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

Sep 24, 2023 – 04:57 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 5KOV |
| Title | : | Crystal structure of the human astrovirus 2 capsid protein spike in complex with a single chain variable fragment of an astrovirus neutralizing antibody at 3.24-A resolution |
| Authors | : | Bogdanoff, W.A.; DuBois, R.M. |
| Deposited on | : | 2016-07-01 |
| Resolution | : | 3.25 Å(reported) |

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

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

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

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

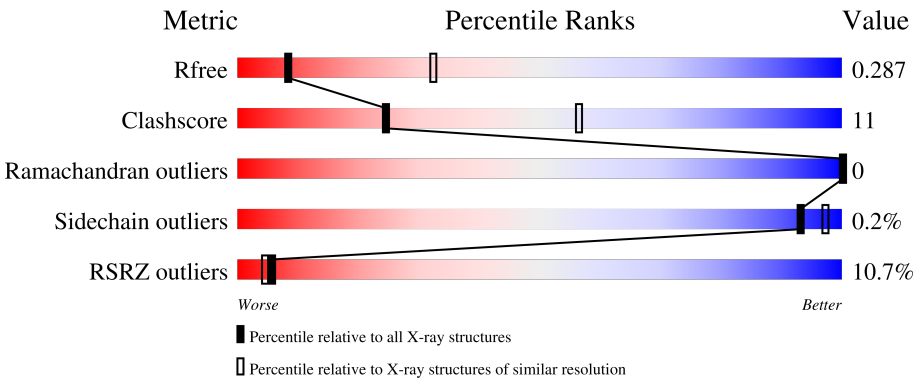
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 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 3.25 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 1619 (3.28-3.20) |
| Clashscore | 141614 | 1755 (3.28-3.20) |
| Ramachandran outliers | 138981 | 1728 (3.28-3.20) |
| Sidechain outliers | 138945 | 1727 (3.28-3.20) |
| RSRZ outliers | 127900 | 1567 (3.28-3.20) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 228 | 5% 69% 25% 5% |
| 1 | B | 228 | 10% 74% 22% . |
| 1 | G | 228 | 13% 68% 28% . |
| 1 | H | 228 | 6% 69% 25% 5% |
| 1 | M | 228 | 11% 74% 21% 5% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | N | 228 | 5% 74% 21% 5% |
| 1 | S | 228 | 8% 75% 20% • |
| 1 | T | 228 | 14% 70% 25% 5% |
| 2 | C | 251 | 4% 66% 23% 11% |
| 2 | E | 251 | 9% 65% 24% 11% |
| 2 | I | 251 | 15% 70% 19% 10% |
| 2 | K | 251 | 5% 68% 21% 11% |
| 2 | O | 251 | 10% 60% 24% • 16% |
| 2 | Q | 251 | 8% 29% 8% 63% |
| 2 | U | 251 | 10% 67% 22% 12% |
| 2 | W | 251 | 14% 30% 12% 58% |

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 |
|---|---|---|---|---|---|---|---|
| 3 | NAG | C | 1201 | - | - | - | X |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25943 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 Capsid polyprotein VP90.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 216 | 1745 | 1118 | 290 | 328 | 9 | 0 | 0 | 0 |
| 1 | B | 218 | 1756 | 1125 | 292 | 330 | 9 | 0 | 0 | 0 |
| 1 | H | 216 | 1745 | 1118 | 290 | 328 | 9 | 0 | 0 | 0 |
| 1 | G | 219 | 1760 | 1127 | 293 | 331 | 9 | 0 | 0 | 0 |
| 1 | N | 217 | 1750 | 1121 | 291 | 329 | 9 | 0 | 0 | 0 |
| 1 | M | 216 | 1745 | 1118 | 290 | 328 | 9 | 0 | 0 | 0 |
| 1 | S | 218 | 1755 | 1124 | 292 | 330 | 9 | 0 | 0 | 0 |
| 1 | T | 216 | 1745 | 1118 | 290 | 328 | 9 | 0 | 0 | 0 |

There are 96 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 427 | MET | - | initiating methionine | UNP Q82446 |
| A | 428 | GLY | - | expression tag | UNP Q82446 |
| A | 645 | ALA | - | expression tag | UNP Q82446 |
| A | 646 | ALA | - | expression tag | UNP Q82446 |
| A | 647 | ALA | - | expression tag | UNP Q82446 |
| A | 648 | GLU | - | expression tag | UNP Q82446 |
| A | 649 | LEU | - | expression tag | UNP Q82446 |
| A | 650 | ALA | - | expression tag | UNP Q82446 |
| A | 651 | LEU | - | expression tag | UNP Q82446 |
| A | 652 | VAL | - | expression tag | UNP Q82446 |
| A | 653 | PRO | - | expression tag | UNP Q82446 |
| A | 654 | ARG | - | expression tag | UNP Q82446 |
| B | 427 | MET | - | initiating methionine | UNP Q82446 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 428 | GLY | - | expression tag | UNP Q82446 |
| B | 645 | ALA | - | expression tag | UNP Q82446 |
| B | 646 | ALA | - | expression tag | UNP Q82446 |
| B | 647 | ALA | - | expression tag | UNP Q82446 |
| B | 648 | GLU | - | expression tag | UNP Q82446 |
| B | 649 | LEU | - | expression tag | UNP Q82446 |
| B | 650 | ALA | - | expression tag | UNP Q82446 |
| B | 651 | LEU | - | expression tag | UNP Q82446 |
| B | 652 | VAL | - | expression tag | UNP Q82446 |
| B | 653 | PRO | - | expression tag | UNP Q82446 |
| B | 654 | ARG | - | expression tag | UNP Q82446 |
| H | 427 | MET | - | initiating methionine | UNP Q82446 |
| H | 428 | GLY | - | expression tag | UNP Q82446 |
| H | 645 | ALA | - | expression tag | UNP Q82446 |
| H | 646 | ALA | - | expression tag | UNP Q82446 |
| H | 647 | ALA | - | expression tag | UNP Q82446 |
| H | 648 | GLU | - | expression tag | UNP Q82446 |
| H | 649 | LEU | - | expression tag | UNP Q82446 |
| H | 650 | ALA | - | expression tag | UNP Q82446 |
| H | 651 | LEU | - | expression tag | UNP Q82446 |
| H | 652 | VAL | - | expression tag | UNP Q82446 |
| H | 653 | PRO | - | expression tag | UNP Q82446 |
| H | 654 | ARG | - | expression tag | UNP Q82446 |
| G | 427 | MET | - | initiating methionine | UNP Q82446 |
| G | 428 | GLY | - | expression tag | UNP Q82446 |
| G | 645 | ALA | - | expression tag | UNP Q82446 |
| G | 646 | ALA | - | expression tag | UNP Q82446 |
| G | 647 | ALA | - | expression tag | UNP Q82446 |
| G | 648 | GLU | - | expression tag | UNP Q82446 |
| G | 649 | LEU | - | expression tag | UNP Q82446 |
| G | 650 | ALA | - | expression tag | UNP Q82446 |
| G | 651 | LEU | - | expression tag | UNP Q82446 |
| G | 652 | VAL | - | expression tag | UNP Q82446 |
| G | 653 | PRO | - | expression tag | UNP Q82446 |
| G | 654 | ARG | - | expression tag | UNP Q82446 |
| N | 427 | MET | - | initiating methionine | UNP Q82446 |
| N | 428 | GLY | - | expression tag | UNP Q82446 |
| N | 645 | ALA | - | expression tag | UNP Q82446 |
| N | 646 | ALA | - | expression tag | UNP Q82446 |
| N | 647 | ALA | - | expression tag | UNP Q82446 |
| N | 648 | GLU | - | expression tag | UNP Q82446 |
| N | 649 | LEU | - | expression tag | UNP Q82446 |

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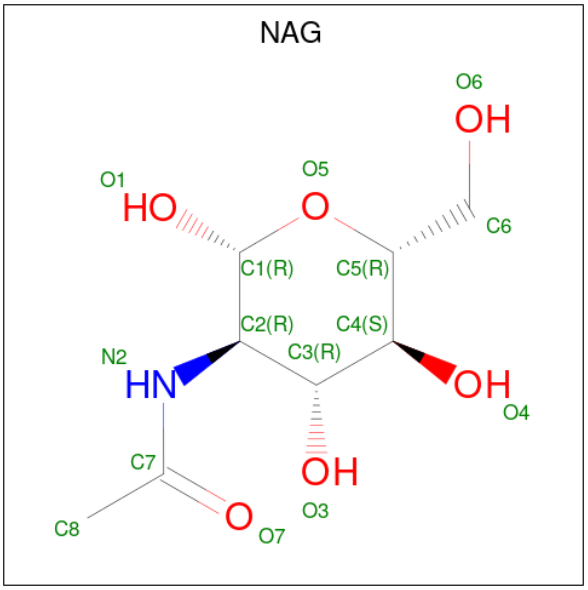
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| N | 650 | ALA | - | expression tag | UNP Q82446 |
| N | 651 | LEU | - | expression tag | UNP Q82446 |
| N | 652 | VAL | - | expression tag | UNP Q82446 |
| N | 653 | PRO | - | expression tag | UNP Q82446 |
| N | 654 | ARG | - | expression tag | UNP Q82446 |
| M | 427 | MET | - | initiating methionine | UNP Q82446 |
| M | 428 | GLY | - | expression tag | UNP Q82446 |
| M | 645 | ALA | - | expression tag | UNP Q82446 |
| M | 646 | ALA | - | expression tag | UNP Q82446 |
| M | 647 | ALA | - | expression tag | UNP Q82446 |
| M | 648 | GLU | - | expression tag | UNP Q82446 |
| M | 649 | LEU | - | expression tag | UNP Q82446 |
| M | 650 | ALA | - | expression tag | UNP Q82446 |
| M | 651 | LEU | - | expression tag | UNP Q82446 |
| M | 652 | VAL | - | expression tag | UNP Q82446 |
| M | 653 | PRO | - | expression tag | UNP Q82446 |
| M | 654 | ARG | - | expression tag | UNP Q82446 |
| S | 427 | MET | - | initiating methionine | UNP Q82446 |
| S | 428 | GLY | - | expression tag | UNP Q82446 |
| S | 645 | ALA | - | expression tag | UNP Q82446 |
| S | 646 | ALA | - | expression tag | UNP Q82446 |
| S | 647 | ALA | - | expression tag | UNP Q82446 |
| S | 648 | GLU | - | expression tag | UNP Q82446 |
| S | 649 | LEU | - | expression tag | UNP Q82446 |
| S | 650 | ALA | - | expression tag | UNP Q82446 |
| S | 651 | LEU | - | expression tag | UNP Q82446 |
| S | 652 | VAL | - | expression tag | UNP Q82446 |
| S | 653 | PRO | - | expression tag | UNP Q82446 |
| S | 654 | ARG | - | expression tag | UNP Q82446 |
| T | 427 | MET | - | initiating methionine | UNP Q82446 |
| T | 428 | GLY | - | expression tag | UNP Q82446 |
| T | 645 | ALA | - | expression tag | UNP Q82446 |
| T | 646 | ALA | - | expression tag | UNP Q82446 |
| T | 647 | ALA | - | expression tag | UNP Q82446 |
| T | 648 | GLU | - | expression tag | UNP Q82446 |
| T | 649 | LEU | - | expression tag | UNP Q82446 |
| T | 650 | ALA | - | expression tag | UNP Q82446 |
| T | 651 | LEU | - | expression tag | UNP Q82446 |
| T | 652 | VAL | - | expression tag | UNP Q82446 |
| T | 653 | PRO | - | expression tag | UNP Q82446 |
| T | 654 | ARG | - | expression tag | UNP Q82446 |

