 207 | ARG | NE-CZ-NH1 | 6.99 | 123.80 | 120.30 |
| 1 | A | 27 | LYS | CD-CE-NZ | 6.90 | 127.57 | 111.70 |
| 2 | N | 160 | ASP | CB-CG-OD2 | 6.46 | 124.11 | 118.30 |
| 2 | B | 160 | ASP | CB-CG-OD2 | 6.42 | 124.08 | 118.30 |
| 2 | F | 160 | ASP | CB-CG-OD2 | 6.39 | 124.05 | 118.30 |
| 2 | B | 163 | ARG | NE-CZ-NH1 | 6.25 | 123.42 | 120.30 |
| 2 | N | 163 | ARG | NE-CZ-NH2 | -6.19 | 117.21 | 120.30 |
| 2 | R | 160 | ASP | CB-CG-OD2 | 6.17 | 123.85 | 118.30 |
| 2 | R | 114 | GLU | N-CA-CB | 6.06 | 121.50 | 110.60 |
| 2 | J | 11 | GLU | CB-CA-C | -6.04 | 98.33 | 110.40 |
| 3 | Y | 104 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 2 | R | 123 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 2 | R | 153 | ARG | NE-CZ-NH2 | -5.85 | 117.37 | 120.30 |
| 2 | V | 163 | ARG | NE-CZ-NH1 | 5.85 | 123.22 | 120.30 |
| 1 | A | 92 | LYS | CB-CA-C | -5.82 | 98.76 | 110.40 |
| 2 | J | 79 | ASP | N-CA-CB | 5.80 | 121.03 | 110.60 |
| 2 | V | 160 | ASP | CB-CG-OD2 | 5.79 | 123.51 | 118.30 |
| 2 | R | 19 | ASP | OD1-CG-OD2 | -5.75 | 112.38 | 123.30 |
| 1 | M | 275 | ASP | CB-CG-OD2 | 5.71 | 123.44 | 118.30 |
| 1 | I | 275 | ASP | CB-CG-OD2 | 5.70 | 123.43 | 118.30 |
| 3 | C | 104 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 3 | Y | 10 | GLU | OE1-CD-OE2 | -5.64 | 116.53 | 123.30 |
| 3 | Y | 2 | VAL | CB-CA-C | -5.63 | 100.69 | 111.40 |
| 3 | G | 2 | VAL | CB-CA-C | -5.62 | 100.72 | 111.40 |
| 2 | V | 153 | ARG | NE-CZ-NH2 | -5.61 | 117.49 | 120.30 |
| 2 | R | 39 | LYS | CB-CA-C | 5.59 | 121.58 | 110.40 |
| 3 | C | 2 | VAL | CB-CA-C | -5.59 | 100.78 | 111.40 |
| 3 | O | 2 | VAL | CB-CA-C | -5.53 | 100.89 | 111.40 |
| 2 | V | 25 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 2 | B | 153 | ARG | NE-CZ-NH2 | -5.45 | 117.57 | 120.30 |
| 1 | I | 150 | ARG | NE-CZ-NH2 | -5.45 | 117.58 | 120.30 |
| 2 | B | 163 | ARG | NE-CZ-NH2 | -5.42 | 117.59 | 120.30 |
| 1 | A | 307 | LYS | CD-CE-NZ | 5.41 | 124.15 | 111.70 |
| 4 | T | 97 | TRP | CA-CB-CG | 5.40 | 123.95 | 113.70 |
| 2 | J | 160 | ASP | CB-CG-OD2 | 5.38 | 123.14 | 118.30 |
| 1 | A | 140 | LYS | CA-CB-CG | -5.37 | 101.58 | 113.40 |
| 1 | M | 150 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 3 | S | 104 | ARG | NE-CZ-NH1 | 5.32 | 122.96 | 120.30 |
| 3 | S | 2 | VAL | CB-CA-C | -5.32 | 101.30 | 111.40 |
| 4 | X | 97 | TRP | CA-CB-CG | 5.31 | 123.80 | 113.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | E | 222 | TRP | CA-CB-CG | 5.30 | 123.78 | 113.70 |
| 3 | K | 2 | VAL | CB-CA-C | -5.30 | 101.32 | 111.40 |
| 2 | F | 153 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 4 | H | 97 | TRP | CA-CB-CG | 5.25 | 123.68 | 113.70 |
| 2 | F | 132 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 2 | B | 132 | ASP | CB-CG-OD2 | 5.23 | 123.00 | 118.30 |
| 2 | V | 132 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 2 | N | 132 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 2 | J | 132 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 4 | L | 97 | TRP | CA-CB-CG | 5.19 | 123.56 | 113.70 |
| 2 | F | 150 | GLU | OE1-CD-OE2 | -5.18 | 117.08 | 123.30 |
| 2 | R | 132 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 4 | P | 97 | TRP | CA-CB-CG | 5.17 | 123.53 | 113.70 |
| 1 | Q | 207 | ARG | N-CA-CB | 5.16 | 119.89 | 110.60 |
| 4 | D | 97 | TRP | CA-CB-CG | 5.16 | 123.50 | 113.70 |
| 3 | C | 10 | GLU | OE1-CD-OE2 | -5.09 | 117.19 | 123.30 |
| 2 | B | 25 | ARG | NE-CZ-NH1 | 5.09 | 122.85 | 120.30 |
| 3 | K | 104 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 1 | A | 207 | ARG | N-CA-CB | 5.05 | 119.70 | 110.60 |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 3 | C | 106 | GLU | Peptide |
| 3 | G | 106 | GLU | Peptide |
| 3 | K | 106 | GLU | Peptide |
| 3 | O | 106 | GLU | Peptide |
| 3 | S | 106 | GLU | Peptide |
| 3 | Y | 106 | GLU | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2470 | 0 | 2419 | 57 | 0 |
| 1 | E | 2470 | 0 | 2422 | 48 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | I | 2445 | 0 | 2393 | 30 | 1 |
| 1 | M | 2470 | 0 | 2421 | 36 | 1 |
| 1 | Q | 2470 | 0 | 2420 | 45 | 0 |
| 1 | U | 2470 | 0 | 2421 | 46 | 0 |
| 2 | B | 1357 | 0 | 1275 | 23 | 0 |
| 2 | F | 1338 | 0 | 1255 | 26 | 0 |
| 2 | J | 1349 | 0 | 1264 | 17 | 0 |
| 2 | N | 1338 | 0 | 1255 | 20 | 0 |
| 2 | R | 1359 | 0 | 1282 | 23 | 0 |
| 2 | V | 1346 | 0 | 1265 | 13 | 0 |
| 3 | C | 1637 | 0 | 1610 | 55 | 0 |
| 3 | G | 1637 | 0 | 1610 | 52 | 0 |
| 3 | K | 1637 | 0 | 1610 | 48 | 0 |
| 3 | O | 1637 | 0 | 1610 | 48 | 0 |
| 3 | S | 1637 | 0 | 1610 | 59 | 0 |
| 3 | Y | 1637 | 0 | 1610 | 52 | 0 |
| 4 | D | 1650 | 0 | 1602 | 20 | 0 |
| 4 | H | 1650 | 0 | 1602 | 24 | 1 |
| 4 | L | 1650 | 0 | 1602 | 23 | 0 |
| 4 | P | 1650 | 0 | 1602 | 23 | 0 |
| 4 | T | 1650 | 0 | 1602 | 23 | 1 |
| 4 | X | 1650 | 0 | 1602 | 17 | 0 |
| 5 | A | 98 | 0 | 87 | 1 | 0 |
| 5 | E | 28 | 0 | 24 | 0 | 0 |
| 5 | F | 14 | 0 | 13 | 0 | 0 |
| 5 | I | 42 | 0 | 37 | 4 | 0 |
| 5 | M | 42 | 0 | 37 | 0 | 0 |
| 5 | Q | 70 | 0 | 62 | 7 | 0 |
| 5 | U | 42 | 0 | 37 | 5 | 0 |
| 5 | V | 14 | 0 | 13 | 0 | 0 |
| 6 | A | 11 | 0 | 9 | 0 | 0 |
| 6 | E | 11 | 0 | 9 | 1 | 0 |
| 6 | I | 11 | 0 | 9 | 0 | 0 |
| 6 | M | 11 | 0 | 9 | 0 | 0 |
| 6 | Q | 11 | 0 | 9 | 0 | 0 |
| 6 | U | 11 | 0 | 9 | 1 | 0 |
| 7 | A | 11 | 0 | 10 | 0 | 0 |
| 7 | E | 11 | 0 | 10 | 1 | 0 |
| 7 | I | 11 | 0 | 10 | 0 | 0 |
| 7 | M | 11 | 0 | 10 | 0 | 0 |
| 7 | Q | 11 | 0 | 10 | 0 | 0 |
| 7 | U | 11 | 0 | 10 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| All | All | 43086 | 0 | 41788 | 704 | 2 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (704) 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) |
|---|---|---|---|
| 1:U:285:ASN:ND2 | 5:U:405:NAG:C1 | 1.71 | 1.51 |
| 1:U:156:LYS:HE2 | 1:U:196:VAL:CG2 | 1.66 | 1.25 |
| 1:A:140:LYS:HD2 | 1:A:140:LYS:N | 1.33 | 1.22 |
| 1:U:156:LYS:CE | 1:U:196:VAL:HG23 | 1.75 | 1.16 |
| 3:G:208:ILE:HA | 3:G:223:LYS:HD3 | 1.21 | 1.11 |
| 3:S:208:ILE:HA | 3:S:223:LYS:HD3 | 1.22 | 1.10 |
| 3:Y:208:ILE:HA | 3:Y:223:LYS:HD3 | 1.21 | 1.10 |
| 3:C:208:ILE:HA | 3:C:223:LYS:HD3 | 1.20 | 1.10 |
| 3:O:208:ILE:HA | 3:O:223:LYS:HD3 | 1.23 | 1.09 |
| 2:R:120:GLU:OE1 | 2:R:123:ARG:NH1 | 1.86 | 1.08 |
| 3:K:208:ILE:HA | 3:K:223:LYS:HD3 | 1.22 | 1.07 |
| 1:A:137:ASN:HA | 1:A:140:LYS:HE2 | 1.39 | 1.03 |
| 2:V:49:ASN:OD1 | 3:Y:106:GLU:HB3 | 1.60 | 1.01 |
| 2:B:49:ASN:OD1 | 3:C:106:GLU:HB3 | 1.63 | 0.98 |
| 1:A:140:LYS:CD | 1:A:140:LYS:N | 2.27 | 0.97 |
| 1:U:156:LYS:HE2 | 1:U:196:VAL:HG23 | 0.98 | 0.96 |
| 1:A:27:LYS:HD2 | 1:A:32:ASP:O | 1.66 | 0.96 |
| 3:S:107:VAL:HB | 3:S:108:GLY:HA2 | 1.47 | 0.95 |
| 3:C:208:ILE:HA | 3:C:223:LYS:CD | 1.97 | 0.94 |
| 1:M:212:THR:HB | 1:Q:216:ASN:HD22 | 1.32 | 0.94 |
| 3:Y:208:ILE:HA | 3:Y:223:LYS:CD | 1.97 | 0.93 |
| 3:G:107:VAL:HB | 3:G:108:GLY:HA2 | 1.49 | 0.93 |
| 2:V:49:ASN:OD1 | 3:Y:106:GLU:CB | 2.17 | 0.93 |
| 3:G:208:ILE:HA | 3:G:223:LYS:CD | 1.99 | 0.92 |
| 3:S:208:ILE:HA | 3:S:223:LYS:CD | 1.99 | 0.92 |
| 3:O:208:ILE:HA | 3:O:223:LYS:CD | 2.00 | 0.91 |
| 1:A:136:SER:O | 1:A:140:LYS:NZ | 2.02 | 0.91 |
| 1:A:139:CYS:C | 1:A:140:LYS:HD2 | 1.91 | 0.91 |
| 3:C:107:VAL:HB | 3:C:108:GLY:HA2 | 1.50 | 0.91 |
| 3:O:107:VAL:HB | 3:O:108:GLY:HA2 | 1.50 | 0.91 |
| 3:K:107:VAL:HB | 3:K:108:GLY:HA2 | 1.49 | 0.90 |
| 3:Y:107:VAL:HB | 3:Y:108:GLY:HA2 | 1.49 | 0.90 |
| 3:K:208:ILE:HA | 3:K:223:LYS:CD | 2.00 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:49:ASN:OD1 | 3:C:106:GLU:CB | 2.20 | 0.90 |
| 2:B:9:PHE:CE1 | 2:B:10:ILE:HD11 | 2.07 | 0.89 |
| 1:Q:27:LYS:HE3 | 4:P:28:ARG:HG3 | 1.55 | 0.89 |
| 2:J:9:PHE:CE1 | 2:J:10:ILE:HD11 | 2.09 | 0.88 |
| 2:R:150:GLU:OE1 | 2:R:150:GLU:HA | 1.71 | 0.87 |
| 1:A:27:LYS:HE2 | 1:A:33:GLN:HE22 | 1.41 | 0.85 |
| 1:A:140:LYS:HE2 | 1:A:145:SER:HB2 | 1.59 | 0.85 |
| 5:Q:406:NAG:C8 | 3:S:104:ARG:HH21 | 1.90 | 0.84 |
| 1:E:27:LYS:HE3 | 4:L:28:ARG:HG3 | 1.59 | 0.84 |
| 1:E:33:GLN:HB2 | 4:L:94:VAL:HG22 | 1.61 | 0.83 |
| 3:S:107:VAL:HB | 3:S:108:GLY:CA | 2.09 | 0.83 |
| 2:R:49:ASN:OD1 | 3:S:106:GLU:HB3 | 1.78 | 0.82 |
| 2:F:49:ASN:OD1 | 3:G:106:GLU:HB3 | 1.80 | 0.82 |
| 2:N:127:ARG:HE | 2:N:159:HIS:CE1 | 1.97 | 0.82 |
| 1:U:285:ASN:ND2 | 5:U:405:NAG:O5 | 2.10 | 0.82 |
| 3:Y:107:VAL:HB | 3:Y:108:GLY:CA | 2.09 | 0.81 |
| 3:G:107:VAL:HB | 3:G:108:GLY:CA | 2.10 | 0.81 |
| 1:U:285:ASN:CG | 5:U:405:NAG:C1 | 2.48 | 0.81 |
| 1:I:40:THR:HA | 5:I:405:NAG:H82 | 1.63 | 0.80 |
| 3:C:107:VAL:HB | 3:C:108:GLY:CA | 2.11 | 0.80 |
| 1:U:156:LYS:HE3 | 1:U:196:VAL:N | 1.97 | 0.79 |
| 2:R:150:GLU:OE1 | 2:R:150:GLU:CA | 2.32 | 0.78 |
| 2:J:49:ASN:OD1 | 3:K:106:GLU:HB3 | 1.83 | 0.77 |
| 3:K:107:VAL:HB | 3:K:108:GLY:CA | 2.14 | 0.77 |
| 1:U:156:LYS:CD | 1:U:196:VAL:HG23 | 2.13 | 0.77 |
| 3:O:107:VAL:HB | 3:O:108:GLY:CA | 2.14 | 0.77 |
| 1:A:137:ASN:C | 1:A:140:LYS:HD3 | 2.06 | 0.75 |
| 1:E:33:GLN:HG2 | 4:L:94:VAL:HG21 | 1.68 | 0.75 |
| 3:C:208:ILE:CA | 3:C:223:LYS:HD3 | 2.11 | 0.74 |
| 2:R:150:GLU:OE2 | 2:R:153:ARG:NH2 | 2.21 | 0.74 |
| 1:A:27:LYS:HE3 | 4:H:28:ARG:HG3 | 1.70 | 0.74 |
| 1:A:216:ASN:CG | 1:E:212:THR:HG21 | 2.09 | 0.74 |
| 1:A:137:ASN:HA | 1:A:140:LYS:CE | 2.15 | 0.73 |
| 3:G:209:CYS:SG | 3:G:223:LYS:NZ | 2.63 | 0.72 |
| 1:A:207:ARG:NH1 | 1:A:242:VAL:HG12 | 2.04 | 0.72 |
| 3:S:209:CYS:SG | 3:S:223:LYS:NZ | 2.63 | 0.72 |
| 3:O:209:CYS:SG | 3:O:223:LYS:NZ | 2.63 | 0.72 |
| 1:U:216:ASN:CG | 1:Q:212:THR:HG21 | 2.11 | 0.72 |
| 1:A:140:LYS:HE3 | 1:A:145:SER:HA | 1.72 | 0.71 |
| 3:K:209:CYS:SG | 3:K:223:LYS:NZ | 2.63 | 0.71 |
| 2:R:49:ASN:OD1 | 3:S:106:GLU:CB | 2.37 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:27:LYS:HE2 | 1:A:33:GLN:NE2 | 2.03 | 0.71 |
| 3:G:208:ILE:CA | 3:G:223:LYS:HD3 | 2.12 | 0.70 |
| 3:S:208:ILE:CA | 3:S:223:LYS:HD3 | 2.13 | 0.70 |
| 3:C:209:CYS:SG | 3:C:223:LYS:NZ | 2.64 | 0.70 |
| 3:Y:209:CYS:SG | 3:Y:223:LYS:NZ | 2.64 | 0.70 |
| 1:U:238:LYS:HE3 | 2:N:72:GLU:OE1 | 1.92 | 0.70 |
| 2:N:127:ARG:NH2 | 2:R:131:GLU:OE1 | 2.25 | 0.70 |
| 2:N:49:ASN:OD1 | 3:O:106:GLU:HB3 | 1.92 | 0.70 |
| 2:F:49:ASN:OD1 | 3:G:106:GLU:CB | 2.39 | 0.69 |
| 1:Q:33:GLN:HB2 | 4:P:94:VAL:HG22 | 1.73 | 0.69 |
| 3:Y:99:ASP:OD1 | 3:Y:112:ARG:HD3 | 1.92 | 0.69 |
| 5:Q:406:NAG:H81 | 3:S:104:ARG:HH21 | 1.57 | 0.69 |
| 1:E:33:GLN:CB | 4:L:94:VAL:HG22 | 2.22 | 0.69 |
| 1:A:140:LYS:HE3 | 1:A:145:SER:CA | 2.23 | 0.69 |
| 1:A:137:ASN:O | 1:A:140:LYS:HD3 | 1.92 | 0.69 |
| 3:Y:208:ILE:CA | 3:Y:223:LYS:HD3 | 2.12 | 0.69 |
| 3:O:208:ILE:CA | 3:O:223:LYS:HD3 | 2.14 | 0.69 |
| 3:S:99:ASP:OD1 | 3:S:112:ARG:HD3 | 1.93 | 0.69 |
| 3:G:99:ASP:OD1 | 3:G:112:ARG:HD3 | 1.93 | 0.69 |
| 3:K:208:ILE:CA | 3:K:223:LYS:HD3 | 2.13 | 0.68 |
| 3:C:99:ASP:OD1 | 3:C:112:ARG:HD3 | 1.94 | 0.68 |
| 3:K:99:ASP:OD1 | 3:K:112:ARG:HD3 | 1.94 | 0.68 |
| 1:A:140:LYS:CE | 1:A:145:SER:HB2 | 2.23 | 0.67 |
| 3:C:207:TYR:C | 3:C:223:LYS:HE2 | 2.14 | 0.67 |
| 3:O:99:ASP:OD1 | 3:O:112:ARG:HD3 | 1.95 | 0.66 |
| 3:S:207:TYR:C | 3:S:223:LYS:HE2 | 2.16 | 0.66 |
| 3:G:207:TYR:C | 3:G:223:LYS:HE2 | 2.16 | 0.66 |
| 1:M:212:THR:CB | 1:Q:216:ASN:HD22 | 2.07 | 0.66 |
| 1:U:156:LYS:CE | 1:U:196:VAL:N | 2.57 | 0.66 |
| 3:Y:207:TYR:C | 3:Y:223:LYS:HE2 | 2.15 | 0.66 |
| 1:A:136:SER:C | 1:A:140:LYS:NZ | 2.48 | 0.66 |
| 3:G:137:LEU:CD1 | 4:H:119:PHE:CG | 2.78 | 0.65 |
| 1:Q:207:ARG:HG2 | 1:Q:241:ASP:OD1 | 1.96 | 0.65 |
| 1:A:137:ASN:CA | 1:A:140:LYS:HE2 | 2.23 | 0.64 |
| 1:A:219:SER:HB2 | 1:E:165:ASN:OD1 | 1.98 | 0.64 |
| 5:Q:406:NAG:C8 | 3:S:104:ARG:NH2 | 2.61 | 0.64 |
| 1:A:207:ARG:HG2 | 1:A:241:ASP:OD1 | 1.96 | 0.64 |
| 3:S:137:LEU:CD1 | 4:T:119:PHE:CG | 2.80 | 0.64 |
| 1:A:27:LYS:CE | 1:A:33:GLN:HE22 | 2.11 | 0.64 |
| 2:J:75:GLY:O | 2:J:79:ASP:OD1 | 2.16 | 0.64 |
| 1:U:219:SER:HB2 | 1:Q:165:ASN:OD1 | 1.98 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:27:LYS:HE3 | 2:N:97:GLU:OE2 | 1.99 | 0.63 |
| 3:G:137:LEU:HD11 | 4:H:119:PHE:CG | 2.33 | 0.63 |
| 2:B:9:PHE:CE1 | 2:B:10:ILE:CD1 | 2.80 | 0.63 |
| 2:J:9:PHE:CE1 | 2:J:10:ILE:CD1 | 2.82 | 0.63 |
| 1:U:140:LYS:HG2 | 1:U:144:GLY:O | 1.98 | 0.63 |
| 1:A:217:ILE:O | 1:E:201:ARG:CZ | 2.45 | 0.63 |
| 3:K:207:TYR:C | 3:K:223:LYS:HE2 | 2.20 | 0.62 |
| 1:E:27:LYS:HG2 | 1:E:32:ASP:O | 1.98 | 0.62 |
| 1:Q:33:GLN:HG2 | 4:P:94:VAL:HG21 | 1.81 | 0.62 |
| 1:I:27:LYS:HG2 | 1:I:32:ASP:O | 1.99 | 0.62 |
| 1:U:217:ILE:O | 1:Q:201:ARG:CZ | 2.46 | 0.62 |
| 1:U:27:LYS:HG2 | 1:U:32:ASP:O | 1.98 | 0.62 |
| 1:Q:27:LYS:HG2 | 1:Q:32:ASP:O | 1.98 | 0.62 |
| 3:Y:201:SER:O | 3:Y:205:GLN:NE2 | 2.32 | 0.62 |
| 3:O:137:LEU:CD1 | 4:P:119:PHE:CG | 2.83 | 0.62 |
| 3:C:201:SER:O | 3:C:205:GLN:NE2 | 2.32 | 0.62 |
| 3:O:207:TYR:C | 3:O:223:LYS:HE2 | 2.20 | 0.61 |
| 2:V:53:ASN:HD21 | 3:Y:108:GLY:HA2 | 1.64 | 0.61 |
| 3:C:137:LEU:CD1 | 4:D:119:PHE:CG | 2.84 | 0.61 |
| 3:O:201:SER:O | 3:O:205:GLN:NE2 | 2.34 | 0.61 |
| 1:M:212:THR:HB | 1:Q:216:ASN:ND2 | 2.12 | 0.60 |
| 3:S:201:SER:O | 3:S:205:GLN:NE2 | 2.34 | 0.60 |
| 3:G:201:SER:O | 3:G:205:GLN:NE2 | 2.34 | 0.60 |
| 1:U:156:LYS:HE3 | 1:U:196:VAL:H | 1.63 | 0.60 |
| 3:S:137:LEU:HD11 | 4:T:119:PHE:CG | 2.36 | 0.60 |
| 1:I:97:CYS:O | 1:I:224:ARG:NH1 | 2.35 | 0.60 |
| 3:C:207:TYR:O | 3:C:223:LYS:HG3 | 2.02 | 0.60 |
| 1:A:37:THR:HG23 | 1:A:319:GLY:HA3 | 1.83 | 0.60 |
| 3:K:201:SER:O | 3:K:205:GLN:NE2 | 2.34 | 0.60 |
| 3:O:111:GLY:HA2 | 3:O:112:ARG:HB2 | 1.84 | 0.60 |
| 1:A:140:LYS:HE3 | 1:A:146:GLY:H | 1.67 | 0.60 |
| 3:O:223:LYS:HA | 3:O:223:LYS:CE | 2.32 | 0.60 |
| 3:Y:207:TYR:O | 3:Y:223:LYS:HG3 | 2.02 | 0.60 |
| 1:M:97:CYS:O | 1:M:224:ARG:NH1 | 2.35 | 0.60 |
| 5:A:405:NAG:O7 | 3:C:105:VAL:CG1 | 2.50 | 0.60 |
| 1:U:156:LYS:HD2 | 1:U:196:VAL:HG23 | 1.84 | 0.59 |
| 3:O:137:LEU:HD11 | 4:P:119:PHE:CG | 2.38 | 0.59 |
| 1:U:37:THR:HG23 | 1:U:319:GLY:HA3 | 1.84 | 0.59 |
| 1:A:182:VAL:HG22 | 1:A:202:VAL:HG21 | 1.84 | 0.59 |
| 3:G:137:LEU:HD11 | 4:H:119:PHE:CD2 | 2.38 | 0.59 |
| 3:O:207:TYR:O | 3:O:223:LYS:HG3 | 2.03 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:K:111:GLY:HA2 | 3:K:112:ARG:HB2 | 1.85 | 0.59 |
| 3:K:223:LYS:HA | 3:K:223:LYS:CE | 2.32 | 0.59 |
| 3:K:207:TYR:O | 3:K:223:LYS:HG3 | 2.02 | 0.59 |
| 1:E:10:THR:HB | 2:F:140:ILE:O | 2.03 | 0.59 |
| 3:G:207:TYR:O | 3:G:223:LYS:HG3 | 2.02 | 0.59 |
| 3:S:207:TYR:O | 3:S:223:LYS:HG3 | 2.02 | 0.59 |
| 3:C:137:LEU:HD11 | 4:D:119:PHE:CD2 | 2.37 | 0.59 |
| 3:O:4:LEU:HD13 | 3:O:24:THR:HG22 | 1.84 | 0.59 |
| 3:G:223:LYS:CE | 3:G:223:LYS:HA | 2.33 | 0.59 |
| 3:C:223:LYS:HA | 3:C:223:LYS:CE | 2.31 | 0.59 |
| 3:G:104:ARG:O | 3:G:105:VAL:O | 2.21 | 0.59 |
| 1:U:325:GLU:HG3 | 2:V:13:GLY:O | 2.03 | 0.59 |
| 3:S:104:ARG:O | 3:S:105:VAL:O | 2.21 | 0.58 |
| 2:N:57:GLU:OE2 | 4:P:31:SER:N | 2.34 | 0.58 |
| 1:Q:184:HIS:CE1 | 1:Q:216:ASN:OD1 | 2.56 | 0.58 |
| 3:Y:137:LEU:CD1 | 4:X:119:PHE:CG | 2.86 | 0.58 |
| 1:I:182:VAL:HG22 | 1:I:202:VAL:HG21 | 1.85 | 0.58 |
| 4:L:164:VAL:HG22 | 4:L:176:LEU:HD13 | 1.85 | 0.58 |
| 3:Y:4:LEU:HD13 | 3:Y:24:THR:HG22 | 1.85 | 0.58 |
| 1:E:37:THR:HG23 | 1:E:319:GLY:HA3 | 1.85 | 0.58 |
| 1:E:97:CYS:O | 1:E:224:ARG:NH1 | 2.35 | 0.58 |
| 1:U:182:VAL:HG22 | 1:U:202:VAL:HG21 | 1.86 | 0.58 |
| 1:A:97:CYS:O | 1:A:224:ARG:NH1 | 2.36 | 0.58 |
| 5:I:405:NAG:H5 | 3:K:105:VAL:HG11 | 1.85 | 0.58 |
| 1:Q:33:GLN:CB | 4:P:94:VAL:HG22 | 2.34 | 0.58 |
| 1:U:97:CYS:O | 1:U:224:ARG:NH1 | 2.36 | 0.58 |
| 3:S:4:LEU:HD13 | 3:S:24:THR:HG22 | 1.85 | 0.58 |
| 3:G:4:LEU:HD13 | 3:G:24:THR:HG22 | 1.84 | 0.58 |
| 1:Q:97:CYS:O | 1:Q:224:ARG:NH1 | 2.35 | 0.58 |
| 1:M:182:VAL:HG22 | 1:M:202:VAL:HG21 | 1.86 | 0.58 |
| 4:P:164:VAL:HG22 | 4:P:176:LEU:HD13 | 1.86 | 0.58 |
| 3:S:218:THR:HG22 | 3:S:220:VAL:HG23 | 1.84 | 0.58 |
| 1:M:27:LYS:HG2 | 1:M:32:ASP:O | 2.04 | 0.58 |
| 3:G:218:THR:HG22 | 3:G:220:VAL:HG23 | 1.84 | 0.58 |
| 1:I:37:THR:HG23 | 1:I:319:GLY:HA3 | 1.86 | 0.58 |
| 1:M:37:THR:HG23 | 1:M:319:GLY:HA3 | 1.86 | 0.58 |
| 3:S:137:LEU:HD11 | 4:T:119:PHE:CD2 | 2.39 | 0.57 |
| 3:S:223:LYS:CE | 3:S:223:LYS:HA | 2.34 | 0.57 |
| 3:K:4:LEU:HD13 | 3:K:24:THR:HG22 | 1.85 | 0.57 |
| 1:Q:182:VAL:HG22 | 1:Q:202:VAL:HG21 | 1.86 | 0.57 |
| 1:U:216:ASN:CB | 1:Q:212:THR:HG21 | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:207:TYR:O | 3:C:223:LYS:HE2 | 2.04 | 0.57 |
| 2:B:53:ASN:HD21 | 3:C:108:GLY:HA2 | 1.68 | 0.57 |
| 4:H:164:VAL:HG22 | 4:H:176:LEU:HD13 | 1.85 | 0.57 |
| 3:Y:207:TYR:O | 3:Y:223:LYS:HE2 | 2.04 | 0.57 |
| 3:O:218:THR:HG22 | 3:O:220:VAL:HG23 | 1.87 | 0.57 |
| 3:G:110:GLY:HA2 | 4:H:50:TYR:CE1 | 2.39 | 0.57 |
| 2:N:42:GLN:O | 2:N:46:ASP:OD1 | 2.23 | 0.57 |
| 1:A:216:ASN:CB | 1:E:212:THR:HG21 | 2.34 | 0.57 |
| 3:Y:223:LYS:CE | 3:Y:223:LYS:HA | 2.33 | 0.57 |
| 3:K:104:ARG:O | 3:K:105:VAL:O | 2.23 | 0.57 |
| 3:C:218:THR:HG22 | 3:C:220:VAL:HG23 | 1.86 | 0.57 |
| 4:T:164:VAL:HG22 | 4:T:176:LEU:HD13 | 1.86 | 0.57 |
| 3:K:218:THR:HG22 | 3:K:220:VAL:HG23 | 1.87 | 0.57 |
| 1:E:176:LYS:HE3 | 1:E:257:TYR:CD2 | 2.39 | 0.57 |
| 1:E:182:VAL:HG22 | 1:E:202:VAL:HG21 | 1.86 | 0.57 |
| 3:S:207:TYR:O | 3:S:223:LYS:HE2 | 2.05 | 0.57 |
| 2:F:38:LEU:HG | 3:G:54:TYR:CZ | 2.39 | 0.57 |
| 3:C:4:LEU:HD13 | 3:C:24:THR:HG22 | 1.86 | 0.57 |
| 3:G:207:TYR:O | 3:G:223:LYS:HE2 | 2.05 | 0.56 |
| 3:Y:104:ARG:O | 3:Y:105:VAL:O | 2.23 | 0.56 |
| 3:Y:137:LEU:HD11 | 4:X:119:PHE:CD2 | 2.40 | 0.56 |
| 3:K:207:TYR:O | 3:K:223:LYS:HE2 | 2.06 | 0.56 |
| 3:K:103:GLY:O | 3:K:104:ARG:O | 2.23 | 0.56 |
| 3:Y:218:THR:HG22 | 3:Y:220:VAL:HG23 | 1.86 | 0.56 |
| 3:C:103:GLY:O | 3:C:104:ARG:O | 2.22 | 0.56 |
| 3:S:107:VAL:CB | 3:S:108:GLY:CA | 2.83 | 0.56 |
| 1:A:325:GLU:HG3 | 2:B:13:GLY:O | 2.05 | 0.56 |
| 1:M:304:ALA:HB2 | 2:N:61:GLU:HG2 | 1.88 | 0.56 |
| 3:O:207:TYR:O | 3:O:223:LYS:HE2 | 2.06 | 0.56 |
| 3:Y:103:GLY:O | 3:Y:104:ARG:O | 2.23 | 0.56 |
| 3:S:107:VAL:CB | 3:S:108:GLY:HA2 | 2.29 | 0.56 |
| 3:C:111:GLY:HA2 | 3:C:112:ARG:HB2 | 1.87 | 0.56 |
| 3:G:107:VAL:CB | 3:G:108:GLY:CA | 2.84 | 0.56 |
| 2:J:49:ASN:OD1 | 3:K:106:GLU:CB | 2.54 | 0.56 |
| 3:Y:107:VAL:CB | 3:Y:108:GLY:HA2 | 2.30 | 0.56 |
| 3:Y:111:GLY:HA2 | 3:Y:112:ARG:HB2 | 1.87 | 0.56 |
| 2:R:42:GLN:O | 2:R:46:ASP:OD1 | 2.23 | 0.56 |
| 3:K:137:LEU:CD1 | 4:L:119:PHE:CG | 2.89 | 0.56 |
| 3:O:104:ARG:O | 3:O:105:VAL:O | 2.23 | 0.55 |
| 3:K:137:LEU:HD11 | 4:L:119:PHE:CG | 2.41 | 0.55 |
| 2:F:57:GLU:OE2 | 4:H:32:THR:HG22 | 2.05 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:104:ARG:O | 3:C:105:VAL:O | 2.24 | 0.55 |
| 4:D:164:VAL:HG22 | 4:D:176:LEU:HD13 | 1.87 | 0.55 |
| 3:G:107:VAL:CB | 3:G:108:GLY:HA2 | 2.29 | 0.55 |
| 1:Q:176:LYS:HE3 | 1:Q:257:TYR:CD2 | 2.41 | 0.55 |
| 2:J:25:ARG:HD3 | 2:J:34:GLN:OE1 | 2.07 | 0.55 |
| 4:X:164:VAL:HG22 | 4:X:176:LEU:HD13 | 1.88 | 0.55 |
| 3:S:103:GLY:O | 3:S:104:ARG:O | 2.25 | 0.55 |
| 3:O:103:GLY:O | 3:O:104:ARG:O | 2.23 | 0.55 |
| 4:X:165:THR:HG22 | 4:X:175:SER:N | 2.21 | 0.55 |
| 1:Q:216:ASN:OD1 | 1:Q:216:ASN:N | 2.39 | 0.55 |
| 3:G:103:GLY:O | 3:G:104:ARG:O | 2.25 | 0.55 |
| 1:M:206:THR:C | 1:Q:221:PRO:HG2 | 2.25 | 0.55 |
| 4:D:165:THR:HG22 | 4:D:175:SER:N | 2.21 | 0.55 |
| 3:C:107:VAL:CB | 3:C:108:GLY:HA2 | 2.31 | 0.55 |
| 1:I:304:ALA:HB2 | 2:J:61:GLU:HG2 | 1.89 | 0.55 |
| 3:C:137:LEU:HD11 | 4:D:119:PHE:CG | 2.42 | 0.55 |
| 5:Q:405:NAG:O3 | 3:S:105:VAL:CG1 | 2.55 | 0.54 |
| 1:Q:248:ASN:C | 1:Q:248:ASN:OD1 | 2.45 | 0.54 |
| 2:B:21:TRP:CE2 | 2:B:45:ILE:HD11 | 2.42 | 0.54 |
| 3:K:107:VAL:CB | 3:K:108:GLY:HA2 | 2.31 | 0.54 |
| 2:N:72:GLU:CA | 2:N:72:GLU:OE1 | 2.54 | 0.54 |
| 5:Q:405:NAG:O3 | 3:S:105:VAL:HG11 | 2.08 | 0.54 |
| 3:O:137:LEU:HD11 | 4:P:119:PHE:CD2 | 2.42 | 0.54 |
| 3:C:208:ILE:HA | 3:C:223:LYS:CE | 2.39 | 0.53 |
| 3:C:223:LYS:HE3 | 3:C:223:LYS:HA | 1.90 | 0.53 |
| 3:O:111:GLY:CA | 3:O:112:ARG:HB2 | 2.38 | 0.53 |
| 2:V:21:TRP:CE2 | 2:V:45:ILE:HD11 | 2.43 | 0.53 |
| 1:E:248:ASN:C | 1:E:248:ASN:OD1 | 2.45 | 0.53 |
| 3:Y:137:LEU:HD11 | 4:X:119:PHE:CG | 2.44 | 0.53 |
| 2:B:49:ASN:OD1 | 3:C:107:VAL:HG13 | 2.08 | 0.53 |
| 3:Y:208:ILE:HA | 3:Y:223:LYS:CE | 2.39 | 0.53 |
| 2:V:49:ASN:OD1 | 3:Y:107:VAL:HG13 | 2.09 | 0.53 |
| 3:S:111:GLY:HA2 | 3:S:112:ARG:HB2 | 1.90 | 0.53 |
| 3:G:111:GLY:HA2 | 3:G:112:ARG:HB2 | 1.90 | 0.53 |
| 4:P:165:THR:HG22 | 4:P:175:SER:N | 2.24 | 0.53 |
| 2:F:53:ASN:HD21 | 3:G:108:GLY:HA2 | 1.74 | 0.53 |
| 2:N:141:TYR:O | 2:N:166:ALA:HA | 2.09 | 0.53 |
| 3:G:105:VAL:O | 3:G:106:GLU:OE1 | 2.27 | 0.52 |
| 1:M:27:LYS:CE | 2:N:97:GLU:OE2 | 2.57 | 0.52 |
| 6:U:403:BMA:O4 | 7:U:404:MAN:H2 | 2.09 | 0.52 |
| 1:U:165:ASN:OD1 | 1:M:219:SER:OG | 2.26 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:141:TYR:O | 2:J:166:ALA:HA | 2.09 | 0.52 |
| 1:Q:10:THR:HB | 2:R:140:ILE:O | 2.08 | 0.52 |
| 1:E:156:LYS:HD2 | 1:E:159:SER:HA | 1.91 | 0.52 |
| 3:O:107:VAL:CB | 3:O:108:GLY:CA | 2.87 | 0.52 |
| 3:O:107:VAL:CB | 3:O:108:GLY:HA2 | 2.32 | 0.52 |
| 1:E:33:GLN:HG2 | 4:L:94:VAL:CG2 | 2.37 | 0.52 |
| 1:M:27:LYS:NZ | 2:N:97:GLU:OE2 | 2.39 | 0.52 |
| 4:L:165:THR:HG22 | 4:L:175:SER:N | 2.25 | 0.52 |
| 3:K:105:VAL:O | 3:K:106:GLU:OE1 | 2.28 | 0.52 |
| 1:U:27:LYS:HE3 | 4:T:28:ARG:HG3 | 1.91 | 0.52 |
| 1:M:16:GLY:HA3 | 2:N:14:TRP:CZ2 | 2.45 | 0.52 |
| 4:D:165:THR:HG22 | 4:D:175:SER:H | 1.74 | 0.52 |
| 4:P:18:ARG:HG3 | 4:P:18:ARG:O | 2.10 | 0.52 |
| 3:O:101:VAL:HG11 | 3:O:104:ARG:HD3 | 1.92 | 0.52 |
| 1:E:208:ARG:HD2 | 1:E:238:LYS:HE2 | 1.92 | 0.52 |
| 2:F:141:TYR:O | 2:F:166:ALA:HA | 2.09 | 0.52 |
| 2:R:114:GLU:HG3 | 2:R:114:GLU:O | 2.08 | 0.52 |
| 4:X:165:THR:HG22 | 4:X:175:SER:H | 1.74 | 0.52 |
| 3:C:2:VAL:HG11 | 3:C:115:TYR:CD2 | 2.45 | 0.52 |
| 4:P:48:LEU:HA | 4:P:59:ILE:CD1 | 2.40 | 0.52 |
| 4:T:165:THR:HG22 | 4:T:175:SER:N | 2.25 | 0.52 |
| 1:M:59:LEU:HD11 | 1:M:82:GLU:HG2 | 1.91 | 0.52 |
| 1:Q:22:ASN:OD1 | 1:Q:22:ASN:N | 2.43 | 0.52 |
| 3:K:111:GLY:CA | 3:K:112:ARG:HB2 | 2.40 | 0.51 |
| 1:E:326:LYS:HG3 | 2:F:12:ASN:HB3 | 1.91 | 0.51 |
| 3:Y:223:LYS:HE3 | 3:Y:223:LYS:HA | 1.92 | 0.51 |
| 3:O:223:LYS:HA | 3:O:223:LYS:HE3 | 1.92 | 0.51 |
| 3:S:105:VAL:O | 3:S:106:GLU:OE1 | 2.28 | 0.51 |
| 1:Q:156:LYS:HD2 | 1:Q:159:SER:HA | 1.92 | 0.51 |
| 4:T:18:ARG:HG3 | 4:T:18:ARG:O | 2.09 | 0.51 |
| 3:G:223:LYS:HA | 3:G:223:LYS:HE3 | 1.92 | 0.51 |
| 4:P:12:ALA:HA | 4:P:106:GLU:O | 2.10 | 0.51 |
| 4:T:48:LEU:HA | 4:T:59:ILE:CD1 | 2.40 | 0.51 |
| 1:U:22:ASN:OD1 | 1:U:22:ASN:N | 2.41 | 0.51 |
| 4:X:48:LEU:HA | 4:X:59:ILE:CD1 | 2.40 | 0.51 |
| 1:M:210:GLN:HG3 | 1:Q:220:ARG:HE | 1.74 | 0.51 |
| 4:H:165:THR:HG22 | 4:H:175:SER:N | 2.26 | 0.51 |
| 2:N:21:TRP:CE2 | 2:N:45:ILE:HD11 | 2.45 | 0.51 |
| 4:L:18:ARG:O | 4:L:18:ARG:HG3 | 2.10 | 0.51 |
| 4:D:18:ARG:HG3 | 4:D:18:ARG:O | 2.10 | 0.51 |
| 4:L:48:LEU:HA | 4:L:59:ILE:CD1 | 2.41 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:X:18:ARG:HG3 | 4:X:18:ARG:O | 2.10 | 0.51 |
| 4:D:48:LEU:HA | 4:D:59:ILE:CD1 | 2.40 | 0.51 |
| 3:K:223:LYS:HE3 | 3:K:223:LYS:HA | 1.91 | 0.51 |
| 3:K:101:VAL:HG11 | 3:K:104:ARG:HD3 | 1.93 | 0.51 |
| 3:O:105:VAL:O | 3:O:106:GLU:OE1 | 2.28 | 0.51 |
| 4:L:12:ALA:HA | 4:L:106:GLU:O | 2.10 | 0.51 |
| 4:H:187:TYR:HA | 4:H:193:TYR:OH | 2.10 | 0.51 |
| 3:O:6:GLN:NE2 | 3:O:120:THR:HG22 | 2.25 | 0.51 |
| 4:T:12:ALA:HA | 4:T:106:GLU:O | 2.11 | 0.51 |
| 4:H:12:ALA:HA | 4:H:106:GLU:O | 2.11 | 0.51 |
| 3:S:223:LYS:HA | 3:S:223:LYS:HE3 | 1.92 | 0.51 |
| 4:H:48:LEU:HA | 4:H:59:ILE:CD1 | 2.40 | 0.51 |
| 4:H:18:ARG:O | 4:H:18:ARG:HG3 | 2.10 | 0.51 |
| 3:G:101:VAL:HG11 | 3:G:104:ARG:HD3 | 1.92 | 0.51 |
| 4:X:187:TYR:HA | 4:X:193:TYR:OH | 2.10 | 0.51 |
| 4:T:187:TYR:HA | 4:T:193:TYR:OH | 2.11 | 0.51 |
| 2:B:143:LYS:N | 2:B:143:LYS:HD2 | 2.26 | 0.51 |
| 3:S:135:PHE:HB3 | 4:T:122:SER:OG | 2.11 | 0.51 |
| 2:R:141:TYR:O | 2:R:166:ALA:HA | 2.10 | 0.51 |
| 1:I:206:THR:C | 1:E:221:PRO:HG2 | 2.30 | 0.51 |
| 1:E:27:LYS:CE | 4:L:28:ARG:HG3 | 2.36 | 0.50 |
| 4:P:48:LEU:HA | 4:P:59:ILE:HD13 | 1.93 | 0.50 |
| 3:Y:2:VAL:HG11 | 3:Y:115:TYR:CD2 | 2.46 | 0.50 |
| 1:M:325:GLU:HG3 | 2:N:13:GLY:O | 2.11 | 0.50 |
| 3:S:101:VAL:HG11 | 3:S:104:ARG:HD3 | 1.92 | 0.50 |
| 1:U:186:SER:HA | 1:U:218:GLY:O | 2.12 | 0.50 |
| 1:M:238:LYS:HD2 | 1:M:239:PRO:HD2 | 1.93 | 0.50 |
| 3:C:101:VAL:HG11 | 3:C:104:ARG:HD3 | 1.93 | 0.50 |
| 1:E:16:GLY:HA3 | 2:F:14:TRP:CZ2 | 2.46 | 0.50 |
| 1:U:285:ASN:ND2 | 5:U:405:NAG:C2 | 2.65 | 0.50 |
| 3:Y:111:GLY:CA | 3:Y:112:ARG:HB2 | 2.42 | 0.50 |
| 1:A:186:SER:HA | 1:A:218:GLY:O | 2.12 | 0.50 |
| 3:G:135:PHE:HB3 | 4:H:122:SER:OG | 2.12 | 0.50 |
| 3:C:105:VAL:O | 3:C:106:GLU:OE1 | 2.30 | 0.50 |
| 1:E:132:GLN:CB | 1:E:133:ASN:HD22 | 2.24 | 0.50 |
| 3:C:222:LYS:C | 3:C:223:LYS:HD2 | 2.32 | 0.50 |
| 3:C:111:GLY:CA | 3:C:112:ARG:HB2 | 2.42 | 0.50 |
| 1:A:97:CYS:SG | 1:A:98:TYR:N | 2.84 | 0.50 |
| 3:C:20:VAL:CG1 | 3:C:120:THR:HG21 | 2.42 | 0.49 |
| 1:I:238:LYS:HD2 | 1:I:239:PRO:HD2 | 1.93 | 0.49 |
| 2:V:141:TYR:O | 2:V:166:ALA:HA | 2.11 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:S:110:GLY:HA2 | 4:T:50:TYR:CE1 | 2.47 | 0.49 |
| 1:M:188:ASN:OD1 | 1:M:188:ASN:N | 2.42 | 0.49 |
| 3:Y:101:VAL:HG11 | 3:Y:104:ARG:HD3 | 1.94 | 0.49 |
| 3:Y:105:VAL:O | 3:Y:106:GLU:OE1 | 2.30 | 0.49 |
| 5:Q:405:NAG:H4 | 3:S:105:VAL:HG11 | 1.93 | 0.49 |
| 3:O:20:VAL:CG1 | 3:O:120:THR:HG21 | 2.42 | 0.49 |
| 3:Y:6:GLN:NE2 | 3:Y:120:THR:HG22 | 2.27 | 0.49 |
| 4:X:48:LEU:HA | 4:X:59:ILE:HD13 | 1.93 | 0.49 |
| 4:X:12:ALA:HA | 4:X:106:GLU:O | 2.11 | 0.49 |
| 1:Q:132:GLN:CB | 1:Q:133:ASN:HD22 | 2.25 | 0.49 |
| 3:S:208:ILE:HA | 3:S:223:LYS:CE | 2.42 | 0.49 |
| 4:P:187:TYR:HA | 4:P:193:TYR:OH | 2.12 | 0.49 |
| 4:D:187:TYR:HA | 4:D:193:TYR:OH | 2.12 | 0.49 |
| 1:Q:186:SER:HA | 1:Q:218:GLY:O | 2.12 | 0.49 |
| 3:G:208:ILE:HA | 3:G:223:LYS:CE | 2.42 | 0.49 |
| 1:U:97:CYS:SG | 1:U:98:TYR:N | 2.84 | 0.49 |
| 3:K:20:VAL:CG1 | 3:K:120:THR:HG21 | 2.43 | 0.49 |
| 3:G:2:VAL:HG11 | 3:G:115:TYR:CD2 | 2.47 | 0.49 |
| 3:Y:20:VAL:CG1 | 3:Y:120:THR:HG21 | 2.42 | 0.49 |
| 4:L:187:TYR:HA | 4:L:193:TYR:OH | 2.12 | 0.49 |
| 1:U:326:LYS:O | 1:U:327:GLN:HB2 | 2.13 | 0.49 |
| 2:J:21:TRP:CE2 | 2:J:45:ILE:HD11 | 2.48 | 0.49 |
| 1:A:139:CYS:H | 1:A:140:LYS:HZ3 | 1.61 | 0.49 |
| 1:A:140:LYS:CE | 1:A:145:SER:CB | 2.89 | 0.49 |
| 3:S:6:GLN:NE2 | 3:S:120:THR:HG22 | 2.28 | 0.49 |
| 4:X:116:VAL:O | 4:X:208:LYS:HD2 | 2.13 | 0.49 |
| 3:O:208:ILE:HA | 3:O:223:LYS:CE | 2.42 | 0.49 |
| 4:T:118:ILE:CG2 | 4:T:119:PHE:N | 2.75 | 0.49 |
| 4:P:165:THR:HG22 | 4:P:175:SER:H | 1.77 | 0.49 |
| 4:D:48:LEU:HA | 4:D:59:ILE:HD13 | 1.93 | 0.49 |
| 4:D:116:VAL:O | 4:D:208:LYS:HD2 | 2.13 | 0.49 |
| 1:I:167:THR:HB | 5:I:401:NAG:H62 | 1.95 | 0.49 |
| 2:B:141:TYR:O | 2:B:166:ALA:HA | 2.12 | 0.48 |
| 1:A:37:THR:CG2 | 1:A:319:GLY:HA3 | 2.43 | 0.48 |
| 3:C:6:GLN:NE2 | 3:C:120:THR:HG22 | 2.28 | 0.48 |
| 1:I:16:GLY:HA3 | 2:J:14:TRP:CZ2 | 2.49 | 0.48 |
| 3:Y:222:LYS:C | 3:Y:223:LYS:HD2 | 2.34 | 0.48 |
| 4:L:48:LEU:HA | 4:L:59:ILE:HD13 | 1.94 | 0.48 |
| 4:T:165:THR:HG22 | 4:T:175:SER:H | 1.78 | 0.48 |
| 1:A:248:ASN:OD1 | 1:A:248:ASN:C | 2.51 | 0.48 |
| 1:E:186:SER:HA | 1:E:218:GLY:O | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:G:111:GLY:CA | 3:G:112:ARG:HB2 | 2.44 | 0.48 |
| 4:L:165:THR:HG22 | 4:L:175:SER:H | 1.78 | 0.48 |
| 1:I:248:ASN:C | 1:I:248:ASN:OD1 | 2.52 | 0.48 |
| 1:Q:170:ASN:CG | 1:Q:176:LYS:HD3 | 2.33 | 0.48 |
| 2:F:171:PHE:CE2 | 2:B:171:PHE:CE2 | 3.01 | 0.48 |
| 1:I:210:GLN:HG3 | 1:E:220:ARG:HE | 1.78 | 0.48 |
| 3:Y:64:PHE:O | 3:Y:65:GLN:C | 2.52 | 0.48 |
| 1:A:140:LYS:NZ | 1:A:146:GLY:O | 2.47 | 0.48 |
| 1:M:20:VAL:HB | 1:M:21:PRO:HD2 | 1.96 | 0.48 |
| 1:E:170:ASN:CG | 1:E:176:LYS:HD3 | 2.34 | 0.47 |
| 4:D:12:ALA:HA | 4:D:106:GLU:O | 2.13 | 0.47 |
| 1:A:327:GLN:OE1 | 1:A:327:GLN:N | 2.47 | 0.47 |
| 1:I:37:THR:CG2 | 1:I:319:GLY:HA3 | 2.44 | 0.47 |
| 4:T:48:LEU:HA | 4:T:59:ILE:HD13 | 1.94 | 0.47 |
| 4:H:48:LEU:HA | 4:H:59:ILE:HD13 | 1.95 | 0.47 |
| 3:K:6:GLN:NE2 | 3:K:120:THR:HG22 | 2.29 | 0.47 |
| 2:N:165:GLU:O | 2:N:169:ASN:OD1 | 2.31 | 0.47 |
| 1:M:248:ASN:C | 1:M:248:ASN:OD1 | 2.52 | 0.47 |
| 1:M:37:THR:CG2 | 1:M:319:GLY:HA3 | 2.44 | 0.47 |
| 3:S:2:VAL:HG11 | 3:S:115:TYR:CD2 | 2.49 | 0.47 |
| 1:M:326:LYS:O | 1:M:327:GLN:CB | 2.61 | 0.47 |
| 3:C:64:PHE:O | 3:C:65:GLN:C | 2.52 | 0.47 |
| 3:K:208:ILE:HA | 3:K:223:LYS:CE | 2.43 | 0.47 |
| 2:R:150:GLU:CD | 2:R:153:ARG:NH2 | 2.66 | 0.47 |
| 3:S:111:GLY:CA | 3:S:112:ARG:HB2 | 2.44 | 0.47 |
| 4:H:165:THR:HG22 | 4:H:175:SER:H | 1.79 | 0.47 |
| 4:L:116:VAL:O | 4:L:208:LYS:HD2 | 2.15 | 0.47 |
| 1:E:37:THR:CG2 | 1:E:319:GLY:HA3 | 2.44 | 0.47 |
| 3:S:135:PHE:CE2 | 4:T:125:GLN:HG3 | 2.49 | 0.47 |
| 3:G:20:VAL:CG1 | 3:G:120:THR:HG21 | 2.43 | 0.47 |
| 2:J:75:GLY:C | 2:J:79:ASP:OD1 | 2.52 | 0.47 |
| 1:U:16:GLY:HA3 | 2:V:14:TRP:CZ2 | 2.50 | 0.47 |
| 3:G:14:PRO:O | 3:G:86:LEU:O | 2.33 | 0.47 |
| 1:I:22:ASN:OD1 | 1:I:22:ASN:O | 2.32 | 0.47 |
| 2:B:58:LYS:HA | 2:B:58:LYS:HD2 | 1.76 | 0.47 |
| 1:A:137:ASN:HA | 1:A:140:LYS:CD | 2.43 | 0.47 |
| 3:S:20:VAL:CG1 | 3:S:120:THR:HG21 | 2.44 | 0.47 |
| 1:U:248:ASN:OD1 | 1:U:248:ASN:C | 2.52 | 0.47 |
| 4:P:116:VAL:O | 4:P:208:LYS:HD2 | 2.15 | 0.47 |
| 1:E:52:CYS:HB2 | 1:E:279:SER:HB3 | 1.96 | 0.47 |
| 1:Q:326:LYS:O | 1:Q:327:GLN:CB | 2.62 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:37:THR:CG2 | 1:U:319:GLY:HA3 | 2.44 | 0.47 |
| 1:M:186:SER:HA | 1:M:218:GLY:O | 2.14 | 0.47 |
| 2:R:53:ASN:HB3 | 4:T:32:THR:HG21 | 1.97 | 0.47 |
| 1:I:20:VAL:HB | 1:I:21:PRO:HD2 | 1.97 | 0.47 |
| 1:I:119:GLU:OE1 | 1:I:261:ARG:NH2 | 2.48 | 0.47 |
| 1:M:119:GLU:OE1 | 1:M:261:ARG:NH2 | 2.48 | 0.47 |
| 3:Y:14:PRO:O | 3:Y:86:LEU:O | 2.31 | 0.47 |
| 1:E:326:LYS:O | 1:E:327:GLN:HG2 | 2.15 | 0.47 |
| 1:Q:325:GLU:HB2 | 2:R:12:ASN:HD22 | 1.80 | 0.47 |
| 3:O:2:VAL:HG11 | 3:O:115:TYR:CD2 | 2.50 | 0.47 |
| 1:A:140:LYS:HE3 | 1:A:145:SER:CB | 2.45 | 0.46 |
| 2:B:9:PHE:CZ | 2:B:10:ILE:HD11 | 2.50 | 0.46 |
| 2:F:21:TRP:CE2 | 2:F:45:ILE:HD11 | 2.51 | 0.46 |
| 1:Q:52:CYS:HB2 | 1:Q:279:SER:HB3 | 1.97 | 0.46 |
| 3:Y:172:LEU:HD21 | 3:Y:195:VAL:HG11 | 1.97 | 0.46 |
| 4:T:116:VAL:O | 4:T:208:LYS:HD2 | 2.14 | 0.46 |
| 3:S:222:LYS:C | 3:S:223:LYS:HD2 | 2.36 | 0.46 |
| 2:B:171:PHE:CD1 | 2:B:171:PHE:N | 2.83 | 0.46 |
| 1:Q:326:LYS:O | 1:Q:327:GLN:HB2 | 2.15 | 0.46 |
| 3:S:14:PRO:O | 3:S:86:LEU:O | 2.34 | 0.46 |
| 3:K:14:PRO:O | 3:K:86:LEU:O | 2.34 | 0.46 |
| 1:U:217:ILE:O | 1:Q:201:ARG:NH1 | 2.49 | 0.46 |
| 4:H:116:VAL:O | 4:H:208:LYS:HD2 | 2.14 | 0.46 |
| 1:U:119:GLU:OE1 | 1:U:261:ARG:NH2 | 2.48 | 0.46 |
| 3:O:14:PRO:O | 3:O:86:LEU:O | 2.33 | 0.46 |
| 1:I:186:SER:HA | 1:I:218:GLY:O | 2.15 | 0.46 |
| 3:C:14:PRO:O | 3:C:86:LEU:O | 2.32 | 0.46 |
| 2:R:21:TRP:CE2 | 2:R:45:ILE:HD11 | 2.51 | 0.46 |
| 1:A:29:ILE:HD11 | 2:B:102:LEU:HD23 | 1.96 | 0.46 |
| 3:K:2:VAL:HG11 | 3:K:115:TYR:CD2 | 2.50 | 0.46 |
| 1:U:156:LYS:HE2 | 1:U:196:VAL:CB | 2.41 | 0.46 |
| 4:H:118:ILE:CG2 | 4:H:119:PHE:N | 2.78 | 0.46 |
| 2:V:163:ARG:O | 2:V:167:LEU:HB2 | 2.16 | 0.46 |
| 1:E:20:VAL:HB | 1:E:21:PRO:HD2 | 1.97 | 0.46 |
| 1:E:97:CYS:SG | 1:E:98:TYR:N | 2.86 | 0.46 |
| 3:C:172:LEU:HD21 | 3:C:195:VAL:HG11 | 1.98 | 0.46 |
| 1:I:156:LYS:HD2 | 1:I:159:SER:HA | 1.96 | 0.46 |
| 2:V:17:MET:O | 2:V:18:ILE:HD13 | 2.15 | 0.46 |
| 3:S:28:SER:OG | 3:S:28:SER:O | 2.34 | 0.46 |
| 1:M:97:CYS:SG | 1:M:98:TYR:N | 2.86 | 0.46 |
| 1:A:9:SER:N | 2:B:143:LYS:HE3 | 2.31 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:119:GLU:OE1 | 1:E:261:ARG:NH2 | 2.49 | 0.46 |
| 5:I:402:NAG:O3 | 1:E:222:TRP:CE3 | 2.63 | 0.46 |
| 1:U:52:CYS:HB2 | 1:U:279:SER:HB3 | 1.98 | 0.46 |
| 2:J:9:PHE:CZ | 2:J:10:ILE:HD11 | 2.51 | 0.45 |
| 1:A:57:ARG:NH1 | 1:A:83:THR:O | 2.49 | 0.45 |
| 1:M:137:ASN:OD1 | 1:M:140:LYS:HE3 | 2.16 | 0.45 |
| 1:E:29:ILE:HD11 | 2:F:102:LEU:HD23 | 1.96 | 0.45 |
| 1:E:326:LYS:HE2 | 2:F:11:GLU:OE1 | 2.16 | 0.45 |
| 1:I:210:GLN:HE21 | 1:E:220:ARG:NH2 | 2.14 | 0.45 |
| 2:B:159:HIS:ND1 | 2:B:160:ASP:N | 2.64 | 0.45 |
| 1:A:270:SER:HB2 | 1:A:284:PRO:HA | 1.98 | 0.45 |
| 3:K:172:LEU:HD21 | 3:K:195:VAL:HG11 | 1.98 | 0.45 |
| 1:I:63:ASP:OD1 | 1:I:92:LYS:HE3 | 2.16 | 0.45 |
| 3:G:222:LYS:C | 3:G:223:LYS:HD2 | 2.37 | 0.45 |
| 1:A:217:ILE:O | 1:E:201:ARG:NH1 | 2.50 | 0.45 |
| 3:G:6:GLN:NE2 | 3:G:120:THR:HG22 | 2.31 | 0.45 |
| 2:B:163:ARG:O | 2:B:167:LEU:HB2 | 2.17 | 0.45 |
| 1:A:52:CYS:HB2 | 1:A:279:SER:HB3 | 1.99 | 0.45 |
| 3:O:172:LEU:HD21 | 3:O:195:VAL:HG11 | 1.98 | 0.45 |
| 1:I:97:CYS:SG | 1:I:98:TYR:N | 2.87 | 0.45 |
| 1:M:57:ARG:NH1 | 1:M:83:THR:O | 2.49 | 0.45 |
| 3:G:105:VAL:C | 3:G:106:GLU:CD | 2.75 | 0.45 |
| 1:E:326:LYS:O | 1:E:327:GLN:CB | 2.64 | 0.45 |
| 3:K:214:LYS:HA | 3:K:214:LYS:HD2 | 1.68 | 0.45 |
| 1:A:136:SER:O | 1:A:138:ALA:N | 2.50 | 0.45 |
| 3:O:222:LYS:C | 3:O:223:LYS:HD2 | 2.37 | 0.45 |
| 2:J:163:ARG:O | 2:J:167:LEU:HB2 | 2.16 | 0.45 |
| 1:U:156:LYS:HE2 | 1:U:196:VAL:CA | 2.46 | 0.45 |
| 1:A:140:LYS:HE3 | 1:A:146:GLY:N | 2.30 | 0.45 |
| 1:Q:184:HIS:ND1 | 1:Q:216:ASN:OD1 | 2.50 | 0.45 |
| 2:R:57:GLU:OE2 | 4:T:32:THR:HG22 | 2.16 | 0.45 |
| 1:Q:97:CYS:SG | 1:Q:98:TYR:N | 2.87 | 0.45 |
| 3:O:20:VAL:HG11 | 3:O:120:THR:HG21 | 1.99 | 0.45 |
| 4:D:80:GLU:HB3 | 4:D:81:PRO:HD2 | 1.99 | 0.45 |
| 3:S:172:LEU:HD21 | 3:S:195:VAL:HG11 | 1.99 | 0.45 |
| 2:B:47:GLN:HB3 | 2:B:110:LEU:HD11 | 1.99 | 0.45 |
| 2:R:163:ARG:O | 2:R:167:LEU:HB2 | 2.17 | 0.45 |
| 3:K:222:LYS:C | 3:K:223:LYS:HD2 | 2.37 | 0.45 |
| 1:Q:57:ARG:NH1 | 1:Q:83:THR:O | 2.50 | 0.45 |
| 1:I:270:SER:HB2 | 1:I:284:PRO:HA | 1.98 | 0.45 |
| 2:F:123:ARG:HH21 | 2:F:132:ASP:HB2 | 1.81 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:O:99:ASP:OD1 | 3:O:112:ARG:HA | 2.17 | 0.45 |
| 1:Q:20:VAL:HB | 1:Q:21:PRO:HD2 | 1.98 | 0.45 |
| 3:G:135:PHE:CE2 | 4:H:125:GLN:HG3 | 2.52 | 0.44 |
| 1:Q:119:GLU:OE1 | 1:Q:261:ARG:NH2 | 2.50 | 0.44 |
| 2:R:49:ASN:OD1 | 3:S:107:VAL:HG13 | 2.17 | 0.44 |
| 1:M:270:SER:HB2 | 1:M:284:PRO:HA | 1.98 | 0.44 |
| 1:M:52:CYS:HB2 | 1:M:279:SER:HB3 | 1.98 | 0.44 |
| 1:U:57:ARG:NH1 | 1:U:83:THR:O | 2.50 | 0.44 |
| 3:O:28:SER:O | 3:O:28:SER:OG | 2.36 | 0.44 |
| 1:E:33:GLN:HB3 | 4:L:94:VAL:HG13 | 1.98 | 0.44 |
| 2:F:38:LEU:HA | 2:F:38:LEU:HD12 | 1.82 | 0.44 |
| 3:K:20:VAL:HG11 | 3:K:120:THR:HG21 | 2.00 | 0.44 |
| 2:N:163:ARG:O | 2:N:167:LEU:HB2 | 2.17 | 0.44 |
| 3:K:91:THR:HG23 | 3:K:123:ILE:HA | 2.00 | 0.44 |
| 4:X:80:GLU:HB3 | 4:X:81:PRO:HD2 | 1.99 | 0.44 |
| 3:S:91:THR:HG23 | 3:S:123:ILE:HA | 1.98 | 0.44 |
| 2:F:163:ARG:O | 2:F:167:LEU:HB2 | 2.18 | 0.44 |
| 1:M:156:LYS:HD2 | 1:M:159:SER:HA | 1.98 | 0.44 |
| 3:S:99:ASP:OD1 | 3:S:112:ARG:HA | 2.17 | 0.44 |
| 4:P:118:ILE:CG2 | 4:P:119:PHE:N | 2.81 | 0.44 |
| 1:U:29:ILE:HD11 | 2:V:102:LEU:HD23 | 1.98 | 0.44 |
| 3:G:99:ASP:OD1 | 3:G:112:ARG:HA | 2.17 | 0.44 |
| 1:E:61:GLY:O | 1:E:62:ILE:C | 2.56 | 0.44 |
| 1:Q:16:GLY:HA3 | 2:R:14:TRP:CZ2 | 2.51 | 0.44 |
| 3:G:172:LEU:HD21 | 3:G:195:VAL:HG11 | 1.99 | 0.44 |
| 1:M:62:ILE:HG22 | 1:M:63:ASP:N | 2.32 | 0.44 |
| 3:Y:28:SER:OG | 3:Y:28:SER:O | 2.35 | 0.44 |
| 3:Y:111:GLY:HA2 | 3:Y:112:ARG:CB | 2.47 | 0.44 |
| 3:C:20:VAL:HG11 | 3:C:120:THR:HG21 | 1.99 | 0.44 |
| 2:V:47:GLN:HB3 | 2:V:110:LEU:HD11 | 2.00 | 0.44 |
| 1:I:57:ARG:NH1 | 1:I:83:THR:O | 2.51 | 0.44 |
| 3:K:105:VAL:C | 3:K:106:GLU:CD | 2.76 | 0.44 |
| 3:K:99:ASP:OD1 | 3:K:112:ARG:HA | 2.18 | 0.44 |
| 3:C:3:GLN:C | 3:C:4:LEU:HD22 | 2.38 | 0.44 |
| 1:E:57:ARG:NH1 | 1:E:83:THR:O | 2.51 | 0.44 |
| 1:A:20:VAL:HB | 1:A:21:PRO:HD2 | 1.99 | 0.44 |
| 3:C:28:SER:OG | 3:C:28:SER:O | 2.35 | 0.44 |
| 2:F:38:LEU:HG | 3:G:54:TYR:CE2 | 2.53 | 0.44 |
| 1:I:52:CYS:HB2 | 1:I:279:SER:HB3 | 1.98 | 0.44 |
| 3:G:64:PHE:O | 3:G:65:GLN:C | 2.55 | 0.44 |
| 3:Y:214:LYS:HA | 3:Y:214:LYS:HD2 | 1.66 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:R:150:GLU:CD | 2:R:153:ARG:HH21 | 2.20 | 0.43 |
| 2:J:47:GLN:HB3 | 2:J:110:LEU:HD11 | 2.00 | 0.43 |
| 1:U:20:VAL:HB | 1:U:21:PRO:HD2 | 2.00 | 0.43 |
| 3:C:111:GLY:HA2 | 3:C:112:ARG:CB | 2.47 | 0.43 |
| 3:K:64:PHE:O | 3:K:65:GLN:C | 2.56 | 0.43 |
| 4:L:118:ILE:CG2 | 4:L:119:PHE:N | 2.81 | 0.43 |
| 1:M:207:ARG:HG3 | 1:Q:223:VAL:HG22 | 2.00 | 0.43 |
| 2:B:38:LEU:HD22 | 3:C:54:TYR:CZ | 2.53 | 0.43 |
| 2:F:125:GLN:HE22 | 2:F:152:ILE:HA | 1.83 | 0.43 |
| 3:O:91:THR:HG23 | 3:O:123:ILE:HA | 2.00 | 0.43 |
| 3:G:167:TRP:HA | 3:G:208:ILE:O | 2.19 | 0.43 |
| 2:R:150:GLU:OE1 | 2:R:153:ARG:NE | 2.52 | 0.43 |
| 2:N:47:GLN:HB3 | 2:N:110:LEU:HD11 | 2.00 | 0.43 |
| 1:U:62:ILE:HG22 | 1:U:63:ASP:N | 2.33 | 0.43 |
| 3:Y:20:VAL:HG11 | 3:Y:120:THR:HG21 | 2.00 | 0.43 |
| 2:F:171:PHE:CE2 | 2:B:171:PHE:HE2 | 2.36 | 0.43 |
| 3:S:64:PHE:O | 3:S:65:GLN:C | 2.55 | 0.43 |
| 3:C:214:LYS:HD2 | 3:C:214:LYS:HA | 1.67 | 0.43 |
| 3:K:137:LEU:HD11 | 4:L:119:PHE:CD2 | 2.53 | 0.43 |
| 1:I:62:ILE:HG22 | 1:I:63:ASP:N | 2.33 | 0.43 |
| 1:A:27:LYS:CE | 1:A:33:GLN:NE2 | 2.77 | 0.43 |
| 2:F:49:ASN:OD1 | 3:G:107:VAL:HG13 | 2.19 | 0.43 |
| 3:G:91:THR:HG23 | 3:G:123:ILE:HA | 1.99 | 0.43 |
| 2:F:58:LYS:NZ | 4:H:54:ASN:HD21 | 2.16 | 0.43 |
| 1:U:270:SER:HB2 | 1:U:284:PRO:HA | 2.01 | 0.43 |
| 3:S:167:TRP:HA | 3:S:208:ILE:O | 2.19 | 0.43 |
| 2:R:47:GLN:HB3 | 2:R:110:LEU:HD11 | 2.00 | 0.43 |
| 3:O:64:PHE:O | 3:O:65:GLN:C | 2.57 | 0.43 |
| 3:Y:99:ASP:OD1 | 3:Y:112:ARG:HA | 2.18 | 0.43 |
| 1:I:61:GLY:O | 1:I:62:ILE:C | 2.56 | 0.43 |
| 1:Q:270:SER:HB2 | 1:Q:284:PRO:HA | 2.00 | 0.43 |
| 3:C:91:THR:HG23 | 3:C:123:ILE:HA | 2.00 | 0.42 |
| 4:X:40:LYS:O | 4:X:43:GLN:HG2 | 2.19 | 0.42 |
| 1:Q:25:LEU:HB2 | 4:P:27:HIS:CE1 | 2.54 | 0.42 |
| 2:N:72:GLU:OE1 | 2:N:72:GLU:N | 2.52 | 0.42 |
| 3:S:20:VAL:HG11 | 3:S:120:THR:HG21 | 2.01 | 0.42 |
| 2:F:16:GLY:O | 2:F:18:ILE:HD12 | 2.19 | 0.42 |
| 2:N:72:GLU:OE1 | 2:N:72:GLU:HA | 2.18 | 0.42 |
| 2:F:47:GLN:HB3 | 2:F:110:LEU:HD11 | 2.00 | 0.42 |
| 1:U:37:THR:HG22 | 1:U:320:MET:N | 2.34 | 0.42 |
| 1:E:62:ILE:HG22 | 1:E:63:ASP:N | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:G:214:LYS:HA | 3:G:214:LYS:HD2 | 1.66 | 0.42 |
| 3:Y:91:THR:HG23 | 3:Y:123:ILE:HA | 2.00 | 0.42 |
| 3:O:54:TYR:HD2 | 3:O:55:THR:HG23 | 1.84 | 0.42 |
| 1:Q:61:GLY:O | 1:Q:62:ILE:C | 2.58 | 0.42 |
| 4:T:162:GLU:HB2 | 4:T:176:LEU:HD11 | 2.01 | 0.42 |
| 3:G:20:VAL:HG11 | 3:G:120:THR:HG21 | 2.01 | 0.42 |
| 1:A:92:LYS:HE2 | 1:A:92:LYS:HB2 | 1.78 | 0.42 |
| 3:S:222:LYS:O | 3:S:223:LYS:HD2 | 2.20 | 0.42 |
| 3:Y:209:CYS:HB3 | 3:Y:211:VAL:HG23 | 2.01 | 0.42 |
| 3:C:209:CYS:HB3 | 3:C:211:VAL:HG23 | 2.01 | 0.42 |
| 3:C:99:ASP:OD1 | 3:C:112:ARG:HA | 2.19 | 0.42 |
| 4:T:118:ILE:HG22 | 4:T:119:PHE:N | 2.33 | 0.42 |
| 4:D:118:ILE:CG2 | 4:D:119:PHE:N | 2.82 | 0.42 |
| 1:Q:62:ILE:HG22 | 1:Q:63:ASP:N | 2.35 | 0.42 |
| 3:G:222:LYS:O | 3:G:223:LYS:HD2 | 2.20 | 0.42 |
| 3:O:209:CYS:HB3 | 3:O:211:VAL:HG23 | 2.02 | 0.42 |
| 3:K:222:LYS:O | 3:K:223:LYS:HD2 | 2.20 | 0.42 |
| 3:Y:107:VAL:CB | 3:Y:108:GLY:CA | 2.84 | 0.42 |
| 4:H:162:GLU:HB2 | 4:H:176:LEU:HD11 | 2.01 | 0.42 |
| 2:R:52:LEU:HD22 | 3:S:107:VAL:HG23 | 2.01 | 0.42 |
| 1:A:207:ARG:NH1 | 1:A:242:VAL:CG1 | 2.80 | 0.42 |
| 4:L:162:GLU:HB2 | 4:L:176:LEU:HD11 | 2.02 | 0.42 |
| 3:Y:3:GLN:C | 3:Y:4:LEU:HD22 | 2.40 | 0.42 |
| 3:S:214:LYS:HA | 3:S:214:LYS:HD2 | 1.66 | 0.42 |
| 6:E:403:BMA:HO2 | 7:E:404:MAN:C1 | 2.32 | 0.42 |
| 1:I:207:ARG:HG3 | 1:E:223:VAL:HG22 | 2.01 | 0.42 |
| 3:S:209:CYS:HB3 | 3:S:211:VAL:HG23 | 2.01 | 0.41 |
| 1:A:110:SER:OG | 2:J:79:ASP:OD2 | 2.33 | 0.41 |
| 4:H:107:ILE:HD12 | 4:H:107:ILE:C | 2.40 | 0.41 |
| 2:B:123:ARG:HH21 | 2:B:132:ASP:HB2 | 1.84 | 0.41 |
| 3:C:110:GLY:HA2 | 4:D:50:TYR:CE1 | 2.55 | 0.41 |
| 3:C:104:ARG:NH1 | 3:C:106:GLU:O | 2.53 | 0.41 |
| 3:S:3:GLN:C | 3:S:4:LEU:HD22 | 2.40 | 0.41 |
| 2:B:171:PHE:HD1 | 2:B:171:PHE:N | 2.18 | 0.41 |
| 1:E:304:ALA:HB2 | 2:F:61:GLU:HG2 | 2.01 | 0.41 |
| 4:T:8:PRO:O | 4:T:103:THR:HG23 | 2.20 | 0.41 |
| 3:O:214:LYS:HD2 | 3:O:214:LYS:HA | 1.69 | 0.41 |
| 4:X:107:ILE:C | 4:X:107:ILE:HD12 | 2.41 | 0.41 |
| 3:O:222:LYS:O | 3:O:223:LYS:HD2 | 2.20 | 0.41 |
| 1:A:37:THR:HG22 | 1:A:320:MET:N | 2.35 | 0.41 |
| 3:Y:214:LYS:N | 3:Y:215:PRO:CD | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:T:107:ILE:C | 4:T:107:ILE:HD12 | 2.40 | 0.41 |
| 1:A:315:LYS:HG3 | 4:H:28:ARG:HH12 | 1.85 | 0.41 |
| 3:S:105:VAL:C | 3:S:106:GLU:CD | 2.79 | 0.41 |
| 1:I:264:LYS:HE3 | 2:J:63:PHE:CE2 | 2.55 | 0.41 |
| 4:H:8:PRO:O | 4:H:103:THR:HG23 | 2.20 | 0.41 |
| 3:C:222:LYS:O | 3:C:223:LYS:HD2 | 2.20 | 0.41 |
| 3:K:209:CYS:HB3 | 3:K:211:VAL:HG23 | 2.02 | 0.41 |
| 3:O:4:LEU:HD12 | 3:O:22:CYS:SG | 2.61 | 0.41 |
| 3:S:214:LYS:N | 3:S:215:PRO:CD | 2.84 | 0.41 |
| 1:E:270:SER:HB2 | 1:E:284:PRO:HA | 2.01 | 0.41 |
| 3:Y:104:ARG:NH1 | 3:Y:106:GLU:O | 2.54 | 0.41 |
| 4:P:162:GLU:HB2 | 4:P:176:LEU:HD11 | 2.02 | 0.41 |
| 1:M:61:GLY:O | 1:M:62:ILE:C | 2.58 | 0.41 |
| 1:I:212:THR:HG21 | 1:E:216:ASN:HB3 | 2.02 | 0.41 |
| 4:P:8:PRO:O | 4:P:103:THR:HG23 | 2.21 | 0.41 |
| 3:C:167:TRP:HA | 3:C:208:ILE:O | 2.21 | 0.41 |
| 1:A:62:ILE:HG22 | 1:A:63:ASP:N | 2.36 | 0.41 |
| 3:G:209:CYS:HB3 | 3:G:211:VAL:HG23 | 2.02 | 0.41 |
| 3:Y:222:LYS:O | 3:Y:223:LYS:HD2 | 2.20 | 0.41 |
| 3:Y:167:TRP:HA | 3:Y:208:ILE:O | 2.21 | 0.41 |
| 3:K:167:TRP:HA | 3:K:208:ILE:O | 2.21 | 0.41 |
| 3:C:105:VAL:HG23 | 3:C:106:GLU:H | 1.84 | 0.41 |
| 1:M:37:THR:HG22 | 1:M:320:MET:N | 2.36 | 0.41 |
| 3:K:195:VAL:HG12 | 3:K:197:VAL:HG13 | 2.03 | 0.41 |
| 1:U:61:GLY:O | 1:U:62:ILE:C | 2.58 | 0.41 |
| 2:F:58:LYS:HG3 | 4:H:53:SER:OG | 2.21 | 0.41 |
| 2:J:24:PHE:CD1 | 2:J:153:ARG:HD3 | 2.55 | 0.41 |
| 4:P:107:ILE:C | 4:P:107:ILE:HD12 | 2.41 | 0.41 |
| 4:D:107:ILE:HD12 | 4:D:107:ILE:C | 2.41 | 0.41 |
| 3:K:104:ARG:NH1 | 3:K:106:GLU:O | 2.54 | 0.41 |
| 1:U:216:ASN:HB3 | 1:Q:212:THR:HG21 | 2.02 | 0.41 |
| 1:A:61:GLY:O | 1:A:62:ILE:C | 2.57 | 0.41 |
| 3:K:135:PHE:HB3 | 4:L:122:SER:OG | 2.21 | 0.41 |
| 3:C:107:VAL:CB | 3:C:108:GLY:CA | 2.85 | 0.40 |
| 3:O:180:PRO:HG2 | 4:P:164:VAL:O | 2.22 | 0.40 |
| 3:K:4:LEU:HD12 | 3:K:22:CYS:SG | 2.61 | 0.40 |
| 1:Q:132:GLN:HB2 | 1:Q:133:ASN:HD22 | 1.86 | 0.40 |
| 3:O:195:VAL:HG12 | 3:O:197:VAL:HG13 | 2.03 | 0.40 |
| 3:Y:105:VAL:C | 3:Y:106:GLU:CD | 2.79 | 0.40 |
| 3:O:3:GLN:C | 3:O:4:LEU:HD22 | 2.41 | 0.40 |
| 4:L:8:PRO:O | 4:L:103:THR:HG23 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:U:285:ASN:OD1 | 5:U:405:NAG:C1 | 2.68 | 0.40 |
| 1:M:115:SER:HA | 1:M:261:ARG:O | 2.21 | 0.40 |
| 3:C:135:PHE:CE2 | 4:D:125:GLN:HG3 | 2.56 | 0.40 |
| 2:V:123:ARG:HH21 | 2:V:132:ASP:HB2 | 1.85 | 0.40 |
| 1:E:318:THR:HG22 | 2:F:52:LEU:HD12 | 2.03 | 0.40 |
| 5:Q:406:NAG:H81 | 3:S:104:ARG:NH2 | 2.29 | 0.40 |
| 1:I:115:SER:HA | 1:I:261:ARG:O | 2.22 | 0.40 |
| 3:Y:135:PHE:CE2 | 4:X:125:GLN:HG3 | 2.56 | 0.40 |
| 3:O:201:SER:C | 3:O:202:LEU:HD12 | 2.42 | 0.40 |
| 1:E:326:LYS:O | 1:E:327:GLN:HB2 | 2.22 | 0.40 |
| 3:G:195:VAL:HG12 | 3:G:197:VAL:HG13 | 2.03 | 0.40 |
| 3:C:135:PHE:HB3 | 4:D:122:SER:OG | 2.22 | 0.40 |
| 4:D:8:PRO:O | 4:D:103:THR:HG23 | 2.21 | 0.40 |
| 4:X:8:PRO:O | 4:X:103:THR:HG23 | 2.21 | 0.40 |
| 4:D:40:LYS:O | 4:D:43:GLN:HG2 | 2.22 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:275:ASP:OD1 | 4:T:188:GLU:OE2[1_445] | 1.91 | 0.29 |
| 1:I:275:ASP:OD1 | 4:H:188:GLU:OE2[1_565] | 1.92 | 0.28 |

## 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 | 318/321 (99%) | 297 (93%) | 18 (6%) | 3 (1%) | 21 | 68 |
| 1 | E | 318/321 (99%) | 300 (94%) | 15 (5%) | 3 (1%) | 21 | 68 |
| 1 | I | 315/321 (98%) | 297 (94%) | 16 (5%) | 2 (1%) | 30 | 75 |
| 1 | M | 318/321 (99%) | 297 (93%) | 18 (6%) | 3 (1%) | 21 | 68 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | Q | 318/321 (99%) | 300 (94%) | 15 (5%) | 3 (1%) | 21 | 68 |
| 1 | U | 318/321 (99%) | 296 (93%) | 19 (6%) | 3 (1%) | 21 | 68 |
| 2 | B | 163/175 (93%) | 150 (92%) | 13 (8%) | 0 | 100 | 100 |
| 2 | F | 161/175 (92%) | 151 (94%) | 10 (6%) | 0 | 100 | 100 |
| 2 | J | 162/175 (93%) | 149 (92%) | 13 (8%) | 0 | 100 | 100 |
| 2 | N | 161/175 (92%) | 150 (93%) | 11 (7%) | 0 | 100 | 100 |
| 2 | R | 164/175 (94%) | 151 (92%) | 12 (7%) | 1 (1%) | 30 | 75 |
| 2 | V | 162/175 (93%) | 149 (92%) | 13 (8%) | 0 | 100 | 100 |
| 3 | C | 215/226 (95%) | 188 (87%) | 16 (7%) | 11 (5%) | 2 | 26 |
| 3 | G | 215/226 (95%) | 188 (87%) | 16 (7%) | 11 (5%) | 2 | 26 |
| 3 | K | 215/226 (95%) | 189 (88%) | 17 (8%) | 9 (4%) | 3 | 32 |
| 3 | O | 215/226 (95%) | 189 (88%) | 16 (7%) | 10 (5%) | 3 | 29 |
| 3 | S | 215/226 (95%) | 188 (87%) | 16 (7%) | 11 (5%) | 2 | 26 |
| 3 | Y | 215/226 (95%) | 189 (88%) | 17 (8%) | 9 (4%) | 3 | 32 |
| 4 | D | 211/215 (98%) | 200 (95%) | 9 (4%) | 2 (1%) | 21 | 68 |
| 4 | H | 211/215 (98%) | 201 (95%) | 8 (4%) | 2 (1%) | 21 | 68 |
| 4 | L | 211/215 (98%) | 200 (95%) | 9 (4%) | 2 (1%) | 21 | 68 |
| 4 | P | 211/215 (98%) | 201 (95%) | 8 (4%) | 2 (1%) | 21 | 68 |
| 4 | T | 211/215 (98%) | 201 (95%) | 8 (4%) | 2 (1%) | 21 | 68 |
| 4 | X | 211/215 (98%) | 202 (96%) | 7 (3%) | 2 (1%) | 21 | 68 |
| All | All | 5434/5622 (97%) | 5023 (92%) | 320 (6%) | 91 (2%) | 11 | 54 |