- Molecule 2 is a protein called PL-2 scFv chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | C | 223 | 1726 | 1087 | 290 | 342 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | E | 224 | 1727 | 1087 | 288 | 345 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | K | 223 | 1726 | 1087 | 290 | 342 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | I | 225 | 1738 | 1093 | 292 | 346 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | Q | 93 | 746 | 482 | 122 | 138 | 4 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | O | 212 | 1651 | 1043 | 276 | 325 | 7 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | W | 105 | 853 | 548 | 141 | 159 | 5 | 0 | 0 | 0 |
| | | | Total | C | N | O | S | | | |
| 2 | U | 222 | 1719 | 1082 | 289 | 341 | 7 | 0 | 0 | 0 |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | C | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| | | | Total | C | N | O | | |
| 3 | E | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| | | | Total | C | N | O | | |
| 3 | K | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

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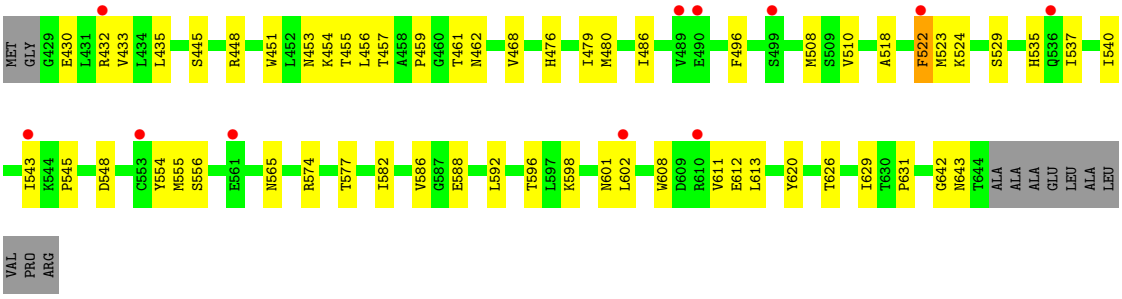
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 3 | I | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