All (91) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 327 | GLN |
| 3 | C | 104 | ARG |
| 3 | C | 105 | VAL |
| 3 | C | 109 | SER |
| 3 | Y | 104 | ARG |
| 3 | Y | 105 | VAL |
| 3 | Y | 109 | SER |
| 3 | G | 104 | ARG |
| 3 | G | 105 | VAL |
| 3 | G | 109 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | S | 104 | ARG |
| 3 | S | 105 | VAL |
| 3 | S | 109 | SER |
| 3 | O | 104 | ARG |
| 3 | O | 105 | VAL |
| 3 | O | 109 | SER |
| 3 | K | 104 | ARG |
| 3 | K | 105 | VAL |
| 3 | K | 109 | SER |
| 1 | A | 62 | ILE |
| 1 | A | 137 | ASN |
| 1 | U | 62 | ILE |
| 1 | U | 326 | LYS |
| 1 | I | 62 | ILE |
| 1 | M | 62 | ILE |
| 1 | M | 327 | GLN |
| 1 | Q | 62 | ILE |
| 1 | E | 62 | ILE |
| 3 | C | 106 | GLU |
| 3 | C | 217 | ASN |
| 3 | Y | 100 | LYS |
| 3 | Y | 106 | GLU |
| 3 | Y | 217 | ASN |
| 3 | G | 106 | GLU |
| 3 | G | 217 | ASN |
| 3 | S | 106 | GLU |
| 3 | O | 106 | GLU |
| 3 | O | 217 | ASN |
| 3 | K | 106 | GLU |
| 3 | K | 217 | ASN |
| 3 | C | 16 | ALA |
| 3 | C | 100 | LYS |
| 4 | D | 205 | PRO |
| 3 | Y | 16 | ALA |
| 4 | X | 205 | PRO |
| 3 | G | 16 | ALA |
| 3 | G | 100 | LYS |
| 4 | H | 205 | PRO |
| 3 | S | 16 | ALA |
| 3 | S | 100 | LYS |
| 3 | S | 217 | ASN |
| 4 | T | 205 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 16 | ALA |
| 3 | O | 100 | LYS |
| 4 | P | 205 | PRO |
| 3 | K | 16 | ALA |
| 3 | K | 100 | LYS |
| 1 | Q | 201 | ARG |
| 1 | Q | 327 | GLN |
| 3 | C | 112 | ARG |
| 3 | Y | 112 | ARG |
| 3 | G | 112 | ARG |
| 3 | S | 112 | ARG |
| 3 | O | 112 | ARG |
| 3 | O | 201 | SER |
| 3 | K | 112 | ARG |
| 4 | L | 205 | PRO |
| 1 | A | 201 | ARG |
| 1 | U | 201 | ARG |
| 1 | I | 201 | ARG |
| 1 | E | 201 | ARG |
| 3 | C | 65 | GLN |
| 3 | Y | 65 | GLN |
| 3 | G | 65 | GLN |
| 3 | G | 201 | SER |
| 3 | S | 201 | SER |
| 3 | K | 201 | SER |
| 1 | M | 201 | ARG |
| 3 | C | 201 | SER |
| 4 | D | 9 | GLY |
| 4 | X | 9 | GLY |
| 3 | S | 65 | GLN |
| 4 | H | 9 | GLY |
| 4 | T | 9 | GLY |
| 4 | P | 9 | GLY |
| 4 | L | 9 | GLY |
| 2 | R | 173 | ILE |
| 3 | C | 14 | PRO |
| 3 | G | 2 | VAL |
| 3 | O | 2 | VAL |
| 3 | S | 2 | VAL |

### 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 | 282/283 (100%) | 269 (95%) | 13 (5%) | 33 | 72 |
| 1 | E | 282/283 (100%) | 270 (96%) | 12 (4%) | 35 | 74 |
| 1 | I | 279/283 (99%) | 271 (97%) | 8 (3%) | 50 | 81 |
| 1 | M | 282/283 (100%) | 272 (96%) | 10 (4%) | 43 | 78 |
| 1 | Q | 282/283 (100%) | 268 (95%) | 14 (5%) | 30 | 69 |
| 1 | U | 282/283 (100%) | 270 (96%) | 12 (4%) | 35 | 74 |
| 2 | B | 145/149 (97%) | 135 (93%) | 10 (7%) | 19 | 59 |
| 2 | F | 143/149 (96%) | 133 (93%) | 10 (7%) | 19 | 59 |
| 2 | J | 144/149 (97%) | 135 (94%) | 9 (6%) | 22 | 63 |
| 2 | N | 143/149 (96%) | 135 (94%) | 8 (6%) | 26 | 66 |
| 2 | R | 145/149 (97%) | 133 (92%) | 12 (8%) | 14 | 50 |
| 2 | V | 144/149 (97%) | 137 (95%) | 7 (5%) | 31 | 70 |
| 3 | C | 181/187 (97%) | 171 (94%) | 10 (6%) | 27 | 67 |
| 3 | G | 181/187 (97%) | 172 (95%) | 9 (5%) | 30 | 69 |
| 3 | K | 181/187 (97%) | 171 (94%) | 10 (6%) | 27 | 67 |
| 3 | O | 181/187 (97%) | 171 (94%) | 10 (6%) | 27 | 67 |
| 3 | S | 181/187 (97%) | 172 (95%) | 9 (5%) | 30 | 69 |
| 3 | Y | 181/187 (97%) | 172 (95%) | 9 (5%) | 30 | 69 |
| 4 | D | 184/186 (99%) | 172 (94%) | 12 (6%) | 21 | 62 |
| 4 | H | 184/186 (99%) | 173 (94%) | 11 (6%) | 24 | 64 |
| 4 | L | 184/186 (99%) | 173 (94%) | 11 (6%) | 24 | 64 |
| 4 | P | 184/186 (99%) | 173 (94%) | 11 (6%) | 24 | 64 |
| 4 | T | 184/186 (99%) | 173 (94%) | 11 (6%) | 24 | 64 |
| 4 | X | 184/186 (99%) | 172 (94%) | 12 (6%) | 21 | 62 |
| All | All | 4743/4830 (98%) | 4493 (95%) | 250 (5%) | 28 | 67 |