# 3 Residue-property plots (i)

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

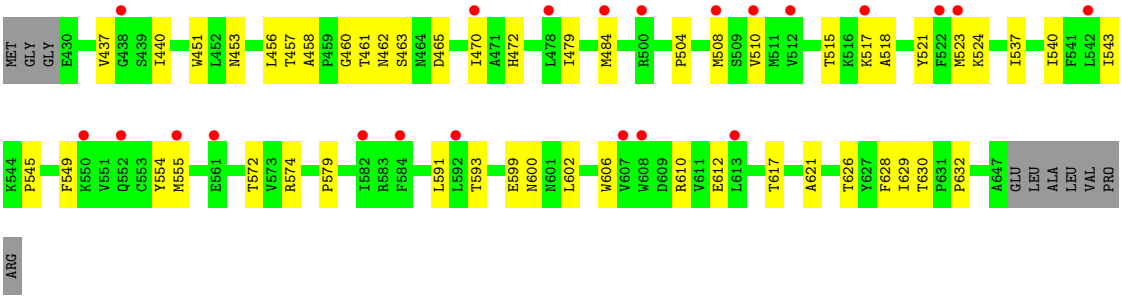
• Molecule 1: Capsid polyprotein VP90

Chain A: 5% 69% 25% 5%



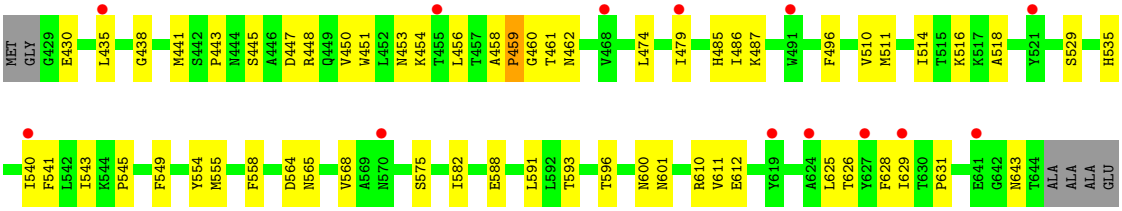

• Molecule 1: Capsid polyprotein VP90

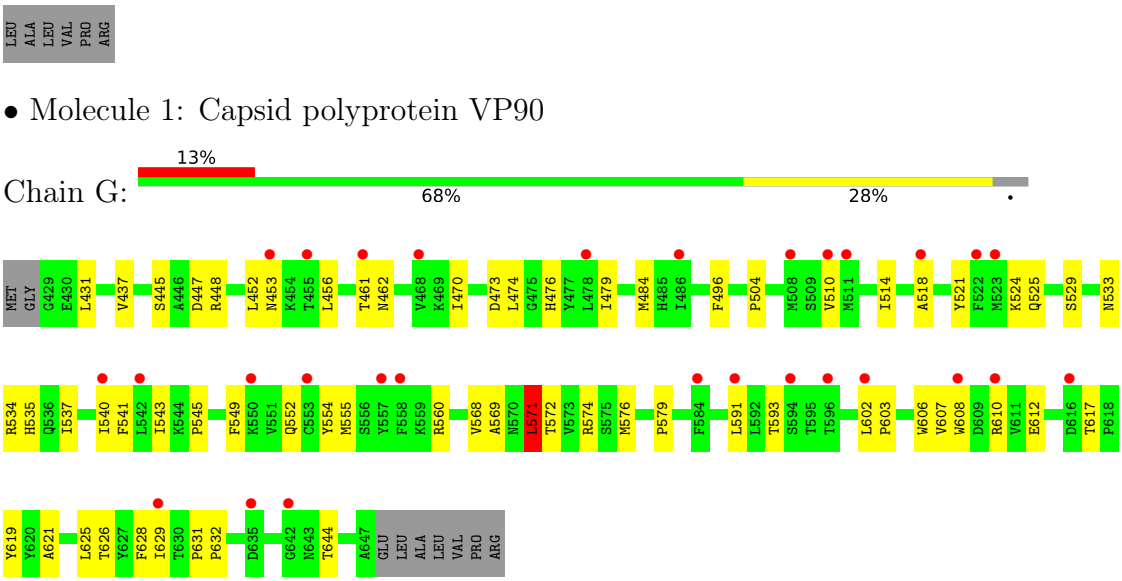
Chain B: 10% 74% 22%

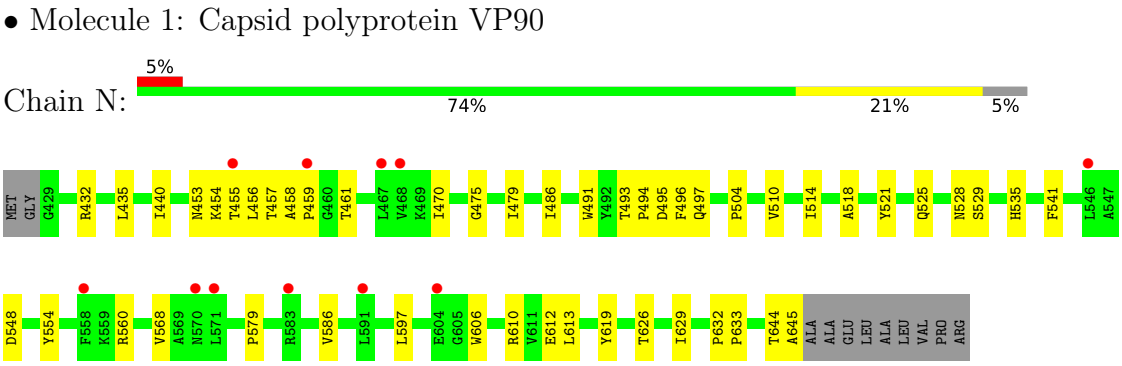


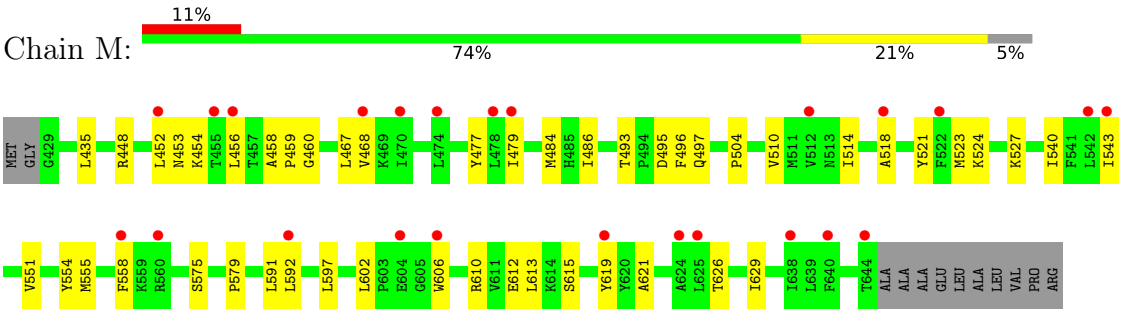

• Molecule 1: Capsid polyprotein VP90

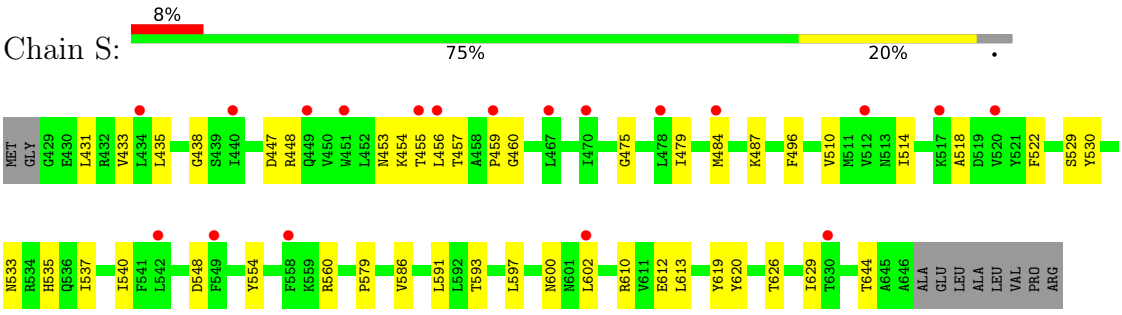
Chain H: 6% 69% 25% 5%




LEU ALA LEU VAL PRO ARG
• Molecule 1: Capsid polyprotein VP90
Chain G:
13%
68%
28%
MET GLY G429 E430 L431 V437 S445 A446 D447 R448 L452 N453 K454 T455 L456 T461 N462 V468 K469 I470 D473 L474 G475 H476 Y477 L478 I479 M484 H485 I486 F496 P504 M508 S509 V510 M511 I514 A518 Y521 F522 M523 K524 Q525 S529 N533
R534 H535 Q536 I537 I540 F541 L542 I543 K544 P545 F549 K550 V551 Q552 C553 Y554 M555 S556 Y557 F558 K559 R560 V568 A569 N570 L571 T572 V573 R574 S575 M576 P579 F584 L591 L592 T593 S594 T595 T596 L602 P603 W606 V607 W608 D609 R610 V611 E612 D616 T617 P618
Y619 Y620 A621 L625 T626 Y627 F628 I629 T630 P631 P632 D635 G642 N643 T644 A647 GLU LEU ALA LEU VAL PRO ARG

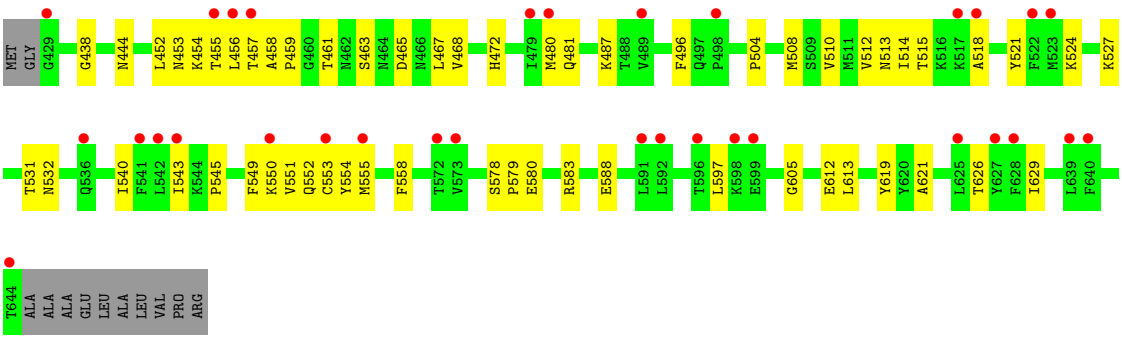

• Molecule 1: Capsid polyprotein VP90
Chain N:
5%
74%
21%
5%
MET GLY G429 R432 L435 I440 N453 K454 T455 L456 T457 A458 P459 G460 T461 L467 V468 K469 I470 G475 I479 I486 W491 Y492 T493 P494 D495 F496 Q497 P504 V510 I514 A518 Y521 Q525 N528 S529 H535 F541 L546 A547
D548 Y554 F558 K559 R560 V568 A569 N570 L571 P579 R583 V586 L591 L597 E604 G605 W606 R610 V611 E612 L613 Y619 T626 I629 P632 P633 T644 A645 ALA ALA GLU LEU ALA LEU VAL PRO ARG


• Molecule 1: Capsid polyprotein VP90
Chain M:
11%
74%
21%
5%
MET GLY G429 L435 R448 L452 N453 K454 T455 L456 T457 A458 P459 G460 L467 V468 K469 I470 L474 Y477 L478 I479 M484 H485 I486 T493 P494 D495 F496 Q497 P504 V510 M511 V512 N513 I514 A518 Y521 F522 M523 K524 K527 I540 F541 L542 I543
V551 Y554 M555 F558 K559 R560 S575 P579 L591 L592 L597 L602 P603 E604 G605 W606 R610 V611 E612 L613 K614 S615 Y619 Y620 A621 A624 L625 T626 I629 I638 L639 F640 T644 ALA ALA ALA GLU LEU ALA LEU VAL PRO ARG


• Molecule 1: Capsid polyprotein VP90
Chain S:
8%
75%
20%
MET GLY G429 E430 L431 R432 V433 L434 L435 G438 S439 I440 D447 R448 Q449 V450 W451 L452 N453 K454 T455 L456 T457 A458 P459 G460 L467 I470 G475 L478 I479 M484 K487 F496 V510 M511 V512 N513 I514 K517 A518 D519 V520 Y521 F522 S529 Y530
N533 R534 H535 Q536 I537 I540 F541 L542 D548 F549 Y554 F558 K559 R560 P579 V586 L591 L592 T593 L597 N600 N601 L602 R610 V611 E612 L613 Y619 Y620 T626 I629 T630 T644 A645 A646 ALA GLU LEU ALA LEU VAL PRO ARG

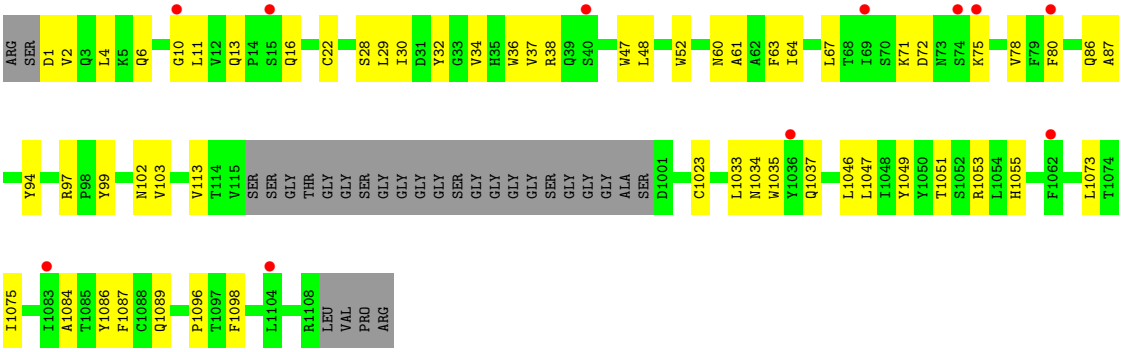
• Molecule 1: Capsid polyprotein VP90

Chain T:



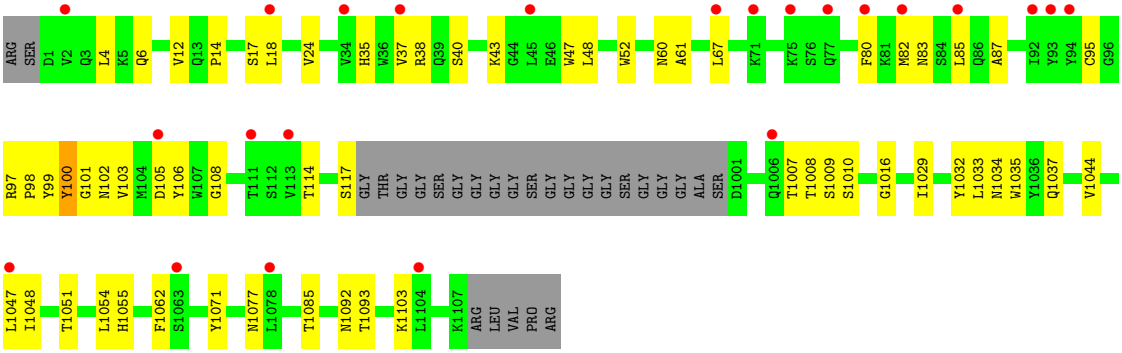

• Molecule 2: PL-2 scFv chain

Chain C:



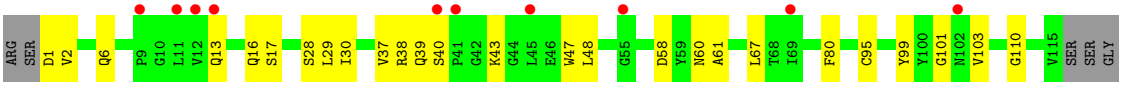

• Molecule 2: PL-2 scFv chain

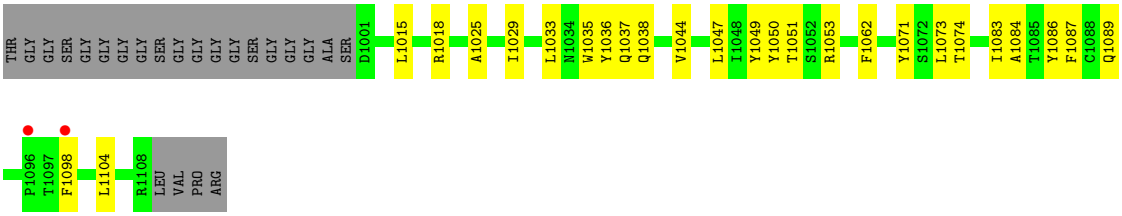
Chain E:




• Molecule 2: PL-2 scFv chain

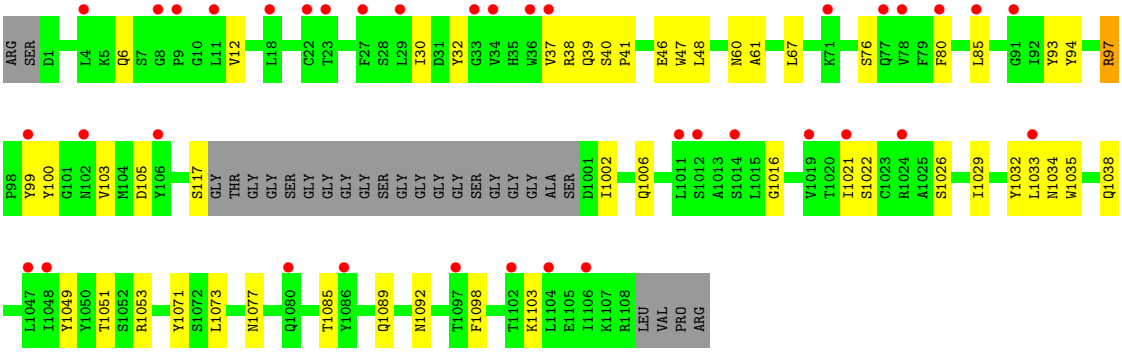
Chain K:





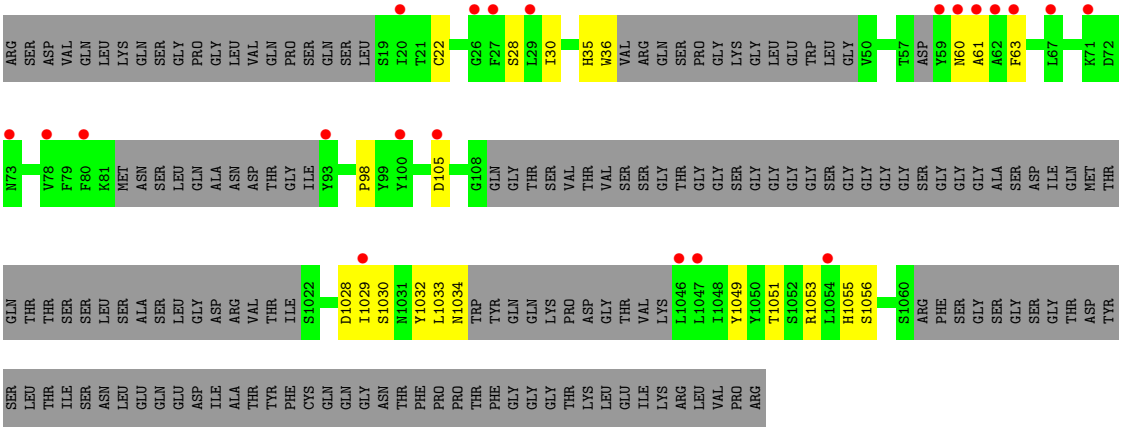

• Molecule 2: PL-2 scFv chain

Chain I:



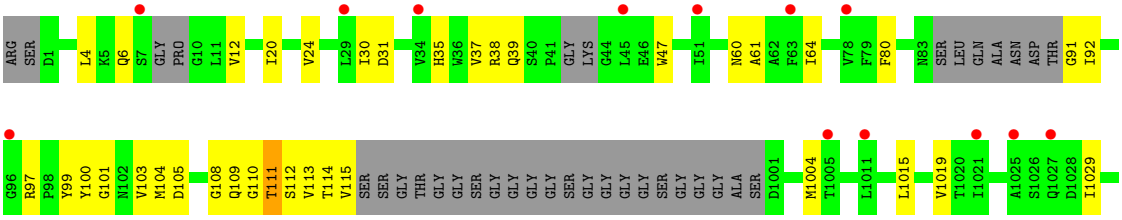

• Molecule 2: PL-2 scFv chain

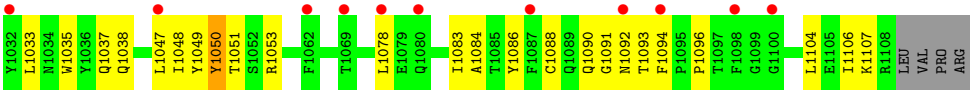
Chain Q:




• Molecule 2: PL-2 scFv chain

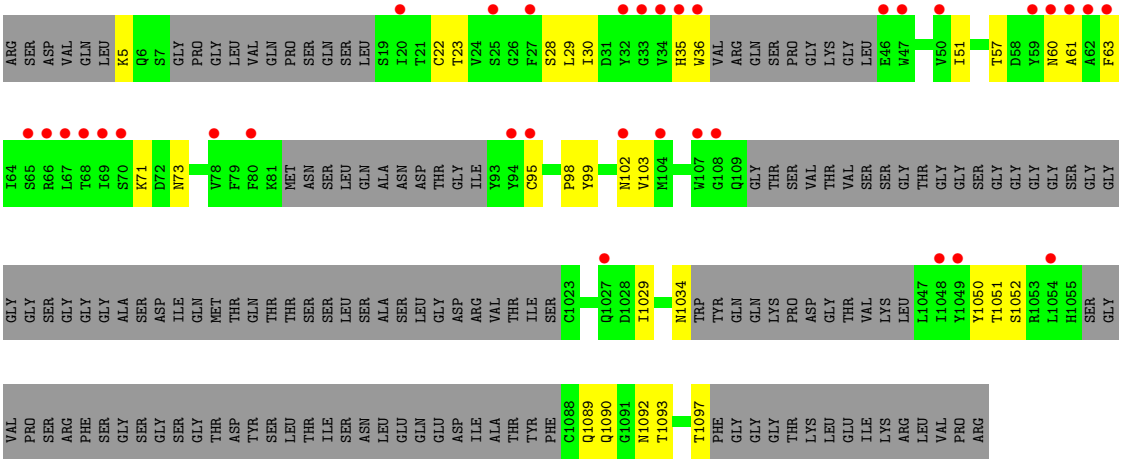
Chain O:





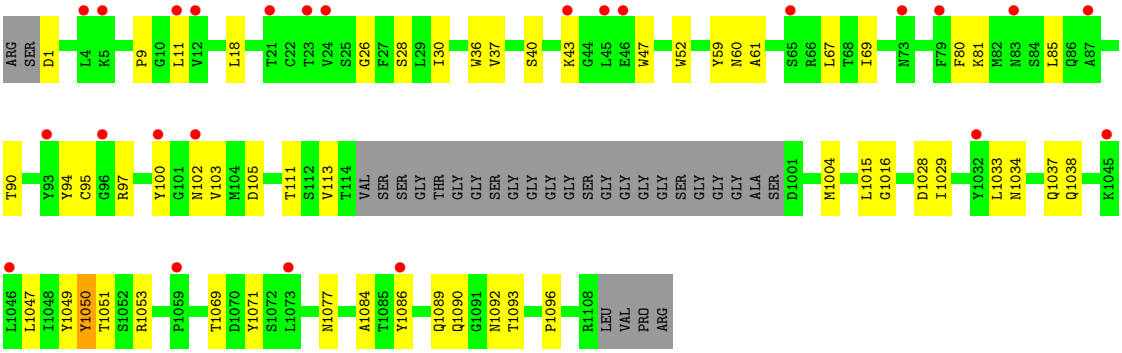

- Molecule 2: PL-2 scFv chain

Chain W:




- Molecule 2: PL-2 scFv chain

Chain U:



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 200.00Å 200.00Å 157.51Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.25<br>50.00 – 3.24 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 88.1 (50.00-3.25)<br>81.5 (50.00-3.24) | Depositor<br>EDS |
| $R_{merge}$ | 0.16 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.56 (at 3.25Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.241 , 0.288<br>0.241 , 0.287 | Depositor<br>DCC |
| $R_{free}$ test set | 4185 reflections (4.84%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 75.5 | Xtriage |
| Anisotropy | 0.523 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.31 , 45.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.46$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.417 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 25943 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 105.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

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 | 0.28 | 0/1792 | 0.54 | 1/2441 (0.0%) |
| 1 | B | 0.30 | 0/1803 | 0.53 | 0/2457 |
| 1 | G | 0.30 | 0/1807 | 0.55 | 1/2462 (0.0%) |
| 1 | H | 0.29 | 0/1792 | 0.52 | 0/2441 |
| 1 | M | 0.27 | 0/1792 | 0.53 | 0/2441 |
| 1 | N | 0.28 | 0/1797 | 0.51 | 0/2448 |
| 1 | S | 0.28 | 0/1802 | 0.55 | 0/2455 |
| 1 | T | 0.29 | 0/1792 | 0.53 | 0/2441 |
| 2 | C | 0.36 | 1/1765 (0.1%) | 0.54 | 0/2395 |
| 2 | E | 0.27 | 0/1766 | 0.52 | 0/2397 |
| 2 | I | 0.29 | 0/1777 | 0.54 | 1/2411 (0.0%) |
| 2 | K | 0.30 | 0/1765 | 0.53 | 0/2395 |
| 2 | O | 0.27 | 0/1686 | 0.53 | 0/2283 |
| 2 | Q | 0.24 | 0/764 | 0.48 | 0/1031 |
| 2 | U | 0.27 | 0/1758 | 0.52 | 0/2385 |
| 2 | W | 0.25 | 0/874 | 0.47 | 0/1179 |
| All | All | 0.29 | 1/26532 (0.0%) | 0.53 | 3/36062 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | H | 0 | 1 |
| 2 | O | 0 | 1 |
| All | All | 0 | 2 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | C | 1087 | PHE | CG-CD2 | -5.03 | 1.31 | 1.38 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | G | 571 | LEU | CA-CB-CG | 6.79 | 130.91 | 115.30 |
| 1 | A | 601 | ASN | C-N-CA | 5.64 | 135.81 | 121.70 |
| 2 | I | 97 | ARG | NE-CZ-NH1 | -5.45 | 117.57 | 120.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | H | 459 | PRO | Peptide |
| 2 | O | 111 | THR | 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 | 1745 | 0 | 1709 | 43 | 0 |
| 1 | B | 1756 | 0 | 1721 | 34 | 0 |
| 1 | G | 1760 | 0 | 1724 | 46 | 0 |
| 1 | H | 1745 | 0 | 1709 | 44 | 0 |
| 1 | M | 1745 | 0 | 1709 | 36 | 0 |
| 1 | N | 1750 | 0 | 1714 | 35 | 0 |
| 1 | S | 1755 | 0 | 1719 | 32 | 0 |
| 1 | T | 1745 | 0 | 1709 | 52 | 0 |
| 2 | C | 1726 | 0 | 1661 | 38 | 0 |
| 2 | E | 1727 | 0 | 1658 | 48 | 0 |
| 2 | I | 1738 | 0 | 1671 | 34 | 0 |
| 2 | K | 1726 | 0 | 1661 | 37 | 0 |
| 2 | O | 1651 | 0 | 1587 | 49 | 0 |
| 2 | Q | 746 | 0 | 701 | 14 | 0 |
| 2 | U | 1719 | 0 | 1653 | 45 | 0 |
| 2 | W | 853 | 0 | 788 | 22 | 0 |
| 3 | C | 14 | 0 | 13 | 1 | 0 |
| 3 | E | 14 | 0 | 13 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | I | 14 | 0 | 13 | 0 | 0 |
| 3 | K | 14 | 0 | 13 | 1 | 0 |
| All | All | 25943 | 0 | 25146 | 555 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (555) 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:H:514:ILE:HD11 | 2:K:30:ILE:HB | 1.54 | 0.90 |
| 1:T:554:TYR:HA | 1:T:579:PRO:HA | 1.55 | 0.89 |
| 1:S:484:MET:HB3 | 1:S:591:LEU:HB3 | 1.56 | 0.88 |
| 1:B:461:THR:HG22 | 1:B:463:SER:H | 1.42 | 0.84 |
| 1:G:461:THR:HG22 | 1:G:462:ASN:H | 1.42 | 0.83 |
| 1:T:552:GLN:HE21 | 1:T:579:PRO:HB2 | 1.42 | 0.82 |
| 1:T:510:VAL:HB | 1:T:518:ALA:HB3 | 1.64 | 0.80 |
| 1:A:461:THR:HG21 | 2:C:52:TRP:CZ2 | 2.19 | 0.78 |
| 1:N:493:THR:HG22 | 1:N:497:GLN:H | 1.49 | 0.77 |
| 1:H:448:ARG:HG2 | 1:G:568:VAL:HG12 | 1.65 | 0.77 |
| 1:M:493:THR:HG22 | 1:M:497:GLN:H | 1.51 | 0.76 |
| 1:M:510:VAL:HB | 1:M:518:ALA:HB3 | 1.67 | 0.76 |
| 2:O:37:VAL:HG12 | 2:O:47:TRP:HA | 1.70 | 0.74 |
| 2:E:37:VAL:HG12 | 2:E:47:TRP:HA | 1.69 | 0.74 |
| 2:O:1033:LEU:HD21 | 2:O:1088:CYS:HB2 | 1.69 | 0.73 |
| 1:S:510:VAL:HB | 1:S:518:ALA:HB3 | 1.71 | 0.71 |
| 2:U:37:VAL:HG12 | 2:U:47:TRP:HA | 1.72 | 0.71 |
| 2:K:1037:GLN:HB2 | 2:K:1047:LEU:HD11 | 1.71 | 0.71 |
| 2:C:102:ASN:ND2 | 2:C:1096:PRO:HG3 | 2.06 | 0.71 |
| 1:H:510:VAL:HB | 1:H:518:ALA:HB3 | 1.72 | 0.71 |
| 1:G:484:MET:HB2 | 1:G:591:LEU:HB3 | 1.72 | 0.70 |
| 2:U:1050:TYR:CE1 | 1:T:579:PRO:HD2 | 2.25 | 0.70 |
| 1:T:552:GLN:NE2 | 1:T:579:PRO:HB2 | 2.05 | 0.70 |
| 2:U:67:LEU:HD21 | 2:U:80:PHE:CE1 | 2.27 | 0.70 |
| 1:M:456:LEU:HG | 1:M:612:GLU:HB3 | 1.74 | 0.69 |
| 1:T:453:ASN:ND2 | 1:T:553:CYS:HB3 | 2.08 | 0.69 |
| 1:N:510:VAL:HB | 1:N:518:ALA:HB3 | 1.75 | 0.69 |
| 1:A:522:PHE:HE2 | 1:A:642:GLY:HA3 | 1.58 | 0.68 |
| 1:H:568:VAL:HG12 | 1:G:448:ARG:HG2 | 1.73 | 0.68 |
| 1:N:493:THR:HG23 | 1:N:495:ASP:H | 1.56 | 0.68 |
| 2:O:92:ILE:HG23 | 2:O:112:SER:HB2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:S:459:PRO:HD3 | 1:S:554:TYR:CZ | 2.29 | 0.67 |
| 1:T:453:ASN:HB3 | 1:T:481:GLN:HA | 1.75 | 0.67 |
| 2:K:6:GLN:NE2 | 2:K:95:CYS:SG | 2.68 | 0.67 |
| 1:H:443:PRO:O | 1:H:448:ARG:NH1 | 2.27 | 0.67 |
| 2:E:14:PRO:HG3 | 2:E:117:SER:H | 1.60 | 0.67 |
| 1:T:468:VAL:HG23 | 1:T:551:VAL:HG21 | 1.76 | 0.67 |
| 2:W:29:LEU:HD21 | 2:W:71:LYS:HD2 | 1.77 | 0.66 |
| 1:T:458:ALA:HB3 | 1:T:461:THR:HB | 1.77 | 0.66 |
| 2:O:12:VAL:O | 2:O:115:VAL:HG11 | 1.97 | 0.65 |
| 2:U:30:ILE:HD11 | 1:T:514:ILE:HD11 | 1.78 | 0.65 |
| 1:B:510:VAL:HB | 1:B:518:ALA:HB3 | 1.78 | 0.65 |
| 1:B:470:ILE:HG12 | 1:B:510:VAL:HG22 | 1.79 | 0.65 |
| 2:O:99:TYR:HB3 | 2:O:103:VAL:HG13 | 1.77 | 0.65 |
| 2:W:51:ILE:HG13 | 2:W:57:THR:HG22 | 1.78 | 0.65 |
| 2:E:105:ASP:OD1 | 2:E:1055:HIS:NE2 | 2.30 | 0.64 |
| 2:C:29:LEU:HD13 | 2:C:71:LYS:HD2 | 1.79 | 0.64 |
| 1:A:468:VAL:HG21 | 1:A:480:MET:HE3 | 1.78 | 0.64 |
| 2:U:103:VAL:HG22 | 2:U:1034:ASN:HD21 | 1.63 | 0.64 |
| 2:I:32:TYR:CD2 | 2:I:97:ARG:HD2 | 2.32 | 0.64 |
| 1:S:629:ILE:HG13 | 1:T:629:ILE:HG13 | 1.80 | 0.64 |
| 1:A:510:VAL:HB | 1:A:518:ALA:HB3 | 1.80 | 0.63 |
| 1:N:629:ILE:HG13 | 1:M:629:ILE:HG13 | 1.79 | 0.63 |
| 2:K:6:GLN:HG3 | 2:K:110:GLY:H | 1.63 | 0.63 |
| 2:W:1092:ASN:OD1 | 2:W:1093:THR:N | 2.29 | 0.63 |
| 1:A:461:THR:HG22 | 1:A:462:ASN:H | 1.63 | 0.63 |
| 1:T:458:ALA:HA | 1:T:554:TYR:HE2 | 1.64 | 0.63 |
| 1:A:529:SER:HB3 | 1:A:535:HIS:CD2 | 2.34 | 0.63 |
| 2:O:99:TYR:C | 2:O:101:GLY:HA2 | 2.18 | 0.62 |
| 1:T:514:ILE:O | 1:T:515:THR:OG1 | 2.18 | 0.62 |
| 1:B:457:THR:OG1 | 1:B:458:ALA:N | 2.32 | 0.62 |
| 2:U:59:TYR:CD2 | 2:U:67:LEU:HD12 | 2.35 | 0.62 |