All (250) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 18 | HIS |
| 1 | A | 27 | LYS |
| 1 | A | 45 | SER |
| 1 | A | 65 | THR |
| 1 | A | 92 | LYS |
| 1 | A | 136 | SER |
| 1 | A | 140 | LYS |
| 1 | A | 145 | SER |
| 1 | A | 160 | THR |
| 1 | A | 207 | ARG |
| 1 | A | 208 | ARG |
| 1 | A | 261 | ARG |
| 1 | A | 315 | LYS |
| 1 | U | 18 | HIS |
| 1 | U | 45 | SER |
| 1 | U | 65 | THR |
| 1 | U | 92 | LYS |
| 1 | U | 136 | SER |
| 1 | U | 145 | SER |
| 1 | U | 160 | THR |
| 1 | U | 189 | GLN |
| 1 | U | 261 | ARG |
| 1 | U | 264 | LYS |
| 1 | U | 299 | LYS |
| 1 | U | 321 | ARG |
| 2 | V | 19 | ASP |
| 2 | V | 57 | GLU |
| 2 | V | 58 | LYS |
| 2 | V | 71 | SER |
| 2 | V | 116 | ASN |
| 2 | V | 128 | GLU |
| 2 | V | 168 | ASN |
| 1 | I | 45 | SER |
| 1 | I | 65 | THR |
| 1 | I | 92 | LYS |
| 1 | I | 136 | SER |
| 1 | I | 145 | SER |
| 1 | I | 160 | THR |
| 1 | I | 238 | LYS |
| 1 | I | 261 | ARG |
| 1 | M | 45 | SER |
| 1 | M | 65 | THR |
| 1 | M | 92 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | M | 145 | SER |
| 1 | M | 160 | THR |
| 1 | M | 188 | ASN |
| 1 | M | 210 | GLN |
| 1 | M | 238 | LYS |
| 1 | M | 261 | ARG |
| 1 | M | 280 | GLU |
| 1 | Q | 9 | SER |
| 1 | Q | 18 | HIS |
| 1 | Q | 45 | SER |
| 1 | Q | 65 | THR |
| 1 | Q | 92 | LYS |
| 1 | Q | 136 | SER |
| 1 | Q | 145 | SER |
| 1 | Q | 160 | THR |
| 1 | Q | 216 | ASN |
| 1 | Q | 222 | TRP |
| 1 | Q | 261 | ARG |
| 1 | Q | 299 | LYS |
| 1 | Q | 310 | LYS |
| 1 | Q | 326 | LYS |
| 1 | E | 9 | SER |
| 1 | E | 18 | HIS |
| 1 | E | 45 | SER |
| 1 | E | 65 | THR |
| 1 | E | 92 | LYS |
| 1 | E | 136 | SER |
| 1 | E | 145 | SER |
| 1 | E | 160 | THR |
| 1 | E | 189 | GLN |
| 1 | E | 208 | ARG |
| 1 | E | 261 | ARG |
| 1 | E | 299 | LYS |
| 2 | F | 10 | ILE |
| 2 | F | 11 | GLU |
| 2 | F | 18 | ILE |
| 2 | F | 19 | ASP |
| 2 | F | 38 | LEU |
| 2 | F | 58 | LYS |
| 2 | F | 71 | SER |
| 2 | F | 116 | ASN |
| 2 | F | 121 | LYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 168 | ASN |
| 2 | B | 9 | PHE |
| 2 | B | 10 | ILE |
| 2 | B | 19 | ASP |
| 2 | B | 57 | GLU |
| 2 | B | 58 | LYS |
| 2 | B | 71 | SER |
| 2 | B | 82 | LYS |
| 2 | B | 116 | ASN |
| 2 | B | 143 | LYS |
| 2 | B | 168 | ASN |
| 2 | J | 9 | PHE |
| 2 | J | 10 | ILE |
| 2 | J | 19 | ASP |
| 2 | J | 58 | LYS |
| 2 | J | 71 | SER |
| 2 | J | 79 | ASP |
| 2 | J | 116 | ASN |
| 2 | J | 124 | ARG |
| 2 | J | 168 | ASN |
| 2 | N | 10 | ILE |
| 2 | N | 46 | ASP |
| 2 | N | 71 | SER |
| 2 | N | 72 | GLU |
| 2 | N | 116 | ASN |
| 2 | N | 124 | ARG |
| 2 | N | 168 | ASN |
| 2 | N | 169 | ASN |
| 2 | R | 10 | ILE |
| 2 | R | 19 | ASP |
| 2 | R | 39 | LYS |
| 2 | R | 46 | ASP |
| 2 | R | 58 | LYS |
| 2 | R | 71 | SER |
| 2 | R | 116 | ASN |
| 2 | R | 123 | ARG |
| 2 | R | 143 | LYS |
| 2 | R | 150 | GLU |
| 2 | R | 168 | ASN |
| 2 | R | 173 | ILE |
| 3 | C | 4 | LEU |
| 3 | C | 89 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | C | 93 | THR |
| 3 | C | 106 | GLU |
| 3 | C | 137 | LEU |
| 3 | C | 153 | CYS |
| 3 | C | 190 | SER |
| 3 | C | 206 | THR |
| 3 | C | 214 | LYS |
| 3 | C | 222 | LYS |
| 4 | D | 5 | THR |
| 4 | D | 17 | GLU |
| 4 | D | 22 | SER |
| 4 | D | 32 | THR |
| 4 | D | 47 | ARG |
| 4 | D | 75 | THR |
| 4 | D | 97 | TRP |
| 4 | D | 122 | SER |
| 4 | D | 160 | SER |
| 4 | D | 165 | THR |
| 4 | D | 178 | SER |
| 4 | D | 183 | SER |
| 3 | Y | 89 | ASP |
| 3 | Y | 93 | THR |
| 3 | Y | 106 | GLU |
| 3 | Y | 137 | LEU |
| 3 | Y | 153 | CYS |
| 3 | Y | 190 | SER |
| 3 | Y | 206 | THR |
| 3 | Y | 214 | LYS |
| 3 | Y | 222 | LYS |
| 4 | X | 5 | THR |
| 4 | X | 17 | GLU |
| 4 | X | 22 | SER |
| 4 | X | 32 | THR |
| 4 | X | 47 | ARG |
| 4 | X | 75 | THR |
| 4 | X | 97 | TRP |
| 4 | X | 122 | SER |
| 4 | X | 160 | SER |
| 4 | X | 165 | THR |
| 4 | X | 178 | SER |
| 4 | X | 183 | SER |
| 3 | G | 89 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | G | 93 | THR |
| 3 | G | 106 | GLU |
| 3 | G | 137 | LEU |
| 3 | G | 153 | CYS |
| 3 | G | 190 | SER |
| 3 | G | 206 | THR |
| 3 | G | 214 | LYS |
| 3 | G | 222 | LYS |
| 4 | H | 5 | THR |
| 4 | H | 17 | GLU |
| 4 | H | 22 | SER |
| 4 | H | 32 | THR |
| 4 | H | 47 | ARG |
| 4 | H | 75 | THR |
| 4 | H | 97 | TRP |
| 4 | H | 122 | SER |
| 4 | H | 160 | SER |
| 4 | H | 178 | SER |
| 4 | H | 183 | SER |
| 3 | S | 89 | ASP |
| 3 | S | 93 | THR |
| 3 | S | 106 | GLU |
| 3 | S | 137 | LEU |
| 3 | S | 153 | CYS |
| 3 | S | 190 | SER |
| 3 | S | 206 | THR |
| 3 | S | 214 | LYS |
| 3 | S | 222 | LYS |
| 4 | T | 5 | THR |
| 4 | T | 17 | GLU |
| 4 | T | 22 | SER |
| 4 | T | 32 | THR |
| 4 | T | 47 | ARG |
| 4 | T | 75 | THR |
| 4 | T | 97 | TRP |
| 4 | T | 122 | SER |
| 4 | T | 160 | SER |
| 4 | T | 178 | SER |
| 4 | T | 183 | SER |
| 3 | O | 28 | SER |
| 3 | O | 89 | ASP |
| 3 | O | 93 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | O | 106 | GLU |
| 3 | O | 137 | LEU |
| 3 | O | 153 | CYS |
| 3 | O | 190 | SER |
| 3 | O | 206 | THR |
| 3 | O | 214 | LYS |
| 3 | O | 222 | LYS |
| 4 | P | 5 | THR |
| 4 | P | 17 | GLU |
| 4 | P | 22 | SER |
| 4 | P | 32 | THR |
| 4 | P | 47 | ARG |
| 4 | P | 75 | THR |
| 4 | P | 97 | TRP |
| 4 | P | 122 | SER |
| 4 | P | 160 | SER |
| 4 | P | 178 | SER |
| 4 | P | 183 | SER |
| 3 | K | 89 | ASP |
| 3 | K | 93 | THR |
| 3 | K | 105 | VAL |
| 3 | K | 106 | GLU |
| 3 | K | 137 | LEU |
| 3 | K | 153 | CYS |
| 3 | K | 190 | SER |
| 3 | K | 206 | THR |
| 3 | K | 214 | LYS |
| 3 | K | 222 | LYS |
| 4 | L | 5 | THR |
| 4 | L | 17 | GLU |
| 4 | L | 22 | SER |
| 4 | L | 32 | THR |
| 4 | L | 47 | ARG |
| 4 | L | 75 | THR |
| 4 | L | 97 | TRP |
| 4 | L | 122 | SER |
| 4 | L | 160 | SER |
| 4 | L | 178 | SER |
| 4 | L | 183 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 33 | GLN |
| 1 | A | 80 | GLN |
| 1 | A | 216 | ASN |
| 1 | U | 216 | ASN |
| 2 | V | 53 | ASN |
| 2 | V | 159 | HIS |
| 1 | M | 33 | GLN |
| 1 | M | 210 | GLN |
| 1 | Q | 33 | GLN |
| 1 | Q | 133 | ASN |
| 1 | Q | 137 | ASN |
| 1 | E | 133 | ASN |
| 2 | F | 53 | ASN |
| 2 | F | 60 | ASN |
| 2 | F | 159 | HIS |
| 2 | B | 53 | ASN |
| 2 | B | 78 | GLN |
| 2 | N | 60 | ASN |
| 2 | N | 159 | HIS |
| 2 | R | 53 | ASN |
| 2 | R | 159 | HIS |
| 3 | C | 113 | HIS |
| 3 | C | 210 | ASN |
| 4 | D | 43 | GLN |
| 4 | D | 139 | ASN |
| 4 | D | 148 | GLN |
| 4 | D | 161 | GLN |
| 3 | Y | 113 | HIS |
| 3 | Y | 210 | ASN |
| 4 | X | 27 | HIS |
| 4 | X | 43 | GLN |
| 4 | X | 139 | ASN |
| 4 | X | 148 | GLN |
| 4 | X | 161 | GLN |
| 3 | G | 113 | HIS |
| 3 | G | 210 | ASN |
| 4 | H | 43 | GLN |
| 4 | H | 54 | ASN |
| 4 | H | 139 | ASN |
| 4 | H | 148 | GLN |
| 3 | S | 113 | HIS |
| 3 | S | 210 | ASN |
| 4 | T | 43 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 4 | T | 139 | ASN |
| 4 | T | 148 | GLN |
| 3 | O | 113 | HIS |
| 3 | O | 210 | ASN |
| 4 | P | 27 | HIS |
| 4 | P | 43 | GLN |
| 4 | P | 139 | ASN |
| 4 | P | 148 | GLN |
| 3 | K | 113 | HIS |
| 3 | K | 210 | ASN |
| 4 | L | 43 | GLN |
| 4 | L | 139 | ASN |
| 4 | L | 148 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

25 non-standard protein/DNA/RNA residues 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 | $\#\|Z\| > 2$ |
| 5 | NAG | A | 401 | 1,5 | 14,14,15 | 0.66 | 0 | 15,19,21 | 1.71 | 4 (26%) |
| 5 | NAG | A | 402 | 5,6 | 14,14,15 | 0.64 | 0 | 15,19,21 | 2.44 | 5 (33%) |
| 5 | NAG | A | 405 | 1,5 | 14,14,15 | 0.86 | 1 (7%) | 15,19,21 | 2.93 | 5 (33%) |
| 5 | NAG | A | 406 | 5 | 14,14,15 | 0.71 | 0 | 15,19,21 | 1.70 | 3 (20%) |
| 5 | NAG | A | 407 | 1,5 | 14,14,15 | 0.94 | 1 (7%) | 15,19,21 | 2.35 | 6 (40%) |
| 5 | NAG | A | 408 | 5 | 14,14,15 | 0.81 | 1 (7%) | 15,19,21 | 1.98 | 4 (26%) |
| 5 | NAG | A | 409 | 1 | 14,14,15 | 1.01 | 1 (7%) | 15,19,21 | 3.33 | 9 (60%) |
| 5 | NAG | E | 401 | 1,5 | 14,14,15 | 0.68 | 0 | 15,19,21 | 1.30 | 3 (20%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | NAG | E | 402 | 5,6 | 14,14,15 | 0.75 | 0 | 15,19,21 | 3.17 | 9 (60%) |
| 5 | NAG | F | 201 | - | 14,14,15 | 0.91 | 0 | 15,19,21 | 2.20 | 6 (40%) |
| 5 | NAG | I | 401 | 1,5 | 14,14,15 | 0.74 | 0 | 15,19,21 | 3.98 | 10 (66%) |
| 5 | NAG | I | 402 | 5,6 | 14,14,15 | 0.78 | 1 (7%) | 15,19,21 | 3.79 | 9 (60%) |
| 5 | NAG | I | 405 | 1 | 14,14,15 | 1.57 | 2 (14%) | 15,19,21 | 2.54 | 8 (53%) |
| 5 | NAG | M | 401 | 1,5 | 14,14,15 | 0.54 | 0 | 15,19,21 | 2.22 | 3 (20%) |
| 5 | NAG | M | 402 | 5,6 | 14,14,15 | 0.65 | 0 | 15,19,21 | 2.45 | 6 (40%) |
| 5 | NAG | M | 405 | 1 | 14,14,15 | 1.02 | 1 (7%) | 15,19,21 | 1.29 | 2 (13%) |
| 5 | NAG | Q | 401 | 1,5 | 14,14,15 | 0.72 | 1 (7%) | 15,19,21 | 1.50 | 4 (26%) |
| 5 | NAG | Q | 402 | 5,6 | 14,14,15 | 0.54 | 0 | 15,19,21 | 2.43 | 5 (33%) |
| 5 | NAG | Q | 405 | 1,5 | 14,14,15 | 1.09 | 1 (7%) | 15,19,21 | 2.79 | 6 (40%) |
| 5 | NAG | Q | 406 | 5 | 14,14,15 | 0.82 | 0 | 15,19,21 | 1.52 | 2 (13%) |
| 5 | NAG | Q | 407 | 1 | 14,14,15 | 1.37 | 2 (14%) | 15,19,21 | 3.38 | 8 (53%) |
| 5 | NAG | U | 401 | 1,5 | 14,14,15 | 0.70 | 0 | 15,19,21 | 1.65 | 3 (20%) |
| 5 | NAG | U | 402 | 5,6 | 14,14,15 | 0.53 | 0 | 15,19,21 | 2.14 | 4 (26%) |
| 5 | NAG | U | 405 | - | 14,14,15 | 1.28 | 2 (14%) | 15,19,21 | 2.95 | 8 (53%) |
| 5 | NAG | V | 201 | 2 | 14,14,15 | 0.98 | 1 (7%) | 15,19,21 | 2.36 | 5 (33%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | NAG | A | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 405 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 406 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 407 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 408 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 409 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | F | 201 | - | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 405 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 5 | NAG | M | 405 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 405 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 406 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 407 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 405 | - | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | V | 201 | 2 | - | 0/6/23/26 | 0/1/1/1 |

All (15) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 401 | NAG | O5-C1 | -2.12 | 1.40 | 1.43 |
| 5 | A | 407 | NAG | C1-C2 | 2.12 | 1.55 | 1.52 |
| 5 | U | 405 | NAG | C4-C5 | 2.17 | 1.57 | 1.53 |
| 5 | A | 409 | NAG | C3-C2 | 2.19 | 1.57 | 1.52 |
| 5 | A | 405 | NAG | C1-C2 | 2.20 | 1.55 | 1.52 |
| 5 | Q | 407 | NAG | C3-C2 | 2.22 | 1.57 | 1.52 |
| 5 | I | 402 | NAG | C3-C2 | 2.23 | 1.57 | 1.52 |
| 5 | I | 405 | NAG | C3-C2 | 2.29 | 1.57 | 1.52 |
| 5 | A | 408 | NAG | C1-C2 | 2.36 | 1.55 | 1.52 |
| 5 | U | 405 | NAG | C3-C2 | 2.68 | 1.58 | 1.52 |
| 5 | V | 201 | NAG | C1-C2 | 2.71 | 1.56 | 1.52 |
| 5 | M | 405 | NAG | C1-C2 | 2.98 | 1.56 | 1.52 |
| 5 | Q | 407 | NAG | C4-C5 | 3.05 | 1.59 | 1.53 |
| 5 | Q | 405 | NAG | C1-C2 | 3.55 | 1.57 | 1.52 |
| 5 | I | 405 | NAG | C1-C2 | 4.44 | 1.58 | 1.52 |