| 1:T:456:LEU:HG | 1:T:612:GLU:HB3 | 1.80 | 0.62 |
| 2:C:86:GLN:HG3 | 2:C:87:ALA:H | 1.65 | 0.62 |
| 1:N:458:ALA:HB3 | 1:N:461:THR:HG22 | 1.81 | 0.62 |
| 1:S:459:PRO:HD3 | 1:S:554:TYR:CE2 | 2.36 | 0.61 |
| 2:E:100:TYR:N | 2:E:101:GLY:HA2 | 2.16 | 0.61 |
| 2:K:103:VAL:O | 2:K:1036:TYR:OH | 2.18 | 0.61 |
| 1:G:456:LEU:HG | 1:G:612:GLU:HB3 | 1.81 | 0.61 |
| 1:A:461:THR:HG21 | 2:C:52:TRP:HZ2 | 1.64 | 0.60 |
| 2:K:39:GLN:OE1 | 2:K:1038:GLN:NE2 | 2.30 | 0.60 |
| 1:T:527:LYS:NZ | 1:T:605:GLY:O | 2.28 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:6:GLN:HE22 | 2:C:94:TYR:HA | 1.66 | 0.60 |
| 2:I:1085:THR:HG22 | 2:I:1103:LYS:HG2 | 1.84 | 0.60 |
| 2:E:12:VAL:HG11 | 2:E:85:LEU:HD22 | 1.84 | 0.60 |
| 2:U:52:TRP:HB3 | 1:T:465:ASP:OD2 | 2.01 | 0.60 |
| 1:B:456:LEU:HG | 1:B:612:GLU:HB3 | 1.83 | 0.59 |
| 1:N:454:LYS:HG3 | 1:N:613:LEU:HB2 | 1.84 | 0.59 |
| 1:N:455:THR:OG1 | 1:N:457:THR:O | 2.19 | 0.59 |
| 2:I:30:ILE:HB | 1:G:514:ILE:HD11 | 1.84 | 0.59 |
| 2:I:103:VAL:CG1 | 2:I:1034:ASN:HD21 | 2.14 | 0.59 |
| 2:O:1015:LEU:O | 1:S:475:GLY:HA3 | 2.02 | 0.59 |
| 2:U:1050:TYR:CD1 | 1:T:579:PRO:HD2 | 2.37 | 0.59 |
| 1:T:461:THR:HG22 | 1:T:463:SER:H | 1.67 | 0.59 |
| 2:E:6:GLN:HE22 | 2:E:108:GLY:HA3 | 1.67 | 0.59 |
| 2:E:1092:ASN:OD1 | 2:E:1093:THR:N | 2.35 | 0.59 |
| 2:C:37:VAL:HG12 | 2:C:47:TRP:HA | 1.83 | 0.59 |
| 2:I:103:VAL:HG12 | 2:I:1034:ASN:HD21 | 1.67 | 0.59 |
| 2:I:37:VAL:HG12 | 2:I:47:TRP:HA | 1.85 | 0.59 |
| 2:K:40:SER:HB2 | 2:K:43:LYS:HB2 | 1.83 | 0.58 |
| 1:A:459:PRO:HD3 | 1:A:554:TYR:CE2 | 2.39 | 0.58 |
| 2:C:1084:ALA:HB3 | 2:C:1086:TYR:HE1 | 1.69 | 0.58 |
| 2:O:91:GLY:N | 2:O:114:THR:HG1 | 2.01 | 0.58 |
| 2:O:100:TYR:N | 2:O:101:GLY:HA2 | 2.19 | 0.58 |
| 2:C:10:GLY:O | 2:C:113:VAL:HA | 2.04 | 0.58 |
| 1:N:496:PHE:HB3 | 1:M:496:PHE:HB3 | 1.84 | 0.58 |
| 2:O:1094:PHE:O | 2:O:1096:PRO:HD3 | 2.04 | 0.57 |
| 2:E:40:SER:HB2 | 2:E:43:LYS:HB2 | 1.86 | 0.57 |
| 1:B:479:ILE:HG12 | 1:B:610:ARG:HD2 | 1.86 | 0.57 |
| 2:U:103:VAL:HG22 | 2:U:1034:ASN:ND2 | 2.19 | 0.57 |
| 2:E:38:ARG:NH1 | 2:E:40:SER:OG | 2.38 | 0.57 |
| 1:B:484:MET:HB3 | 1:B:591:LEU:HB3 | 1.85 | 0.57 |
| 1:H:447:ASP:OD1 | 1:H:448:ARG:N | 2.37 | 0.57 |
| 1:S:479:ILE:HG12 | 1:S:610:ARG:HD2 | 1.87 | 0.57 |
| 2:E:1029:ILE:HA | 2:E:1092:ASN:ND2 | 2.20 | 0.57 |
| 2:O:1029:ILE:HD13 | 2:O:1090:GLN:HB2 | 1.85 | 0.57 |
| 1:S:456:LEU:HG | 1:S:612:GLU:HB3 | 1.87 | 0.57 |
| 2:E:35:HIS:HE2 | 2:E:102:ASN:HA | 1.70 | 0.56 |
| 2:C:99:TYR:O | 2:C:103:VAL:HB | 2.05 | 0.56 |
| 2:K:37:VAL:HG12 | 2:K:47:TRP:HA | 1.86 | 0.56 |
| 2:I:1002:ILE:HG23 | 2:I:1026:SER:HB3 | 1.87 | 0.56 |
| 1:G:484:MET:HG2 | 1:G:628:PHE:HE1 | 1.70 | 0.56 |
| 2:C:1037:GLN:HB3 | 2:C:1047:LEU:HD11 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:453:ASN:HA | 1:B:554:TYR:O | 2.06 | 0.56 |
| 1:H:629:ILE:HG13 | 1:G:629:ILE:HG13 | 1.88 | 0.56 |
| 1:G:560:ARG:HB2 | 1:G:571:LEU:HB3 | 1.87 | 0.56 |
| 2:E:87:ALA:HB2 | 2:E:117:SER:HB3 | 1.88 | 0.56 |
| 1:A:430:GLU:HA | 1:A:643:ASN:HA | 1.88 | 0.56 |
| 2:O:111:THR:O | 2:O:113:VAL:HG23 | 2.05 | 0.56 |
| 1:S:431:LEU:HD12 | 1:S:644:THR:HG21 | 1.87 | 0.56 |
| 1:H:496:PHE:HB3 | 1:G:496:PHE:HB3 | 1.88 | 0.55 |
| 1:M:454:LYS:NZ | 1:M:615:SER:HB3 | 2.20 | 0.55 |
| 1:S:460:GLY:O | 2:W:102:ASN:ND2 | 2.39 | 0.55 |
| 2:U:1037:GLN:HB2 | 2:U:1047:LEU:HD11 | 1.87 | 0.55 |
| 2:K:1035:TRP:CE2 | 2:K:1073:LEU:HB2 | 2.42 | 0.55 |
| 2:I:48:LEU:O | 2:I:60:ASN:N | 2.39 | 0.55 |
| 2:I:100:TYR:HD1 | 1:G:552:GLN:HB3 | 1.71 | 0.55 |
| 2:I:6:GLN:HE22 | 2:I:94:TYR:HA | 1.72 | 0.55 |
| 1:G:529:SER:HB3 | 1:G:535:HIS:ND1 | 2.22 | 0.55 |
| 2:E:1016:GLY:HA2 | 2:E:1077:ASN:HB2 | 1.88 | 0.55 |
| 1:G:572:THR:HG22 | 1:G:617:THR:O | 2.06 | 0.55 |
| 2:Q:1055:HIS:CD2 | 2:Q:1056:SER:H | 2.24 | 0.55 |
| 2:W:1090:GLN:HE22 | 2:W:1097:THR:HG22 | 1.71 | 0.55 |
| 1:A:626:THR:O | 1:B:626:THR:OG1 | 2.24 | 0.55 |
| 1:T:455:THR:OG1 | 1:T:457:THR:O | 2.18 | 0.55 |
| 2:C:1033:LEU:HB3 | 2:C:1051:THR:HG22 | 1.89 | 0.55 |
| 1:N:432:ARG:NH1 | 1:N:494:PRO:O | 2.40 | 0.55 |
| 2:O:1004:MET:SD | 2:O:1090:GLN:HB3 | 2.47 | 0.55 |
| 2:O:6:GLN:NE2 | 2:O:110:GLY:H | 2.05 | 0.55 |
| 2:O:38:ARG:HA | 2:O:92:ILE:O | 2.05 | 0.55 |
| 2:E:99:TYR:C | 2:E:101:GLY:HA2 | 2.27 | 0.54 |
| 1:T:459:PRO:HD3 | 1:T:554:TYR:CE2 | 2.42 | 0.54 |
| 1:T:531:THR:HG22 | 1:T:532:ASN:H | 1.72 | 0.54 |
| 1:T:550:LYS:HB3 | 1:T:583:ARG:HG2 | 1.89 | 0.54 |
| 1:A:629:ILE:HG13 | 1:B:629:ILE:HG13 | 1.88 | 0.54 |
| 2:K:13:GLN:HB3 | 2:K:16:GLN:HG3 | 1.89 | 0.54 |
| 1:G:537:ILE:HD11 | 1:G:602:LEU:HD22 | 1.88 | 0.54 |
| 1:M:453:ASN:HA | 1:M:554:TYR:O | 2.07 | 0.54 |
| 2:U:11:LEU:H | 2:U:11:LEU:HD12 | 1.73 | 0.54 |
| 2:C:28:SER:HB3 | 2:C:30:ILE:HG22 | 1.87 | 0.54 |
| 2:I:1016:GLY:HA2 | 2:I:1077:ASN:HB2 | 1.89 | 0.54 |
| 1:G:510:VAL:HB | 1:G:518:ALA:HB3 | 1.89 | 0.54 |
| 1:N:597:LEU:HD11 | 1:N:619:TYR:CE1 | 2.43 | 0.54 |
| 2:O:1037:GLN:HG3 | 2:O:1086:TYR:CE1 | 2.42 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:470:ILE:HG12 | 1:G:510:VAL:HG22 | 1.89 | 0.54 |
| 2:O:1050:TYR:CE2 | 1:M:579:PRO:HD2 | 2.43 | 0.54 |
| 1:A:555:MET:HE1 | 1:A:582:ILE:HD11 | 1.90 | 0.54 |
| 1:B:572:THR:HG22 | 1:B:617:THR:O | 2.08 | 0.54 |
| 1:S:453:ASN:HA | 1:S:554:TYR:O | 2.07 | 0.54 |
| 2:O:30:ILE:HG23 | 2:O:31:ASP:OD1 | 2.07 | 0.53 |
| 2:W:60:ASN:OD1 | 2:W:61:ALA:N | 2.41 | 0.53 |
| 2:U:1050:TYR:HE1 | 1:T:579:PRO:HD2 | 1.70 | 0.53 |
| 2:O:35:HIS:NE2 | 2:O:101:GLY:O | 2.31 | 0.53 |
| 1:A:620:TYR:HB3 | 1:B:630:THR:HG21 | 1.89 | 0.53 |
| 2:E:38:ARG:HH12 | 2:E:40:SER:HG | 1.57 | 0.53 |
| 1:T:458:ALA:HA | 1:T:554:TYR:CE2 | 2.43 | 0.53 |