All (137) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 402 | NAG | O3-C3-C4 | -5.40 | 98.17 | 110.36 |
| 5 | U | 405 | NAG | O3-C3-C4 | -5.27 | 98.47 | 110.36 |
| 5 | A | 409 | NAG | O3-C3-C4 | -5.27 | 98.49 | 110.36 |
| 5 | A | 402 | NAG | O3-C3-C4 | -5.17 | 98.70 | 110.36 |
| 5 | I | 402 | NAG | O3-C3-C4 | -5.16 | 98.73 | 110.36 |
| 5 | U | 402 | NAG | O3-C3-C4 | -5.11 | 98.85 | 110.36 |
| 5 | E | 402 | NAG | O3-C3-C4 | -4.94 | 99.23 | 110.36 |
| 5 | U | 405 | NAG | O7-C7-C8 | -4.93 | 113.00 | 122.07 |
| 5 | I | 402 | NAG | C3-C4-C5 | -4.42 | 102.35 | 110.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 407 | NAG | O7-C7-C8 | -3.87 | 114.94 | 122.07 |
| 5 | A | 407 | NAG | O5-C5-C4 | -3.70 | 104.00 | 110.13 |
| 5 | E | 402 | NAG | O7-C7-C8 | -3.60 | 115.44 | 122.07 |
| 5 | F | 201 | NAG | O7-C7-C8 | -3.46 | 115.70 | 122.07 |
| 5 | I | 405 | NAG | O5-C5-C4 | -3.40 | 104.50 | 110.13 |
| 5 | I | 405 | NAG | O7-C7-C8 | -3.34 | 115.92 | 122.07 |
| 5 | I | 405 | NAG | C4-C3-C2 | -3.32 | 106.18 | 111.34 |
| 5 | A | 405 | NAG | C2-N2-C7 | -3.29 | 118.82 | 123.11 |
| 5 | M | 402 | NAG | C3-C4-C5 | -3.27 | 104.39 | 110.23 |
| 5 | E | 402 | NAG | C3-C4-C5 | -3.23 | 104.47 | 110.23 |
| 5 | M | 401 | NAG | O3-C3-C2 | -3.14 | 102.65 | 109.37 |
| 5 | M | 402 | NAG | O3-C3-C4 | -2.91 | 103.80 | 110.36 |
| 5 | A | 402 | NAG | O7-C7-C8 | -2.88 | 116.77 | 122.07 |
| 5 | I | 405 | NAG | C3-C4-C5 | -2.87 | 105.10 | 110.23 |
| 5 | A | 409 | NAG | O7-C7-C8 | -2.79 | 116.93 | 122.07 |
| 5 | A | 407 | NAG | C3-C4-C5 | -2.77 | 105.28 | 110.23 |
| 5 | I | 402 | NAG | C6-C5-C4 | -2.65 | 106.36 | 112.99 |
| 5 | V | 201 | NAG | O7-C7-C8 | -2.54 | 117.39 | 122.07 |
| 5 | E | 402 | NAG | O5-C5-C6 | -2.51 | 101.96 | 107.34 |
| 5 | M | 402 | NAG | C2-N2-C7 | -2.50 | 119.85 | 123.11 |
| 5 | I | 401 | NAG | O7-C7-C8 | -2.49 | 117.49 | 122.07 |
| 5 | Q | 407 | NAG | O3-C3-C4 | -2.43 | 104.88 | 110.36 |
| 5 | A | 407 | NAG | O7-C7-C8 | -2.41 | 117.63 | 122.07 |
| 5 | Q | 401 | NAG | O7-C7-C8 | -2.37 | 117.71 | 122.07 |
| 5 | A | 401 | NAG | O3-C3-C4 | -2.36 | 105.03 | 110.36 |
| 5 | A | 405 | NAG | C6-C5-C4 | -2.33 | 107.15 | 112.99 |
| 5 | I | 401 | NAG | O3-C3-C2 | -2.33 | 104.40 | 109.37 |
| 5 | Q | 405 | NAG | O4-C4-C5 | -2.31 | 103.15 | 109.23 |
| 5 | Q | 401 | NAG | O3-C3-C4 | -2.30 | 105.16 | 110.36 |
| 5 | E | 401 | NAG | O5-C5-C4 | -2.21 | 106.47 | 110.13 |
| 5 | A | 408 | NAG | O7-C7-C8 | -2.20 | 118.02 | 122.07 |
| 5 | Q | 402 | NAG | O7-C7-C8 | -2.19 | 118.03 | 122.07 |
| 5 | I | 402 | NAG | O7-C7-C8 | -2.19 | 118.05 | 122.07 |
| 5 | E | 401 | NAG | C1-O5-C5 | -2.18 | 108.93 | 112.14 |
| 5 | I | 401 | NAG | O3-C3-C4 | -2.17 | 105.47 | 110.36 |
| 5 | Q | 402 | NAG | C3-C4-C5 | -2.16 | 106.38 | 110.23 |
| 5 | I | 402 | NAG | C2-N2-C7 | -2.14 | 120.32 | 123.11 |
| 5 | F | 201 | NAG | O5-C5-C4 | -2.13 | 106.60 | 110.13 |
| 5 | Q | 401 | NAG | C1-O5-C5 | -2.13 | 109.01 | 112.14 |
| 5 | I | 405 | NAG | O5-C5-C6 | -2.07 | 102.92 | 107.34 |
| 5 | U | 402 | NAG | C2-N2-C7 | -2.05 | 120.44 | 123.11 |
| 5 | V | 201 | NAG | O5-C5-C6 | 2.00 | 111.62 | 107.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 409 | NAG | C4-C3-C2 | 2.02 | 114.48 | 111.34 |
| 5 | I | 401 | NAG | O6-C6-C5 | 2.03 | 118.09 | 111.30 |
| 5 | E | 401 | NAG | C6-C5-C4 | 2.04 | 118.09 | 112.99 |
| 5 | A | 401 | NAG | C3-C4-C5 | 2.04 | 113.87 | 110.23 |
| 5 | A | 407 | NAG | O3-C3-C2 | 2.09 | 113.85 | 109.37 |
| 5 | Q | 405 | NAG | O5-C5-C6 | 2.12 | 111.87 | 107.34 |
| 5 | U | 405 | NAG | C4-C3-C2 | 2.12 | 114.63 | 111.34 |
| 5 | M | 405 | NAG | O4-C4-C5 | 2.18 | 114.97 | 109.23 |
| 5 | Q | 401 | NAG | C4-C3-C2 | 2.23 | 114.80 | 111.34 |
| 5 | A | 408 | NAG | C2-N2-C7 | 2.27 | 126.06 | 123.11 |
| 5 | A | 409 | NAG | O5-C5-C4 | 2.29 | 113.93 | 110.13 |
| 5 | Q | 406 | NAG | O3-C3-C4 | 2.29 | 115.53 | 110.36 |
| 5 | A | 405 | NAG | O4-C4-C5 | 2.32 | 115.33 | 109.23 |
| 5 | U | 401 | NAG | C3-C4-C5 | 2.33 | 114.39 | 110.23 |
| 5 | A | 408 | NAG | O5-C5-C6 | 2.38 | 112.43 | 107.34 |
| 5 | M | 405 | NAG | O3-C3-C2 | 2.49 | 114.70 | 109.37 |
| 5 | M | 402 | NAG | O4-C4-C5 | 2.50 | 115.82 | 109.23 |
| 5 | I | 405 | NAG | O4-C4-C5 | 2.54 | 115.91 | 109.23 |
| 5 | A | 401 | NAG | C4-C3-C2 | 2.62 | 115.41 | 111.34 |
| 5 | A | 406 | NAG | C4-C3-C2 | 2.65 | 115.45 | 111.34 |
| 5 | F | 201 | NAG | C1-O5-C5 | 2.69 | 116.10 | 112.14 |
| 5 | A | 407 | NAG | O4-C4-C5 | 2.70 | 116.33 | 109.23 |
| 5 | F | 201 | NAG | C2-N2-C7 | 2.70 | 126.62 | 123.11 |
| 5 | E | 402 | NAG | O7-C7-N2 | 2.76 | 127.47 | 121.84 |
| 5 | F | 201 | NAG | O5-C5-C6 | 2.79 | 113.31 | 107.34 |
| 5 | M | 402 | NAG | O5-C5-C4 | 2.98 | 115.07 | 110.13 |
| 5 | Q | 405 | NAG | O5-C5-C4 | 2.99 | 115.08 | 110.13 |
| 5 | U | 402 | NAG | C4-C3-C2 | 3.00 | 115.99 | 111.34 |
| 5 | U | 401 | NAG | C4-C3-C2 | 3.03 | 116.04 | 111.34 |
| 5 | V | 201 | NAG | O4-C4-C3 | 3.06 | 117.25 | 110.36 |
| 5 | U | 405 | NAG | O7-C7-N2 | 3.07 | 128.10 | 121.84 |
| 5 | Q | 407 | NAG | O7-C7-N2 | 3.10 | 128.16 | 121.84 |
| 5 | V | 201 | NAG | C2-N2-C7 | 3.16 | 127.22 | 123.11 |
| 5 | Q | 402 | NAG | O4-C4-C5 | 3.17 | 117.56 | 109.23 |
| 5 | A | 409 | NAG | O3-C3-C2 | 3.19 | 116.20 | 109.37 |
| 5 | A | 401 | NAG | C1-O5-C5 | 3.20 | 116.84 | 112.14 |
| 5 | I | 402 | NAG | O4-C4-C5 | 3.29 | 117.88 | 109.23 |
| 5 | Q | 407 | NAG | C6-C5-C4 | 3.29 | 121.24 | 112.99 |
| 5 | U | 405 | NAG | O3-C3-C2 | 3.32 | 116.48 | 109.37 |
| 5 | M | 401 | NAG | O5-C5-C4 | 3.37 | 115.71 | 110.13 |
| 5 | U | 405 | NAG | O5-C5-C4 | 3.43 | 115.81 | 110.13 |
| 5 | I | 401 | NAG | O7-C7-N2 | 3.62 | 129.22 | 121.84 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | Q | 405 | NAG | O3-C3-C4 | 3.69 | 118.69 | 110.36 |
| 5 | A | 406 | NAG | O5-C5-C6 | 3.71 | 115.27 | 107.34 |
| 5 | I | 401 | NAG | O5-C5-C6 | 3.72 | 115.31 | 107.34 |
| 5 | U | 405 | NAG | O4-C4-C5 | 3.73 | 119.06 | 109.23 |
| 5 | A | 409 | NAG | O7-C7-N2 | 3.74 | 129.47 | 121.84 |
| 5 | I | 405 | NAG | C6-C5-C4 | 3.76 | 122.40 | 112.99 |
| 5 | A | 402 | NAG | O4-C4-C5 | 3.80 | 119.24 | 109.23 |
| 5 | I | 401 | NAG | O5-C5-C4 | 3.80 | 116.43 | 110.13 |
| 5 | A | 406 | NAG | C1-O5-C5 | 3.80 | 117.73 | 112.14 |
| 5 | A | 402 | NAG | C4-C3-C2 | 3.82 | 117.26 | 111.34 |
| 5 | E | 402 | NAG | C4-C3-C2 | 3.99 | 117.53 | 111.34 |
| 5 | Q | 406 | NAG | C1-O5-C5 | 4.04 | 118.08 | 112.14 |
| 5 | U | 401 | NAG | C1-O5-C5 | 4.07 | 118.12 | 112.14 |
| 5 | U | 402 | NAG | O4-C4-C5 | 4.11 | 120.06 | 109.23 |
| 5 | A | 409 | NAG | C2-N2-C7 | 4.11 | 128.46 | 123.11 |
| 5 | E | 402 | NAG | O5-C5-C4 | 4.16 | 117.03 | 110.13 |
| 5 | E | 402 | NAG | O4-C4-C5 | 4.26 | 120.45 | 109.23 |
| 5 | A | 402 | NAG | C1-O5-C5 | 4.33 | 118.50 | 112.14 |
| 5 | I | 405 | NAG | O3-C3-C2 | 4.36 | 118.71 | 109.37 |
| 5 | U | 405 | NAG | C2-N2-C7 | 4.48 | 128.93 | 123.11 |
| 5 | I | 401 | NAG | C2-N2-C7 | 4.60 | 129.09 | 123.11 |
| 5 | Q | 402 | NAG | C4-C3-C2 | 4.62 | 118.52 | 111.34 |
| 5 | I | 401 | NAG | O4-C4-C3 | 4.65 | 120.85 | 110.36 |
| 5 | Q | 407 | NAG | O3-C3-C2 | 4.73 | 119.50 | 109.37 |
| 5 | F | 201 | NAG | C4-C3-C2 | 4.78 | 118.76 | 111.34 |
| 5 | A | 409 | NAG | O4-C4-C5 | 4.87 | 122.06 | 109.23 |
| 5 | Q | 407 | NAG | C2-N2-C7 | 4.96 | 129.56 | 123.11 |
| 5 | I | 402 | NAG | O5-C5-C4 | 4.97 | 118.37 | 110.13 |
| 5 | Q | 407 | NAG | O4-C4-C5 | 5.34 | 123.28 | 109.23 |
| 5 | A | 407 | NAG | C1-O5-C5 | 5.40 | 120.08 | 112.14 |
| 5 | E | 402 | NAG | C1-O5-C5 | 5.80 | 120.68 | 112.14 |
| 5 | A | 408 | NAG | C1-O5-C5 | 5.91 | 120.82 | 112.14 |
| 5 | Q | 405 | NAG | C3-C4-C5 | 5.99 | 120.91 | 110.23 |
| 5 | V | 201 | NAG | C1-O5-C5 | 6.35 | 121.47 | 112.14 |
| 5 | A | 405 | NAG | O5-C5-C4 | 6.36 | 120.67 | 110.13 |
| 5 | I | 402 | NAG | C4-C3-C2 | 6.36 | 121.21 | 111.34 |
| 5 | M | 401 | NAG | C1-O5-C5 | 6.38 | 121.52 | 112.14 |
| 5 | Q | 407 | NAG | C1-O5-C5 | 6.39 | 121.54 | 112.14 |
| 5 | Q | 405 | NAG | C1-O5-C5 | 6.43 | 121.60 | 112.14 |
| 5 | M | 402 | NAG | C1-O5-C5 | 6.55 | 121.78 | 112.14 |
| 5 | A | 409 | NAG | C1-O5-C5 | 7.27 | 122.83 | 112.14 |
| 5 | A | 405 | NAG | C1-O5-C5 | 7.49 | 123.15 | 112.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 402 | NAG | C1-O5-C5 | 8.31 | 124.36 | 112.14 |
| 5 | I | 401 | NAG | C1-O5-C5 | 11.20 | 128.61 | 112.14 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 17 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | A | 405 | NAG | 1 | 0 |
| 5 | I | 401 | NAG | 1 | 0 |
| 5 | I | 402 | NAG | 1 | 0 |
| 5 | I | 405 | NAG | 2 | 0 |
| 5 | Q | 405 | NAG | 3 | 0 |
| 5 | Q | 406 | NAG | 4 | 0 |
| 5 | U | 405 | NAG | 5 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

37 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 | $\#\|Z\| > 2$ |
| 5 | NAG | A | 401 | 1,5 | 14,14,15 | 0.66 | 0 | 15,19,21 | 1.71 | 4 (26%) |
| 5 | NAG | A | 402 | 5,6 | 14,14,15 | 0.64 | 0 | 15,19,21 | 2.44 | 5 (33%) |
| 6 | BMA | A | 403 | 5,7 | 11,11,12 | 1.08 | 0 | 15,15,17 | 3.24 | 8 (53%) |
| 7 | MAN | A | 404 | 6 | 11,11,12 | 0.75 | 0 | 15,15,17 | 2.77 | 4 (26%) |
| 5 | NAG | A | 405 | 1,5 | 14,14,15 | 0.86 | 1 (7%) | 15,19,21 | 2.93 | 5 (33%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 5 | NAG | A | 406 | 5 | 14,14,15 | 0.71 | 0 | 15,19,21 | 1.70 | 3 (20%) |
| 5 | NAG | A | 407 | 1,5 | 14,14,15 | 0.94 | 1 (7%) | 15,19,21 | 2.35 | 6 (40%) |
| 5 | NAG | A | 408 | 5 | 14,14,15 | 0.81 | 1 (7%) | 15,19,21 | 1.98 | 4 (26%) |
| 5 | NAG | A | 409 | 1 | 14,14,15 | 1.01 | 1 (7%) | 15,19,21 | 3.33 | 9 (60%) |
| 5 | NAG | E | 401 | 1,5 | 14,14,15 | 0.68 | 0 | 15,19,21 | 1.30 | 3 (20%) |
| 5 | NAG | E | 402 | 5,6 | 14,14,15 | 0.75 | 0 | 15,19,21 | 3.17 | 9 (60%) |
| 6 | BMA | E | 403 | 5,7 | 11,11,12 | 1.24 | 1 (9%) | 15,15,17 | 3.22 | 6 (40%) |
| 7 | MAN | E | 404 | 6 | 11,11,12 | 0.70 | 0 | 15,15,17 | 2.04 | 5 (33%) |
| 5 | NAG | F | 201 | - | 14,14,15 | 0.91 | 0 | 15,19,21 | 2.20 | 6 (40%) |
| 5 | NAG | I | 401 | 1,5 | 14,14,15 | 0.74 | 0 | 15,19,21 | 3.98 | 10 (66%) |
| 5 | NAG | I | 402 | 5,6 | 14,14,15 | 0.78 | 1 (7%) | 15,19,21 | 3.79 | 9 (60%) |
| 6 | BMA | I | 403 | 5,7 | 11,11,12 | 0.94 | 0 | 15,15,17 | 3.66 | 9 (60%) |
| 7 | MAN | I | 404 | 6 | 11,11,12 | 1.24 | 2 (18%) | 15,15,17 | 2.66 | 5 (33%) |
| 5 | NAG | I | 405 | 1 | 14,14,15 | 1.57 | 2 (14%) | 15,19,21 | 2.54 | 8 (53%) |
| 5 | NAG | M | 401 | 1,5 | 14,14,15 | 0.54 | 0 | 15,19,21 | 2.22 | 3 (20%) |
| 5 | NAG | M | 402 | 5,6 | 14,14,15 | 0.65 | 0 | 15,19,21 | 2.45 | 6 (40%) |
| 6 | BMA | M | 403 | 5,7 | 11,11,12 | 0.51 | 0 | 15,15,17 | 2.78 | 6 (40%) |
| 7 | MAN | M | 404 | 6 | 11,11,12 | 0.75 | 0 | 15,15,17 | 1.80 | 5 (33%) |
| 5 | NAG | M | 405 | 1 | 14,14,15 | 1.02 | 1 (7%) | 15,19,21 | 1.29 | 2 (13%) |
| 5 | NAG | Q | 401 | 1,5 | 14,14,15 | 0.72 | 1 (7%) | 15,19,21 | 1.50 | 4 (26%) |
| 5 | NAG | Q | 402 | 5,6 | 14,14,15 | 0.54 | 0 | 15,19,21 | 2.43 | 5 (33%) |
| 6 | BMA | Q | 403 | 5,7 | 11,11,12 | 1.21 | 1 (9%) | 15,15,17 | 2.74 | 6 (40%) |
| 7 | MAN | Q | 404 | 6 | 11,11,12 | 1.02 | 1 (9%) | 15,15,17 | 2.29 | 7 (46%) |
| 5 | NAG | Q | 405 | 1,5 | 14,14,15 | 1.09 | 1 (7%) | 15,19,21 | 2.79 | 6 (40%) |
| 5 | NAG | Q | 406 | 5 | 14,14,15 | 0.82 | 0 | 15,19,21 | 1.52 | 2 (13%) |
| 5 | NAG | Q | 407 | 1 | 14,14,15 | 1.37 | 2 (14%) | 15,19,21 | 3.38 | 8 (53%) |
| 5 | NAG | U | 401 | 1,5 | 14,14,15 | 0.70 | 0 | 15,19,21 | 1.65 | 3 (20%) |
| 5 | NAG | U | 402 | 5,6 | 14,14,15 | 0.53 | 0 | 15,19,21 | 2.14 | 4 (26%) |
| 6 | BMA | U | 403 | 5,7 | 11,11,12 | 1.00 | 0 | 15,15,17 | 2.97 | 6 (40%) |
| 7 | MAN | U | 404 | 6 | 11,11,12 | 0.77 | 0 | 15,15,17 | 2.65 | 6 (40%) |
| 5 | NAG | U | 405 | - | 14,14,15 | 1.28 | 2 (14%) | 15,19,21 | 2.95 | 8 (53%) |
| 5 | NAG | V | 201 | 2 | 14,14,15 | 0.98 | 1 (7%) | 15,19,21 | 2.36 | 5 (33%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | NAG | A | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | A | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | A | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | A | 405 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 406 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 407 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 408 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 409 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | E | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | E | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | E | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | F | 201 | - | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | I | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | I | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | I | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | I | 405 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | M | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | M | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | M | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | M | 405 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | Q | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | Q | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | Q | 405 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 406 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | Q | 407 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 401 | 1,5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | U | 402 | 5,6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | BMA | U | 403 | 5,7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | U | 404 | 6 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 5 | NAG | U | 405 | - | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | V | 201 | 2 | - | 0/6/23/26 | 0/1/1/1 |

All (20) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | I | 404 | MAN | O5-C1 | -2.18 | 1.40 | 1.43 |
| 5 | Q | 401 | NAG | O5-C1 | -2.12 | 1.40 | 1.43 |
| 5 | A | 407 | NAG | C1-C2 | 2.12 | 1.55 | 1.52 |
| 5 | U | 405 | NAG | C4-C5 | 2.17 | 1.57 | 1.53 |
| 5 | A | 409 | NAG | C3-C2 | 2.19 | 1.57 | 1.52 |
| 5 | A | 405 | NAG | C1-C2 | 2.20 | 1.55 | 1.52 |
| 5 | Q | 407 | NAG | C3-C2 | 2.22 | 1.57 | 1.52 |
| 5 | I | 402 | NAG | C3-C2 | 2.23 | 1.57 | 1.52 |
| 5 | I | 405 | NAG | C3-C2 | 2.29 | 1.57 | 1.52 |
| 7 | Q | 404 | MAN | C1-C2 | 2.30 | 1.57 | 1.52 |
| 5 | A | 408 | NAG | C1-C2 | 2.36 | 1.55 | 1.52 |
| 6 | E | 403 | BMA | C2-C3 | 2.56 | 1.56 | 1.52 |
| 7 | I | 404 | MAN | C2-C3 | 2.66 | 1.56 | 1.52 |
| 5 | U | 405 | NAG | C3-C2 | 2.68 | 1.58 | 1.52 |
| 5 | V | 201 | NAG | C1-C2 | 2.71 | 1.56 | 1.52 |
| 6 | Q | 403 | BMA | C2-C3 | 2.79 | 1.56 | 1.52 |
| 5 | M | 405 | NAG | C1-C2 | 2.98 | 1.56 | 1.52 |
| 5 | Q | 407 | NAG | C4-C5 | 3.05 | 1.59 | 1.53 |
| 5 | Q | 405 | NAG | C1-C2 | 3.55 | 1.57 | 1.52 |
| 5 | I | 405 | NAG | C1-C2 | 4.44 | 1.58 | 1.52 |