| 2:U:1050:TYR:HD2 | 2:U:1050:TYR:O | 1.92 | 0.53 |
| 2:E:6:GLN:NE2 | 2:E:108:GLY:HA3 | 2.23 | 0.53 |
| 2:U:97:ARG:NH2 | 2:U:105:ASP:OD2 | 2.36 | 0.53 |
| 1:B:537:ILE:HD11 | 1:B:602:LEU:HD22 | 1.90 | 0.53 |
| 2:Q:60:ASN:OD1 | 2:Q:61:ALA:N | 2.42 | 0.53 |
| 2:O:39:GLN:HB3 | 2:O:92:ILE:HB | 1.90 | 0.53 |
| 1:S:455:THR:OG1 | 1:S:457:THR:O | 2.23 | 0.53 |
| 2:K:1037:GLN:HG3 | 2:K:1086:TYR:CE1 | 2.44 | 0.53 |
| 2:I:38:ARG:NH2 | 2:I:46:GLU:OE1 | 2.41 | 0.53 |
| 1:S:537:ILE:HD11 | 1:S:602:LEU:HD22 | 1.90 | 0.53 |
| 2:W:60:ASN:HB3 | 2:W:63:PHE:HD2 | 1.74 | 0.53 |
| 1:N:440:ILE:HD12 | 1:N:440:ILE:H | 1.73 | 0.53 |
| 1:N:456:LEU:HG | 1:N:612:GLU:HB3 | 1.91 | 0.52 |
| 2:I:100:TYR:O | 1:G:554:TYR:OH | 2.19 | 0.52 |
| 2:W:1051:THR:HG23 | 2:W:1052:SER:H | 1.73 | 0.52 |
| 1:N:470:ILE:HD13 | 1:N:541:PHE:CD2 | 2.44 | 0.52 |
| 1:S:529:SER:HB3 | 1:S:535:HIS:CD2 | 2.44 | 0.52 |
| 1:H:514:ILE:HD11 | 2:K:30:ILE:CB | 2.35 | 0.52 |
| 2:U:30:ILE:HD11 | 1:T:514:ILE:CD1 | 2.40 | 0.52 |
| 2:K:1084:ALA:HB3 | 2:K:1086:TYR:HE1 | 1.74 | 0.52 |
| 1:S:454:LYS:HG3 | 1:S:613:LEU:HB2 | 1.91 | 0.52 |
| 1:B:440:ILE:HD12 | 1:B:440:ILE:H | 1.73 | 0.52 |
| 2:E:4:LEU:HD22 | 2:E:24:VAL:HG12 | 1.92 | 0.52 |
| 1:H:626:THR:O | 1:G:626:THR:OG1 | 2.27 | 0.52 |
| 2:I:1021:ILE:HD11 | 2:I:1073:LEU:HD23 | 1.91 | 0.52 |
| 1:S:597:LEU:HD11 | 1:S:619:TYR:CE1 | 2.45 | 0.52 |
| 2:U:1:ASP:HA | 2:U:26:GLY:HA3 | 1.90 | 0.52 |
| 1:A:456:LEU:O | 1:A:479:ILE:HD13 | 2.10 | 0.52 |
| 2:E:97:ARG:HE | 2:E:106:TYR:HD2 | 1.56 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:1029:ILE:HD11 | 2:E:1071:TYR:CE2 | 2.45 | 0.52 |
| 2:W:35:HIS:CD2 | 2:W:98:PRO:HB3 | 2.45 | 0.52 |
| 1:A:522:PHE:HD2 | 1:A:523:MET:N | 2.07 | 0.52 |
| 2:Q:1030:SER:HB2 | 2:Q:1032:TYR:HD2 | 1.74 | 0.52 |
| 2:O:1050:TYR:O | 2:O:1051:THR:HG22 | 2.09 | 0.52 |
| 2:E:35:HIS:NE2 | 2:E:102:ASN:HA | 2.25 | 0.51 |
| 2:E:98:PRO:HB3 | 2:E:102:ASN:H | 1.75 | 0.51 |
| 2:O:35:HIS:HD2 | 2:O:104:MET:HG2 | 1.75 | 0.51 |
| 1:A:461:THR:HG22 | 1:A:462:ASN:N | 2.26 | 0.51 |
| 2:K:1050:TYR:O | 2:K:1051:THR:HG22 | 2.11 | 0.51 |
| 2:Q:1033:LEU:HB3 | 2:Q:1051:THR:HG22 | 1.92 | 0.51 |
| 1:M:493:THR:HG23 | 1:M:495:ASP:H | 1.75 | 0.51 |
| 2:U:1004:MET:SD | 2:U:1090:GLN:HB3 | 2.51 | 0.51 |
| 1:A:555:MET:CE | 1:A:582:ILE:HD11 | 2.40 | 0.51 |
| 1:S:496:PHE:HB3 | 1:T:496:PHE:HB3 | 1.91 | 0.51 |
| 1:S:533:ASN:O | 1:S:600:ASN:N | 2.42 | 0.51 |
| 1:B:460:GLY:O | 1:B:461:THR:OG1 | 2.27 | 0.51 |
| 1:H:600:ASN:OD1 | 1:H:601:ASN:N | 2.44 | 0.51 |
| 2:Q:105:ASP:HB2 | 2:Q:1055:HIS:HE1 | 1.76 | 0.51 |
| 1:S:548:ASP:OD1 | 1:S:586:VAL:N | 2.41 | 0.51 |
| 1:A:456:LEU:HG | 1:A:612:GLU:HB3 | 1.92 | 0.51 |
| 1:B:504:PRO:HG3 | 1:B:521:TYR:HE1 | 1.76 | 0.51 |
| 2:I:1033:LEU:HB2 | 2:I:1051:THR:HG22 | 1.92 | 0.51 |
| 2:C:1035:TRP:CE2 | 2:C:1073:LEU:HB2 | 2.46 | 0.51 |
| 1:G:543:ILE:HD12 | 1:G:545:PRO:HD3 | 1.92 | 0.51 |
| 1:A:524:LYS:HB3 | 1:A:540:ILE:HG12 | 1.93 | 0.50 |
| 1:N:479:ILE:HG12 | 1:N:610:ARG:HD2 | 1.93 | 0.50 |
| 2:O:99:TYR:O | 2:O:103:VAL:HG12 | 2.11 | 0.50 |
| 1:M:468:VAL:HG23 | 1:M:551:VAL:HG11 | 1.92 | 0.50 |
| 1:S:530:TYR:CE2 | 1:S:620:TYR:HB2 | 2.46 | 0.50 |
| 1:A:453:ASN:HA | 1:A:554:TYR:O | 2.11 | 0.50 |
| 2:I:1029:ILE:HD11 | 2:I:1071:TYR:CE2 | 2.46 | 0.50 |
| 2:C:60:ASN:HB3 | 2:C:63:PHE:HD2 | 1.75 | 0.50 |
| 1:H:529:SER:HB3 | 1:H:535:HIS:ND1 | 2.25 | 0.50 |
| 1:G:479:ILE:HG12 | 1:G:610:ARG:HD2 | 1.94 | 0.50 |
| 1:M:454:LYS:NZ | 1:M:575:SER:O | 2.44 | 0.50 |
| 1:A:522:PHE:HD2 | 1:A:523:MET:H | 1.59 | 0.50 |
| 2:E:99:TYR:O | 2:E:100:TYR:HB2 | 2.11 | 0.50 |
| 1:N:453:ASN:HA | 1:N:554:TYR:O | 2.12 | 0.50 |
| 1:M:479:ILE:HG12 | 1:M:610:ARG:HD2 | 1.93 | 0.50 |
| 1:H:453:ASN:HA | 1:H:554:TYR:O | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:C:103:VAL:HG22 | 2:C:1034:ASN:OD1 | 2.11 | 0.50 |
| 1:H:445:SER:O | 1:H:631:PRO:HG2 | 2.10 | 0.50 |
| 1:H:510:VAL:HG21 | 1:H:543:ILE:HG21 | 1.94 | 0.50 |
| 2:W:99:TYR:O | 2:W:103:VAL:HB | 2.11 | 0.50 |
| 2:E:17:SER:HA | 2:E:83:ASN:HA | 1.92 | 0.50 |
| 2:E:1009:SER:O | 2:E:1103:LYS:N | 2.43 | 0.50 |
| 1:B:543:ILE:HD12 | 1:B:545:PRO:HD3 | 1.92 | 0.50 |
| 2:I:1032:TYR:HE1 | 1:G:579:PRO:HD3 | 1.77 | 0.50 |
| 1:N:456:LEU:HD13 | 1:N:610:ARG:HG2 | 1.94 | 0.50 |
| 2:O:60:ASN:O | 2:O:64:ILE:HG23 | 2.12 | 0.50 |
| 2:C:47:TRP:CD2 | 2:C:1096:PRO:HD2 | 2.47 | 0.49 |
| 2:C:67:LEU:HD11 | 2:C:80:PHE:CE1 | 2.47 | 0.49 |
| 1:H:462:ASN:HD21 | 2:K:58:ASP:HB3 | 1.77 | 0.49 |
| 2:Q:1033:LEU:HD23 | 2:Q:1034:ASN:N | 2.27 | 0.49 |
| 2:U:40:SER:OG | 2:U:43:LYS:HB2 | 2.12 | 0.49 |
| 1:T:552:GLN:HG3 | 1:T:580:GLU:O | 2.12 | 0.49 |
| 2:E:1037:GLN:HB2 | 2:E:1047:LEU:HD11 | 1.95 | 0.49 |
| 1:N:491:TRP:HZ3 | 1:N:644:THR:HG21 | 1.76 | 0.49 |
| 1:N:475:GLY:HA3 | 2:U:1015:LEU:O | 2.12 | 0.49 |
| 2:U:1016:GLY:HA2 | 2:U:1077:ASN:HB2 | 1.94 | 0.49 |
| 1:T:545:PRO:HB3 | 1:T:549:PHE:HE1 | 1.77 | 0.49 |
| 1:G:453:ASN:HA | 1:G:554:TYR:O | 2.12 | 0.49 |
| 1:G:545:PRO:HB3 | 1:G:549:PHE:HE1 | 1.78 | 0.49 |
| 2:E:103:VAL:HG22 | 2:E:1034:ASN:OD1 | 2.13 | 0.49 |
| 1:N:644:THR:OG1 | 1:N:645:ALA:N | 2.45 | 0.49 |
| 2:U:67:LEU:HD21 | 2:U:80:PHE:HE1 | 1.75 | 0.49 |
| 1:N:568:VAL:HG22 | 1:M:448:ARG:HG2 | 1.95 | 0.49 |
| 2:Q:1028:ASP:OD1 | 2:Q:1029:ILE:N | 2.46 | 0.49 |
| 1:T:621:ALA:HB1 | 1:T:626:THR:HA | 1.95 | 0.49 |
| 2:O:6:GLN:OE1 | 2:O:108:GLY:HA3 | 2.13 | 0.49 |
| 2:I:40:SER:OG | 2:I:41:PRO:HD2 | 2.13 | 0.49 |
| 2:O:1037:GLN:HB2 | 2:O:1047:LEU:HD11 | 1.95 | 0.49 |
| 1:M:454:LYS:HG3 | 1:M:613:LEU:HB2 | 1.94 | 0.49 |
| 2:C:60:ASN:OD1 | 2:C:61:ALA:N | 2.44 | 0.48 |
| 2:U:1028:ASP:HA | 2:U:1069:THR:HG22 | 1.95 | 0.48 |
| 1:T:543:ILE:HD12 | 1:T:545:PRO:HD3 | 1.94 | 0.48 |