All (210) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | A | 404 | MAN | C1-C2-C3 | -7.83 | 100.07 | 109.55 |
| 7 | I | 404 | MAN | C1-O5-C5 | -7.63 | 100.91 | 112.14 |
| 5 | Q | 402 | NAG | O3-C3-C4 | -5.40 | 98.17 | 110.36 |
| 6 | M | 403 | BMA | O3-C3-C4 | -5.36 | 98.26 | 110.36 |
| 5 | U | 405 | NAG | O3-C3-C4 | -5.27 | 98.47 | 110.36 |
| 5 | A | 409 | NAG | O3-C3-C4 | -5.27 | 98.49 | 110.36 |
| 5 | A | 402 | NAG | O3-C3-C4 | -5.17 | 98.70 | 110.36 |
| 5 | I | 402 | NAG | O3-C3-C4 | -5.16 | 98.73 | 110.36 |
| 5 | U | 402 | NAG | O3-C3-C4 | -5.11 | 98.85 | 110.36 |
| 7 | U | 404 | MAN | C1-C2-C3 | -5.06 | 103.42 | 109.55 |
| 5 | E | 402 | NAG | O3-C3-C4 | -4.94 | 99.23 | 110.36 |
| 5 | U | 405 | NAG | O7-C7-C8 | -4.93 | 113.00 | 122.07 |
| 6 | I | 403 | BMA | O3-C3-C4 | -4.70 | 99.77 | 110.36 |
| 5 | I | 402 | NAG | C3-C4-C5 | -4.42 | 102.35 | 110.23 |
| 6 | U | 403 | BMA | O3-C3-C2 | -4.32 | 102.08 | 110.01 |
| 6 | A | 403 | BMA | O3-C3-C4 | -3.94 | 101.47 | 110.36 |
| 5 | Q | 407 | NAG | O7-C7-C8 | -3.87 | 114.94 | 122.07 |
| 5 | A | 407 | NAG | O5-C5-C4 | -3.70 | 104.00 | 110.13 |
| 5 | E | 402 | NAG | O7-C7-C8 | -3.60 | 115.44 | 122.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | F | 201 | NAG | O7-C7-C8 | -3.46 | 115.70 | 122.07 |
| 6 | I | 403 | BMA | O4-C4-C3 | -3.44 | 102.59 | 110.36 |
| 5 | I | 405 | NAG | O5-C5-C4 | -3.40 | 104.50 | 110.13 |
| 7 | M | 404 | MAN | C1-O5-C5 | -3.34 | 107.22 | 112.14 |
| 5 | I | 405 | NAG | O7-C7-C8 | -3.34 | 115.92 | 122.07 |
| 5 | I | 405 | NAG | C4-C3-C2 | -3.32 | 106.18 | 111.34 |
| 5 | A | 405 | NAG | C2-N2-C7 | -3.29 | 118.82 | 123.11 |
| 5 | M | 402 | NAG | C3-C4-C5 | -3.27 | 104.39 | 110.23 |
| 5 | E | 402 | NAG | C3-C4-C5 | -3.23 | 104.47 | 110.23 |
| 6 | A | 403 | BMA | O4-C4-C3 | -3.19 | 103.16 | 110.36 |
| 5 | M | 401 | NAG | O3-C3-C2 | -3.14 | 102.65 | 109.37 |
| 6 | Q | 403 | BMA | O3-C3-C4 | -3.11 | 103.34 | 110.36 |
| 7 | A | 404 | MAN | C1-O5-C5 | -3.00 | 107.73 | 112.14 |
| 5 | M | 402 | NAG | O3-C3-C4 | -2.91 | 103.80 | 110.36 |
| 5 | A | 402 | NAG | O7-C7-C8 | -2.88 | 116.77 | 122.07 |
| 6 | I | 403 | BMA | O2-C2-C3 | -2.88 | 104.38 | 110.19 |
| 5 | I | 405 | NAG | C3-C4-C5 | -2.87 | 105.10 | 110.23 |
| 5 | A | 409 | NAG | O7-C7-C8 | -2.79 | 116.93 | 122.07 |
| 5 | A | 407 | NAG | C3-C4-C5 | -2.77 | 105.28 | 110.23 |
| 6 | E | 403 | BMA | O3-C3-C4 | -2.77 | 104.11 | 110.36 |
| 7 | E | 404 | MAN | O2-C2-C3 | -2.66 | 104.82 | 110.19 |
| 5 | I | 402 | NAG | C6-C5-C4 | -2.65 | 106.36 | 112.99 |
| 6 | M | 403 | BMA | O5-C5-C4 | -2.55 | 105.92 | 110.13 |
| 5 | V | 201 | NAG | O7-C7-C8 | -2.54 | 117.39 | 122.07 |
| 5 | E | 402 | NAG | O5-C5-C6 | -2.51 | 101.96 | 107.34 |
| 5 | M | 402 | NAG | C2-N2-C7 | -2.50 | 119.85 | 123.11 |
| 5 | I | 401 | NAG | O7-C7-C8 | -2.49 | 117.49 | 122.07 |
| 6 | M | 403 | BMA | O4-C4-C3 | -2.44 | 104.86 | 110.36 |
| 5 | Q | 407 | NAG | O3-C3-C4 | -2.43 | 104.88 | 110.36 |
| 5 | A | 407 | NAG | O7-C7-C8 | -2.41 | 117.63 | 122.07 |
| 5 | Q | 401 | NAG | O7-C7-C8 | -2.37 | 117.71 | 122.07 |
| 5 | A | 401 | NAG | O3-C3-C4 | -2.36 | 105.03 | 110.36 |
| 5 | A | 405 | NAG | C6-C5-C4 | -2.33 | 107.15 | 112.99 |
| 5 | I | 401 | NAG | O3-C3-C2 | -2.33 | 104.40 | 109.37 |
| 5 | Q | 405 | NAG | O4-C4-C5 | -2.31 | 103.15 | 109.23 |
| 5 | Q | 401 | NAG | O3-C3-C4 | -2.30 | 105.16 | 110.36 |
| 7 | U | 404 | MAN | C1-O5-C5 | -2.23 | 108.86 | 112.14 |
| 5 | E | 401 | NAG | O5-C5-C4 | -2.21 | 106.47 | 110.13 |
| 5 | A | 408 | NAG | O7-C7-C8 | -2.20 | 118.02 | 122.07 |
| 6 | E | 403 | BMA | O2-C2-C1 | -2.20 | 104.83 | 109.23 |
| 5 | Q | 402 | NAG | O7-C7-C8 | -2.19 | 118.03 | 122.07 |
| 5 | I | 402 | NAG | O7-C7-C8 | -2.19 | 118.05 | 122.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | E | 401 | NAG | C1-O5-C5 | -2.18 | 108.93 | 112.14 |
| 5 | I | 401 | NAG | O3-C3-C4 | -2.17 | 105.47 | 110.36 |
| 5 | Q | 402 | NAG | C3-C4-C5 | -2.16 | 106.38 | 110.23 |
| 5 | I | 402 | NAG | C2-N2-C7 | -2.14 | 120.32 | 123.11 |
| 5 | F | 201 | NAG | O5-C5-C4 | -2.13 | 106.60 | 110.13 |
| 5 | Q | 401 | NAG | C1-O5-C5 | -2.13 | 109.01 | 112.14 |
| 6 | Q | 403 | BMA | O5-C5-C4 | -2.12 | 106.63 | 110.13 |
| 7 | M | 404 | MAN | O6-C6-C5 | -2.07 | 104.39 | 111.30 |
| 5 | I | 405 | NAG | O5-C5-C6 | -2.07 | 102.92 | 107.34 |
| 5 | U | 402 | NAG | C2-N2-C7 | -2.05 | 120.44 | 123.11 |
| 7 | Q | 404 | MAN | O3-C3-C4 | -2.03 | 105.78 | 110.36 |
| 5 | V | 201 | NAG | O5-C5-C6 | 2.00 | 111.62 | 107.34 |
| 5 | A | 409 | NAG | C4-C3-C2 | 2.02 | 114.48 | 111.34 |
| 7 | E | 404 | MAN | O2-C2-C1 | 2.02 | 113.28 | 109.23 |
| 7 | Q | 404 | MAN | O2-C2-C1 | 2.02 | 113.29 | 109.23 |
| 5 | I | 401 | NAG | O6-C6-C5 | 2.03 | 118.09 | 111.30 |
| 5 | E | 401 | NAG | C6-C5-C4 | 2.04 | 118.09 | 112.99 |
| 5 | A | 401 | NAG | C3-C4-C5 | 2.04 | 113.87 | 110.23 |
| 7 | A | 404 | MAN | O3-C3-C4 | 2.05 | 114.99 | 110.36 |
| 7 | M | 404 | MAN | O5-C5-C4 | 2.07 | 113.57 | 110.13 |
| 5 | A | 407 | NAG | O3-C3-C2 | 2.09 | 113.85 | 109.37 |
| 7 | Q | 404 | MAN | O5-C5-C6 | 2.09 | 111.82 | 107.34 |
| 6 | I | 403 | BMA | O4-C4-C5 | 2.10 | 114.76 | 109.23 |
| 7 | E | 404 | MAN | O6-C6-C5 | 2.10 | 118.33 | 111.30 |
| 5 | Q | 405 | NAG | O5-C5-C6 | 2.12 | 111.87 | 107.34 |
| 5 | U | 405 | NAG | C4-C3-C2 | 2.12 | 114.63 | 111.34 |
| 6 | U | 403 | BMA | O5-C1-C2 | 2.16 | 114.36 | 110.89 |
| 5 | M | 405 | NAG | O4-C4-C5 | 2.18 | 114.97 | 109.23 |
| 6 | A | 403 | BMA | O6-C6-C5 | 2.21 | 118.69 | 111.30 |
| 5 | Q | 401 | NAG | C4-C3-C2 | 2.23 | 114.80 | 111.34 |
| 6 | I | 403 | BMA | O6-C6-C5 | 2.27 | 118.89 | 111.30 |
| 5 | A | 408 | NAG | C2-N2-C7 | 2.27 | 126.06 | 123.11 |
| 7 | I | 404 | MAN | O3-C3-C2 | 2.29 | 114.19 | 110.01 |
| 5 | A | 409 | NAG | O5-C5-C4 | 2.29 | 113.93 | 110.13 |
| 5 | Q | 406 | NAG | O3-C3-C4 | 2.29 | 115.53 | 110.36 |
| 7 | I | 404 | MAN | C1-C2-C3 | 2.31 | 112.35 | 109.55 |
| 5 | A | 405 | NAG | O4-C4-C5 | 2.32 | 115.33 | 109.23 |
| 5 | U | 401 | NAG | C3-C4-C5 | 2.33 | 114.39 | 110.23 |
| 5 | A | 408 | NAG | O5-C5-C6 | 2.38 | 112.43 | 107.34 |
| 5 | M | 405 | NAG | O3-C3-C2 | 2.49 | 114.70 | 109.37 |
| 5 | M | 402 | NAG | O4-C4-C5 | 2.50 | 115.82 | 109.23 |
| 6 | I | 403 | BMA | O5-C1-C2 | 2.53 | 114.94 | 110.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 405 | NAG | O4-C4-C5 | 2.54 | 115.91 | 109.23 |
| 5 | A | 401 | NAG | C4-C3-C2 | 2.62 | 115.41 | 111.34 |
| 5 | A | 406 | NAG | C4-C3-C2 | 2.65 | 115.45 | 111.34 |
| 6 | E | 403 | BMA | C2-C3-C4 | 2.69 | 115.74 | 111.05 |
| 5 | F | 201 | NAG | C1-O5-C5 | 2.69 | 116.10 | 112.14 |
| 5 | A | 407 | NAG | O4-C4-C5 | 2.70 | 116.33 | 109.23 |
| 5 | F | 201 | NAG | C2-N2-C7 | 2.70 | 126.62 | 123.11 |
| 7 | E | 404 | MAN | O5-C1-C2 | 2.74 | 115.28 | 110.89 |
| 7 | M | 404 | MAN | O5-C1-C2 | 2.75 | 115.29 | 110.89 |
| 5 | E | 402 | NAG | O7-C7-N2 | 2.76 | 127.47 | 121.84 |
| 5 | F | 201 | NAG | O5-C5-C6 | 2.79 | 113.31 | 107.34 |
| 5 | M | 402 | NAG | O5-C5-C4 | 2.98 | 115.07 | 110.13 |
| 5 | Q | 405 | NAG | O5-C5-C4 | 2.99 | 115.08 | 110.13 |
| 5 | U | 402 | NAG | C4-C3-C2 | 3.00 | 115.99 | 111.34 |
| 5 | U | 401 | NAG | C4-C3-C2 | 3.03 | 116.04 | 111.34 |
| 7 | Q | 404 | MAN | C1-C2-C3 | 3.04 | 113.24 | 109.55 |
| 5 | V | 201 | NAG | O4-C4-C3 | 3.06 | 117.25 | 110.36 |
| 5 | U | 405 | NAG | O7-C7-N2 | 3.07 | 128.10 | 121.84 |
| 5 | Q | 407 | NAG | O7-C7-N2 | 3.10 | 128.16 | 121.84 |
| 7 | Q | 404 | MAN | C3-C4-C5 | 3.13 | 115.81 | 110.23 |
| 5 | V | 201 | NAG | C2-N2-C7 | 3.16 | 127.22 | 123.11 |
| 5 | Q | 402 | NAG | O4-C4-C5 | 3.17 | 117.56 | 109.23 |
| 5 | A | 409 | NAG | O3-C3-C2 | 3.19 | 116.20 | 109.37 |
| 5 | A | 401 | NAG | C1-O5-C5 | 3.20 | 116.84 | 112.14 |
| 7 | M | 404 | MAN | C3-C4-C5 | 3.25 | 116.03 | 110.23 |
| 7 | U | 404 | MAN | O2-C2-C1 | 3.25 | 115.75 | 109.23 |
| 5 | I | 402 | NAG | O4-C4-C5 | 3.29 | 117.88 | 109.23 |
| 5 | Q | 407 | NAG | C6-C5-C4 | 3.29 | 121.24 | 112.99 |
| 7 | I | 404 | MAN | C3-C4-C5 | 3.30 | 116.11 | 110.23 |
| 5 | U | 405 | NAG | O3-C3-C2 | 3.32 | 116.48 | 109.37 |
| 5 | M | 401 | NAG | O5-C5-C4 | 3.37 | 115.71 | 110.13 |
| 7 | Q | 404 | MAN | C2-C3-C4 | 3.38 | 116.94 | 111.05 |
| 6 | U | 403 | BMA | C3-C4-C5 | 3.39 | 116.27 | 110.23 |
| 6 | A | 403 | BMA | C2-C3-C4 | 3.42 | 117.02 | 111.05 |
| 5 | U | 405 | NAG | O5-C5-C4 | 3.43 | 115.81 | 110.13 |
| 7 | I | 404 | MAN | O5-C1-C2 | 3.43 | 116.38 | 110.89 |
| 7 | U | 404 | MAN | O3-C3-C4 | 3.45 | 118.14 | 110.36 |
| 6 | U | 403 | BMA | O3-C3-C4 | 3.50 | 118.25 | 110.36 |
| 5 | I | 401 | NAG | O7-C7-N2 | 3.62 | 129.22 | 121.84 |
| 6 | Q | 403 | BMA | C2-C3-C4 | 3.69 | 117.48 | 111.05 |
| 5 | Q | 405 | NAG | O3-C3-C4 | 3.69 | 118.69 | 110.36 |
| 5 | A | 406 | NAG | O5-C5-C6 | 3.71 | 115.27 | 107.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | I | 401 | NAG | O5-C5-C6 | 3.72 | 115.31 | 107.34 |
| 5 | U | 405 | NAG | O4-C4-C5 | 3.73 | 119.06 | 109.23 |
| 5 | A | 409 | NAG | O7-C7-N2 | 3.74 | 129.47 | 121.84 |
| 5 | I | 405 | NAG | C6-C5-C4 | 3.76 | 122.40 | 112.99 |
| 6 | A | 403 | BMA | C3-C4-C5 | 3.77 | 116.94 | 110.23 |
| 5 | A | 402 | NAG | O4-C4-C5 | 3.80 | 119.24 | 109.23 |
| 5 | I | 401 | NAG | O5-C5-C4 | 3.80 | 116.43 | 110.13 |
| 5 | A | 406 | NAG | C1-O5-C5 | 3.80 | 117.73 | 112.14 |
| 6 | Q | 403 | BMA | C3-C4-C5 | 3.81 | 117.02 | 110.23 |
| 7 | U | 404 | MAN | O5-C1-C2 | 3.81 | 116.99 | 110.89 |
| 5 | A | 402 | NAG | C4-C3-C2 | 3.82 | 117.26 | 111.34 |
| 6 | U | 403 | BMA | C1-O5-C5 | 3.82 | 117.76 | 112.14 |
| 6 | M | 403 | BMA | C1-C2-C3 | 3.89 | 114.26 | 109.55 |
| 6 | M | 403 | BMA | C3-C4-C5 | 3.94 | 117.26 | 110.23 |
| 5 | E | 402 | NAG | C4-C3-C2 | 3.99 | 117.53 | 111.34 |
| 5 | Q | 406 | NAG | C1-O5-C5 | 4.04 | 118.08 | 112.14 |
| 6 | Q | 403 | BMA | C1-O5-C5 | 4.06 | 118.11 | 112.14 |
| 5 | U | 401 | NAG | C1-O5-C5 | 4.07 | 118.12 | 112.14 |
| 5 | U | 402 | NAG | O4-C4-C5 | 4.11 | 120.06 | 109.23 |
| 5 | A | 409 | NAG | C2-N2-C7 | 4.11 | 128.46 | 123.11 |
| 5 | E | 402 | NAG | O5-C5-C4 | 4.16 | 117.03 | 110.13 |
| 6 | A | 403 | BMA | C1-C2-C3 | 4.18 | 114.62 | 109.55 |
| 5 | E | 402 | NAG | O4-C4-C5 | 4.26 | 120.45 | 109.23 |
| 6 | E | 403 | BMA | C3-C4-C5 | 4.27 | 117.84 | 110.23 |
| 5 | A | 402 | NAG | C1-O5-C5 | 4.33 | 118.50 | 112.14 |
| 5 | I | 405 | NAG | O3-C3-C2 | 4.36 | 118.71 | 109.37 |
| 6 | A | 403 | BMA | O5-C1-C2 | 4.40 | 117.94 | 110.89 |
| 5 | U | 405 | NAG | C2-N2-C7 | 4.48 | 128.93 | 123.11 |
| 5 | I | 401 | NAG | C2-N2-C7 | 4.60 | 129.09 | 123.11 |
| 5 | Q | 402 | NAG | C4-C3-C2 | 4.62 | 118.52 | 111.34 |
| 6 | I | 403 | BMA | C3-C4-C5 | 4.64 | 118.51 | 110.23 |
| 5 | I | 401 | NAG | O4-C4-C3 | 4.65 | 120.85 | 110.36 |
| 5 | Q | 407 | NAG | O3-C3-C2 | 4.73 | 119.50 | 109.37 |
| 5 | F | 201 | NAG | C4-C3-C2 | 4.78 | 118.76 | 111.34 |
| 7 | U | 404 | MAN | O5-C5-C6 | 4.86 | 117.75 | 107.34 |
| 5 | A | 409 | NAG | O4-C4-C5 | 4.87 | 122.06 | 109.23 |
| 5 | Q | 407 | NAG | C2-N2-C7 | 4.96 | 129.56 | 123.11 |
| 5 | I | 402 | NAG | O5-C5-C4 | 4.97 | 118.37 | 110.13 |
| 6 | E | 403 | BMA | C1-O5-C5 | 5.33 | 119.98 | 112.14 |
| 5 | Q | 407 | NAG | O4-C4-C5 | 5.34 | 123.28 | 109.23 |
| 7 | E | 404 | MAN | O5-C5-C6 | 5.35 | 118.79 | 107.34 |
| 7 | Q | 404 | MAN | O5-C1-C2 | 5.36 | 119.46 | 110.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 407 | NAG | C1-O5-C5 | 5.40 | 120.08 | 112.14 |
| 6 | M | 403 | BMA | C1-O5-C5 | 5.46 | 120.17 | 112.14 |
| 7 | A | 404 | MAN | O5-C1-C2 | 5.62 | 119.88 | 110.89 |
| 6 | I | 403 | BMA | C1-C2-C3 | 5.73 | 116.49 | 109.55 |
| 5 | E | 402 | NAG | C1-O5-C5 | 5.80 | 120.68 | 112.14 |
| 5 | A | 408 | NAG | C1-O5-C5 | 5.91 | 120.82 | 112.14 |
| 5 | Q | 405 | NAG | C3-C4-C5 | 5.99 | 120.91 | 110.23 |
| 6 | Q | 403 | BMA | C1-C2-C3 | 6.14 | 116.99 | 109.55 |
| 5 | V | 201 | NAG | C1-O5-C5 | 6.35 | 121.47 | 112.14 |
| 5 | A | 405 | NAG | O5-C5-C4 | 6.36 | 120.67 | 110.13 |
| 5 | I | 402 | NAG | C4-C3-C2 | 6.36 | 121.21 | 111.34 |
| 5 | M | 401 | NAG | C1-O5-C5 | 6.38 | 121.52 | 112.14 |
| 5 | Q | 407 | NAG | C1-O5-C5 | 6.39 | 121.54 | 112.14 |
| 5 | Q | 405 | NAG | C1-O5-C5 | 6.43 | 121.60 | 112.14 |
| 5 | M | 402 | NAG | C1-O5-C5 | 6.55 | 121.78 | 112.14 |
| 6 | A | 403 | BMA | C1-O5-C5 | 7.15 | 122.65 | 112.14 |
| 5 | A | 409 | NAG | C1-O5-C5 | 7.27 | 122.83 | 112.14 |
| 5 | A | 405 | NAG | C1-O5-C5 | 7.49 | 123.15 | 112.14 |
| 6 | U | 403 | BMA | C1-C2-C3 | 7.95 | 119.18 | 109.55 |
| 5 | I | 402 | NAG | C1-O5-C5 | 8.31 | 124.36 | 112.14 |
| 6 | E | 403 | BMA | C1-C2-C3 | 8.96 | 120.41 | 109.55 |
| 6 | I | 403 | BMA | C1-O5-C5 | 9.12 | 125.55 | 112.14 |
| 5 | I | 401 | NAG | C1-O5-C5 | 11.20 | 128.61 | 112.14 |

All (6) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 7 | U | 404 | MAN | C1 |
| 7 | Q | 404 | MAN | C1 |
| 7 | M | 404 | MAN | C1 |
| 7 | E | 404 | MAN | C1 |
| 7 | I | 404 | MAN | C1 |
| 7 | A | 404 | MAN | C1 |

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | A | 405 | NAG | 1 | 0 |
| 6 | E | 403 | BMA | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | E | 404 | MAN | 1 | 0 |
| 5 | I | 401 | NAG | 1 | 0 |
| 5 | I | 402 | NAG | 1 | 0 |
| 5 | I | 405 | NAG | 2 | 0 |
| 5 | Q | 405 | NAG | 3 | 0 |
| 5 | Q | 406 | NAG | 4 | 0 |
| 6 | U | 403 | BMA | 1 | 0 |
| 7 | U | 404 | MAN | 1 | 0 |
| 5 | U | 405 | NAG | 5 | 0 |

## 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 | 320/321 (99%) | -0.20 | 2 (0%) 90 85 | 68, 103, 128, 172 | 0 |
| 1 | E | 320/321 (99%) | -0.11 | 1 (0%) 94 91 | 57, 99, 124, 184 | 0 |
| 1 | I | 317/321 (98%) | -0.09 | 1 (0%) 94 91 | 57, 93, 117, 143 | 0 |
| 1 | M | 320/321 (99%) | -0.07 | 1 (0%) 94 91 | 60, 94, 118, 199 | 0 |
| 1 | Q | 320/321 (99%) | -0.14 | 0 100 100 | 57, 99, 129, 188 | 0 |
| 1 | U | 320/321 (99%) | -0.19 | 2 (0%) 90 85 | 67, 103, 132, 177 | 0 |
| 2 | B | 165/175 (94%) | -0.07 | 1 (0%) 90 85 | 58, 94, 129, 183 | 0 |
| 2 | F | 163/175 (93%) | -0.07 | 0 100 100 | 66, 104, 139, 175 | 0 |
| 2 | J | 164/175 (93%) | -0.07 | 4 (2%) 62 52 | 63, 104, 138, 178 | 0 |
| 2 | N | 163/175 (93%) | -0.12 | 2 (1%) 81 72 | 64, 102, 135, 163 | 0 |
| 2 | R | 166/175 (94%) | -0.06 | 1 (0%) 90 85 | 64, 103, 141, 185 | 0 |
| 2 | V | 164/175 (93%) | -0.11 | 1 (0%) 90 85 | 59, 94, 129, 171 | 0 |
| 3 | C | 219/226 (96%) | -0.14 | 0 100 100 | 70, 96, 142, 202 | 0 |
| 3 | G | 219/226 (96%) | -0.07 | 4 (1%) 71 62 | 77, 117, 170, 219 | 0 |
| 3 | K | 219/226 (96%) | 0.79 | 43 (19%) 1 2 | 100, 175, 253, 286 | 0 |
| 3 | O | 219/226 (96%) | 1.25 | 54 (24%) 1 1 | 111, 189, 304, 357 | 0 |
| 3 | S | 219/226 (96%) | 0.01 | 5 (2%) 64 54 | 83, 117, 169, 217 | 0 |
| 3 | Y | 219/226 (96%) | -0.11 | 1 (0%) 91 88 | 70, 95, 145, 206 | 0 |
| 4 | D | 213/215 (99%) | -0.03 | 0 100 100 | 69, 96, 127, 156 | 0 |
| 4 | H | 213/215 (99%) | -0.00 | 1 (0%) 91 88 | 75, 115, 164, 197 | 0 |
| 4 | L | 213/215 (99%) | 0.63 | 31 (14%) 3 3 | 99, 186, 239, 267 | 0 |
| 4 | P | 213/215 (99%) | 0.87 | 46 (21%) 1 1 | 96, 205, 273, 317 | 0 |
| 4 | T | 213/215 (99%) | 0.05 | 5 (2%) 64 54 | 76, 115, 170, 216 | 0 |
| 4 | X | 213/215 (99%) | 0.01 | 3 (1%) 78 68 | 69, 95, 126, 157 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| All | All | 5494/5622 (97%) | 0.07 | 209 (3%) 44 36 | 57, 105, 215, 357 | 0 |

All (209) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | O | 197 | VAL | 12.1 |
| 3 | O | 226 | PRO | 11.3 |
| 3 | O | 167 | TRP | 10.8 |
| 3 | O | 198 | PRO | 10.1 |
| 4 | P | 118 | ILE | 9.1 |
| 3 | O | 192 | SER | 9.1 |
| 4 | L | 195 | CYS | 9.0 |
| 3 | O | 196 | THR | 8.9 |
| 3 | K | 192 | SER | 8.7 |
| 4 | L | 118 | ILE | 8.5 |
| 3 | K | 198 | PRO | 8.3 |
| 3 | O | 151 | LEU | 8.1 |
| 3 | K | 193 | SER | 8.1 |
| 4 | P | 119 | PHE | 6.9 |
| 4 | L | 135 | CYS | 6.8 |
| 3 | O | 164 | THR | 6.8 |
| 4 | P | 178 | SER | 6.6 |
| 3 | K | 194 | VAL | 6.5 |
| 3 | O | 166 | SER | 6.5 |
| 4 | P | 136 | LEU | 6.5 |
| 4 | P | 135 | CYS | 6.3 |
| 4 | L | 137 | LEU | 6.2 |
| 3 | K | 152 | GLY | 6.1 |
| 4 | P | 184 | LYS | 6.1 |
| 3 | O | 207 | TYR | 6.1 |
| 3 | O | 193 | SER | 6.0 |
| 3 | O | 194 | VAL | 6.0 |
| 3 | K | 191 | LEU | 5.9 |
| 3 | K | 201 | SER | 5.9 |
| 3 | K | 151 | LEU | 5.8 |
| 3 | O | 204 | THR | 5.7 |
| 3 | O | 208 | ILE | 5.7 |
| 3 | K | 204 | THR | 5.5 |
| 3 | O | 104 | ARG | 5.4 |
| 3 | K | 150 | ALA | 5.3 |
| 2 | J | 141 | TYR | 5.2 |
| 4 | P | 116 | VAL | 5.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | O | 173 | THR | 5.2 |
| 3 | O | 150 | ALA | 5.1 |
| 4 | L | 136 | LEU | 5.1 |
| 4 | P | 117 | PHE | 5.1 |
| 4 | P | 134 | VAL | 5.1 |
| 4 | L | 134 | VAL | 5.1 |
| 4 | L | 116 | VAL | 5.1 |
| 3 | O | 168 | ASN | 5.0 |
| 4 | L | 119 | PHE | 5.0 |
| 4 | P | 137 | LEU | 4.9 |
| 3 | O | 174 | SER | 4.8 |
| 4 | P | 177 | SER | 4.8 |
| 4 | P | 120 | PRO | 4.8 |
| 3 | O | 165 | VAL | 4.6 |
| 3 | O | 225 | GLU | 4.5 |
| 4 | P | 195 | CYS | 4.4 |
| 4 | P | 182 | LEU | 4.3 |
| 3 | O | 178 | THR | 4.3 |
| 4 | P | 131 | ALA | 4.2 |
| 4 | L | 117 | PHE | 4.1 |
| 4 | L | 131 | ALA | 4.1 |
| 4 | P | 147 | VAL | 4.0 |
| 3 | K | 162 | PRO | 4.0 |
| 4 | P | 197 | VAL | 4.0 |
| 4 | P | 176 | LEU | 4.0 |
| 3 | K | 148 | THR | 3.9 |
| 4 | P | 37 | TYR | 3.9 |
| 3 | O | 125 | SER | 3.9 |
| 4 | L | 178 | SER | 3.9 |
| 3 | K | 147 | GLY | 3.9 |
| 3 | K | 197 | VAL | 3.9 |
| 3 | O | 199 | SER | 3.8 |
| 4 | L | 149 | TRP | 3.8 |
| 3 | O | 29 | PHE | 3.8 |
| 4 | P | 181 | THR | 3.7 |
| 4 | P | 161 | GLN | 3.7 |
| 3 | O | 206 | THR | 3.7 |
| 3 | O | 195 | VAL | 3.6 |
| 3 | O | 149 | ALA | 3.6 |
| 4 | P | 163 | SER | 3.6 |
| 3 | O | 163 | VAL | 3.5 |
| 3 | O | 205 | GLN | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | O | 179 | PHE | 3.5 |
| 4 | P | 202 | LEU | 3.5 |
| 4 | L | 176 | LEU | 3.4 |
| 4 | L | 177 | SER | 3.4 |
| 4 | P | 162 | GLU | 3.4 |
| 4 | L | 184 | LYS | 3.3 |
| 2 | N | 141 | TYR | 3.3 |
| 4 | L | 191 | LYS | 3.3 |
| 3 | K | 104 | ARG | 3.2 |
| 3 | K | 170 | GLY | 3.2 |
| 3 | O | 191 | LEU | 3.2 |
| 4 | P | 115 | SER | 3.2 |
| 3 | K | 20 | VAL | 3.2 |
| 3 | O | 169 | SER | 3.2 |
| 4 | P | 188 | GLU | 3.2 |
| 4 | P | 49 | ILE | 3.1 |
| 4 | P | 179 | THR | 3.1 |
| 4 | L | 206 | VAL | 3.1 |
| 2 | J | 140 | ILE | 3.1 |
| 2 | N | 130 | ALA | 3.1 |
| 3 | K | 166 | SER | 3.0 |
| 3 | K | 179 | PHE | 3.0 |
| 4 | P | 63 | PHE | 3.0 |
| 4 | P | 48 | LEU | 2.9 |
| 3 | K | 219 | LYS | 2.9 |
| 3 | K | 226 | PRO | 2.9 |
| 4 | P | 132 | SER | 2.9 |
| 3 | O | 171 | ALA | 2.9 |
| 4 | P | 79 | LEU | 2.8 |
| 4 | L | 49 | ILE | 2.8 |
| 3 | S | 193 | SER | 2.8 |
| 4 | P | 18 | ARG | 2.8 |
| 2 | J | 171 | PHE | 2.8 |
| 3 | O | 162 | PRO | 2.8 |
| 3 | K | 164 | THR | 2.8 |
| 3 | O | 170 | GLY | 2.8 |
| 4 | P | 180 | LEU | 2.8 |
| 3 | O | 210 | ASN | 2.8 |
| 3 | O | 138 | ALA | 2.8 |
| 4 | P | 209 | SER | 2.8 |
| 3 | O | 152 | GLY | 2.8 |
| 4 | L | 132 | SER | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | O | 172 | LEU | 2.7 |
| 4 | L | 197 | VAL | 2.7 |
| 3 | O | 153 | CYS | 2.7 |
| 1 | I | 9 | SER | 2.6 |
| 3 | O | 32 | TYR | 2.6 |
| 3 | K | 160 | PRO | 2.6 |
| 4 | T | 136 | LEU | 2.6 |
| 3 | O | 113 | HIS | 2.6 |
| 2 | B | 173 | ILE | 2.6 |
| 3 | K | 190 | SER | 2.6 |
| 3 | O | 177 | HIS | 2.6 |
| 3 | K | 90 | ASP | 2.6 |
| 4 | L | 146 | LYS | 2.6 |
| 3 | O | 139 | PRO | 2.6 |
| 3 | K | 155 | VAL | 2.5 |
| 3 | O | 53 | ALA | 2.5 |
| 3 | K | 29 | PHE | 2.5 |
| 3 | K | 169 | SER | 2.5 |
| 4 | L | 41 | SER | 2.5 |
| 4 | L | 130 | THR | 2.5 |
| 4 | H | 136 | LEU | 2.5 |
| 4 | L | 48 | LEU | 2.5 |
| 3 | O | 31 | THR | 2.5 |
| 3 | O | 221 | ASP | 2.5 |
| 3 | O | 27 | TYR | 2.5 |
| 3 | S | 194 | VAL | 2.5 |
| 4 | L | 156 | GLN | 2.4 |
| 4 | L | 114 | PRO | 2.4 |
| 3 | G | 1 | GLN | 2.4 |
| 3 | S | 149 | ALA | 2.4 |
| 4 | L | 147 | VAL | 2.4 |
| 3 | G | 193 | SER | 2.4 |
| 4 | T | 177 | SER | 2.4 |
| 1 | U | 127 | TRP | 2.3 |
| 3 | K | 165 | VAL | 2.3 |
| 3 | S | 177 | HIS | 2.3 |
| 4 | T | 149 | TRP | 2.3 |
| 1 | A | 251 | LEU | 2.3 |
| 4 | P | 123 | ASP | 2.3 |
| 4 | P | 196 | GLU | 2.3 |
| 3 | K | 189 | TYR | 2.3 |
| 3 | K | 205 | GLN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | P | 38 | GLN | 2.3 |
| 3 | K | 161 | GLU | 2.3 |
| 4 | X | 28 | ARG | 2.3 |
| 3 | K | 195 | VAL | 2.3 |
| 3 | S | 150 | ALA | 2.3 |
| 4 | P | 76 | ILE | 2.3 |
| 4 | X | 195 | CYS | 2.3 |
| 4 | P | 130 | THR | 2.3 |
| 1 | A | 245 | ILE | 2.2 |
| 3 | G | 194 | VAL | 2.2 |
| 4 | T | 189 | LYS | 2.2 |
| 4 | P | 41 | SER | 2.2 |
| 3 | O | 48 | VAL | 2.2 |
| 4 | P | 39 | GLN | 2.2 |
| 3 | K | 178 | THR | 2.2 |
| 4 | L | 211 | ASN | 2.2 |
| 3 | O | 154 | LEU | 2.2 |
| 4 | L | 209 | SER | 2.2 |
| 4 | T | 156 | GLN | 2.2 |
| 2 | R | 138 | PHE | 2.1 |
| 2 | V | 61 | GLU | 2.1 |
| 3 | K | 153 | CYS | 2.1 |
| 3 | Y | 204 | THR | 2.1 |
| 4 | L | 115 | SER | 2.1 |
| 3 | K | 207 | TYR | 2.1 |
| 3 | K | 114 | ASP | 2.1 |
| 3 | K | 200 | SER | 2.1 |
| 4 | P | 160 | SER | 2.1 |
| 4 | L | 187 | TYR | 2.1 |
| 3 | K | 19 | LYS | 2.1 |
| 3 | K | 139 | PRO | 2.1 |
| 3 | K | 138 | ALA | 2.1 |
| 3 | K | 214 | LYS | 2.1 |
| 1 | E | 12 | THR | 2.1 |
| 3 | O | 161 | GLU | 2.1 |
| 3 | K | 167 | TRP | 2.1 |
| 4 | X | 150 | LYS | 2.0 |
| 3 | G | 170 | GLY | 2.0 |
| 2 | J | 124 | ARG | 2.0 |
| 1 | M | 9 | SER | 2.0 |
| 1 | U | 245 | ILE | 2.0 |
| 4 | P | 35 | ALA | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 4 | P | 189 | LYS | 2.0 |
| 4 | P | 148 | GLN | 2.0 |
| 3 | O | 36 | TRP | 2.0 |
| 3 | O | 155 | VAL | 2.0 |

## 6.2 Non-standard residues in protein, DNA, RNA chains (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 5 | NAG | V | 201 | 14/15 | 0.76 | 0.30 | 2.55 | 103,112,121,121 | 0 |
| 5 | NAG | Q | 407 | 14/15 | 0.88 | 0.26 | 2.29 | 85,101,107,107 | 0 |
| 5 | NAG | M | 405 | 14/15 | 0.89 | 0.24 | 0.24 | 101,119,136,138 | 0 |
| 5 | NAG | A | 409 | 14/15 | 0.88 | 0.19 | -0.33 | 89,104,118,124 | 0 |
| 5 | NAG | U | 401 | 14/15 | 0.90 | 0.18 | -0.83 | 120,124,127,128 | 0 |
| 5 | NAG | I | 405 | 14/15 | 0.84 | 0.21 | -1.00 | 106,126,133,137 | 0 |
| 5 | NAG | A | 401 | 14/15 | 0.91 | 0.17 | -1.14 | 105,108,112,113 | 0 |
| 5 | NAG | U | 402 | 14/15 | 0.94 | 0.18 | -1.20 | 102,125,137,141 | 0 |
| 5 | NAG | A | 402 | 14/15 | 0.85 | 0.20 | -1.47 | 108,122,129,133 | 0 |
| 5 | NAG | M | 401 | 14/15 | 0.93 | 0.16 | -1.71 | 90,94,96,97 | 0 |
| 5 | NAG | I | 402 | 14/15 | 0.94 | 0.25 | -1.89 | 101,107,116,121 | 0 |
| 5 | NAG | E | 402 | 14/15 | 0.91 | 0.22 | -2.34 | 102,121,142,146 | 0 |
| 5 | NAG | Q | 402 | 14/15 | 0.93 | 0.21 | -4.20 | 107,116,134,136 | 0 |
| 5 | NAG | Q | 406 | 14/15 | 0.57 | 0.27 | - | 152,179,197,197 | 0 |
| 5 | NAG | A | 408 | 14/15 | 0.83 | 0.18 | - | 151,173,185,190 | 0 |
| 5 | NAG | U | 405 | 14/15 | 0.89 | 0.20 | - | 84,97,121,129 | 0 |
| 5 | NAG | A | 406 | 14/15 | 0.83 | 0.24 | - | 147,155,164,165 | 0 |
| 5 | NAG | I | 401 | 14/15 | 0.92 | 0.16 | - | 85,91,92,92 | 0 |
| 5 | NAG | M | 402 | 14/15 | 0.96 | 0.16 | - | 94,104,111,111 | 0 |
| 5 | NAG | A | 405 | 14/15 | 0.93 | 0.20 | - | 130,133,144,145 | 0 |
| 5 | NAG | A | 407 | 14/15 | 0.73 | 0.20 | - | 179,195,202,203 | 0 |
| 5 | NAG | Q | 401 | 14/15 | 0.93 | 0.17 | - | 96,104,115,116 | 0 |
| 5 | NAG | E | 401 | 14/15 | 0.91 | 0.19 | - | 101,108,117,119 | 0 |
| 5 | NAG | F | 201 | 14/15 | 0.58 | 0.27 | - | 155,185,196,198 | 0 |
| 5 | NAG | Q | 405 | 14/15 | 0.96 | 0.18 | - | 112,128,138,152 | 0 |

## 6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 5 | NAG | V | 201 | 14/15 | 0.76 | 0.30 | 2.55 | 103,112,121,121 | 0 |
| 5 | NAG | Q | 407 | 14/15 | 0.88 | 0.26 | 2.29 | 85,101,107,107 | 0 |
| 5 | NAG | M | 405 | 14/15 | 0.89 | 0.24 | 0.24 | 101,119,136,138 | 0 |
| 5 | NAG | A | 409 | 14/15 | 0.88 | 0.19 | -0.33 | 89,104,118,124 | 0 |
| 5 | NAG | U | 401 | 14/15 | 0.90 | 0.18 | -0.83 | 120,124,127,128 | 0 |
| 5 | NAG | I | 405 | 14/15 | 0.84 | 0.21 | -1.00 | 106,126,133,137 | 0 |
| 5 | NAG | A | 401 | 14/15 | 0.91 | 0.17 | -1.14 | 105,108,112,113 | 0 |
| 5 | NAG | U | 402 | 14/15 | 0.94 | 0.18 | -1.20 | 102,125,137,141 | 0 |
| 5 | NAG | A | 402 | 14/15 | 0.85 | 0.20 | -1.47 | 108,122,129,133 | 0 |
| 5 | NAG | M | 401 | 14/15 | 0.93 | 0.16 | -1.71 | 90,94,96,97 | 0 |
| 5 | NAG | I | 402 | 14/15 | 0.94 | 0.25 | -1.89 | 101,107,116,121 | 0 |
| 5 | NAG | E | 402 | 14/15 | 0.91 | 0.22 | -2.34 | 102,121,142,146 | 0 |
| 5 | NAG | Q | 402 | 14/15 | 0.93 | 0.21 | -4.20 | 107,116,134,136 | 0 |
| 5 | NAG | I | 401 | 14/15 | 0.92 | 0.16 | - | 85,91,92,92 | 0 |
| 7 | MAN | M | 404 | 11/12 | 0.84 | 0.20 | - | 141,147,157,173 | 0 |
| 6 | BMA | E | 403 | 11/12 | 0.66 | 0.19 | - | 116,129,135,137 | 0 |
| 6 | BMA | A | 403 | 11/12 | 0.72 | 0.21 | - | 109,123,131,147 | 0 |
| 5 | NAG | F | 201 | 14/15 | 0.58 | 0.27 | - | 155,185,196,198 | 0 |
| 6 | BMA | Q | 403 | 11/12 | 0.70 | 0.19 | - | 107,121,124,132 | 0 |
| 7 | MAN | U | 404 | 11/12 | 0.77 | 0.19 | - | 135,149,150,150 | 0 |
| 7 | MAN | Q | 404 | 11/12 | 0.77 | 0.36 | - | 129,145,149,150 | 0 |
| 5 | NAG | U | 405 | 14/15 | 0.89 | 0.20 | - | 84,97,121,129 | 0 |
| 6 | BMA | I | 403 | 11/12 | 0.83 | 0.17 | - | 104,110,118,121 | 0 |
| 5 | NAG | Q | 401 | 14/15 | 0.93 | 0.17 | - | 96,104,115,116 | 0 |
| 5 | NAG | Q | 406 | 14/15 | 0.57 | 0.27 | - | 152,179,197,197 | 0 |
| 5 | NAG | M | 402 | 14/15 | 0.96 | 0.16 | - | 94,104,111,111 | 0 |
| 6 | BMA | U | 403 | 11/12 | 0.80 | 0.14 | - | 114,124,135,146 | 0 |
| 5 | NAG | A | 405 | 14/15 | 0.93 | 0.20 | - | 130,133,144,145 | 0 |
| 7 | MAN | E | 404 | 11/12 | 0.91 | 0.14 | - | 125,138,145,146 | 0 |
| 5 | NAG | A | 407 | 14/15 | 0.73 | 0.20 | - | 179,195,202,203 | 0 |

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*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 5 | NAG | A | 408 | 14/15 | 0.83 | 0.18 | - | 151,173,185,190 | 0 |
| 7 | MAN | I | 404 | 11/12 | 0.81 | 0.18 | - | 134,140,148,169 | 0 |
| 5 | NAG | E | 401 | 14/15 | 0.91 | 0.19 | - | 101,108,117,119 | 0 |
| 5 | NAG | A | 406 | 14/15 | 0.83 | 0.24 | - | 147,155,164,165 | 0 |
| 7 | MAN | A | 404 | 11/12 | 0.85 | 0.23 | - | 147,149,156,160 | 0 |
| 6 | BMA | M | 403 | 11/12 | 0.93 | 0.14 | - | 106,111,126,130 | 0 |
| 5 | NAG | Q | 405 | 14/15 | 0.96 | 0.18 | - | 112,128,138,152 | 0 |

## 6.5 Other polymers

There are no such residues in this entry.