| 2:E:6:GLN:HE21 | 2:E:95:CYS:H | 1.60 | 0.48 |
| 1:H:456:LEU:HG | 1:H:612:GLU:HB3 | 1.94 | 0.48 |
| 2:K:67:LEU:HD11 | 2:K:80:PHE:CE1 | 2.48 | 0.48 |
| 1:B:515:THR:OG1 | 1:B:517:LYS:HD3 | 2.14 | 0.48 |
| 1:T:524:LYS:HB3 | 1:T:540:ILE:HG12 | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:T:554:TYR:C | 1:T:555:MET:HG2 | 2.34 | 0.48 |
| 2:I:1035:TRP:CE2 | 2:I:1073:LEU:HB2 | 2.49 | 0.48 |
| 1:M:527:LYS:HD3 | 1:M:602:LEU:HD13 | 1.96 | 0.48 |
| 1:A:435:LEU:HD13 | 1:A:486:ILE:HD12 | 1.96 | 0.48 |
| 2:O:1092:ASN:OD1 | 2:O:1093:THR:N | 2.46 | 0.48 |
| 2:U:1037:GLN:HG3 | 2:U:1086:TYR:CE1 | 2.49 | 0.48 |
| 1:A:565:ASN:O | 1:B:574:ARG:NH1 | 2.47 | 0.48 |
| 1:S:514:ILE:HG13 | 2:W:30:ILE:HD11 | 1.95 | 0.48 |
| 1:A:445:SER:O | 1:A:631:PRO:HG2 | 2.14 | 0.48 |
| 2:K:99:TYR:C | 2:K:101:GLY:H | 2.17 | 0.48 |
| 2:U:60:ASN:OD1 | 2:U:61:ALA:N | 2.46 | 0.48 |
| 2:W:29:LEU:HD23 | 2:W:73:ASN:HA | 1.94 | 0.48 |
| 2:U:1050:TYR:HE1 | 1:T:578:SER:HA | 1.77 | 0.48 |
| 1:A:522:PHE:CD2 | 1:A:523:MET:N | 2.82 | 0.48 |
| 1:N:528:ASN:O | 1:N:529:SER:OG | 2.30 | 0.48 |
| 2:W:103:VAL:HG22 | 2:W:1034:ASN:ND2 | 2.29 | 0.48 |
| 1:A:455:THR:OG1 | 1:A:457:THR:O | 2.20 | 0.47 |
| 1:H:555:MET:CE | 1:H:582:ILE:HD11 | 2.44 | 0.47 |
| 1:S:433:VAL:HG22 | 1:S:435:LEU:HD12 | 1.95 | 0.47 |
| 1:A:448:ARG:HH12 | 1:A:451:TRP:HE1 | 1.61 | 0.47 |
| 1:B:599:GLU:HG3 | 1:B:600:ASN:H | 1.79 | 0.47 |
| 1:G:461:THR:HG22 | 1:G:462:ASN:N | 2.21 | 0.47 |
| 1:S:579:PRO:HD2 | 2:W:1050:TYR:CE1 | 2.49 | 0.47 |
| 2:C:13:GLN:HB3 | 2:C:16:GLN:HG3 | 1.96 | 0.47 |
| 1:B:463:SER:OG | 1:B:465:ASP:OD1 | 2.32 | 0.47 |
| 2:E:114:THR:HG21 | 1:M:477:TYR:HE1 | 1.80 | 0.47 |
| 1:G:431:LEU:HD12 | 1:G:644:THR:HG21 | 1.97 | 0.47 |
| 2:C:86:GLN:HG2 | 3:C:1201:NAG:H61 | 1.97 | 0.47 |
| 1:H:435:LEU:HD13 | 1:H:486:ILE:HD12 | 1.97 | 0.47 |
| 2:Q:35:HIS:NE2 | 2:Q:98:PRO:HB3 | 2.30 | 0.47 |
| 1:A:522:PHE:CE2 | 1:A:642:GLY:HA3 | 2.44 | 0.47 |
| 2:E:99:TYR:N | 2:E:103:VAL:O | 2.48 | 0.47 |
| 1:H:458:ALA:O | 1:H:461:THR:HG22 | 2.14 | 0.47 |
| 1:H:626:THR:OG1 | 1:G:626:THR:O | 2.32 | 0.47 |
| 2:U:1033:LEU:HA | 2:U:1089:GLN:O | 2.14 | 0.47 |
| 1:T:454:LYS:HG3 | 1:T:613:LEU:HB2 | 1.96 | 0.47 |
| 2:K:60:ASN:OD1 | 2:K:61:ALA:N | 2.47 | 0.47 |
| 1:N:579:PRO:HD3 | 2:Q:1032:TYR:CE1 | 2.50 | 0.47 |
| 2:U:9:PRO:HB3 | 2:U:111:THR:HG23 | 1.97 | 0.47 |
| 1:T:472:HIS:HB2 | 1:T:508:MET:SD | 2.55 | 0.47 |
| 1:T:512:VAL:HG11 | 1:T:551:VAL:HG12 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:448:ARG:NH2 | 1:H:451:TRP:HE1 | 2.12 | 0.46 |
| 2:O:1106:ILE:HG22 | 2:O:1107:LYS:N | 2.30 | 0.46 |
| 1:M:543:ILE:HD13 | 1:M:592:LEU:HD11 | 1.96 | 0.46 |
| 2:U:85:LEU:H | 2:U:85:LEU:HD23 | 1.80 | 0.46 |
| 2:U:1033:LEU:HB3 | 2:U:1051:THR:HG22 | 1.97 | 0.46 |
| 1:A:543:ILE:HD13 | 1:A:592:LEU:HD11 | 1.97 | 0.46 |
| 2:E:99:TYR:O | 2:E:103:VAL:HB | 2.15 | 0.46 |
| 1:H:438:GLY:HA2 | 1:H:487:LYS:HB2 | 1.97 | 0.46 |
| 1:T:504:PRO:HG3 | 1:T:521:TYR:CE1 | 2.50 | 0.46 |
| 1:H:558:PHE:O | 1:G:560:ARG:NH2 | 2.36 | 0.46 |
| 2:O:92:ILE:HA | 2:O:112:SER:HB2 | 1.96 | 0.46 |
| 2:U:59:TYR:CE2 | 2:U:67:LEU:HD12 | 2.51 | 0.46 |
| 1:T:597:LEU:HD11 | 1:T:619:TYR:CE1 | 2.50 | 0.46 |
| 1:H:462:ASN:OD1 | 1:H:462:ASN:N | 2.46 | 0.46 |
| 2:C:28:SER:CB | 2:C:30:ILE:HG22 | 2.45 | 0.46 |
| 1:G:593:THR:HG21 | 1:G:628:PHE:HE2 | 1.81 | 0.46 |
| 1:G:603:PRO:HG2 | 1:G:607:VAL:HG22 | 1.96 | 0.46 |
| 2:O:39:GLN:O | 2:O:92:ILE:N | 2.38 | 0.46 |
| 1:A:598:LYS:HD3 | 1:A:602:LEU:HD23 | 1.98 | 0.46 |
| 2:I:97:ARG:NH2 | 2:I:105:ASP:OD2 | 2.47 | 0.46 |
| 2:O:30:ILE:HD11 | 1:M:514:ILE:HG13 | 1.98 | 0.46 |
| 1:T:513:ASN:OD1 | 1:T:514:ILE:N | 2.49 | 0.46 |
| 2:K:38:ARG:HB3 | 2:K:48:LEU:HD11 | 1.97 | 0.46 |
| 2:I:1089:GLN:HB2 | 2:I:1098:PHE:CD2 | 2.51 | 0.46 |
| 2:U:1051:THR:HG21 | 2:U:1071:TYR:CD1 | 2.51 | 0.46 |
| 2:C:1:ASP:OD1 | 2:C:2:VAL:N | 2.49 | 0.46 |
| 2:E:1032:TYR:HE1 | 1:B:579:PRO:HD3 | 1.79 | 0.46 |
| 1:N:529:SER:HB3 | 1:N:535:HIS:CD2 | 2.50 | 0.46 |
| 2:K:43:LYS:HE3 | 3:K:1201:NAG:H81 | 1.97 | 0.46 |
| 2:O:1029:ILE:HA | 2:O:1092:ASN:ND2 | 2.31 | 0.46 |
| 1:A:545:PRO:HD2 | 1:A:588:GLU:O | 2.16 | 0.45 |
| 2:E:1007:THR:OG1 | 2:E:1008:THR:N | 2.49 | 0.45 |
| 2:K:1038:GLN:HG3 | 2:K:1044:VAL:HG22 | 1.98 | 0.45 |
| 1:G:625:LEU:HD23 | 1:G:628:PHE:HD2 | 1.81 | 0.45 |
| 2:O:60:ASN:OD1 | 2:O:61:ALA:N | 2.49 | 0.45 |
| 1:T:467:LEU:HD22 | 1:T:553:CYS:HA | 1.98 | 0.45 |
| 2:I:12:VAL:HG21 | 2:I:85:LEU:HD22 | 1.98 | 0.45 |
| 1:N:454:LYS:HA | 1:N:613:LEU:HD12 | 1.98 | 0.45 |
| 2:U:1049:TYR:O | 2:U:1053:ARG:HB2 | 2.16 | 0.45 |
| 2:C:1049:TYR:O | 2:C:1053:ARG:HB2 | 2.16 | 0.45 |
| 2:K:1083:ILE:HG23 | 2:K:1104:LEU:O | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:437:VAL:HG21 | 1:G:632:PRO:HB2 | 1.97 | 0.45 |
| 1:A:598:LYS:HB3 | 1:A:602:LEU:HD21 | 1.99 | 0.45 |
| 1:G:525:GLN:HG3 | 1:G:606:TRP:CH2 | 2.52 | 0.45 |
| 1:A:454:LYS:HG3 | 1:A:613:LEU:HB2 | 1.99 | 0.45 |
| 2:C:32:TYR:CD2 | 2:C:97:ARG:HD2 | 2.52 | 0.45 |
| 2:C:72:ASP:OD2 | 2:C:75:LYS:HE2 | 2.15 | 0.45 |
| 2:I:60:ASN:OD1 | 2:I:61:ALA:N | 2.49 | 0.45 |
| 2:I:1033:LEU:HD12 | 2:I:1071:TYR:CG | 2.51 | 0.45 |
| 1:N:435:LEU:HD13 | 1:N:486:ILE:HD12 | 1.99 | 0.45 |
| 2:O:20:ILE:HB | 2:O:80:PHE:HB3 | 1.99 | 0.45 |
| 2:O:1019:VAL:HG21 | 2:O:1078:LEU:HD11 | 1.99 | 0.45 |
| 1:M:524:LYS:HB3 | 1:M:540:ILE:HG12 | 1.99 | 0.45 |
| 2:U:1092:ASN:OD1 | 2:U:1093:THR:N | 2.49 | 0.45 |
| 1:T:554:TYR:CD1 | 1:T:554:TYR:N | 2.82 | 0.45 |
| 2:E:52:TRP:CZ2 | 1:B:461:THR:HG21 | 2.51 | 0.45 |
| 2:E:1010:SER:HA | 2:E:1103:LYS:O | 2.16 | 0.45 |
| 1:H:456:LEU:HD13 | 1:H:610:ARG:HG2 | 1.98 | 0.45 |
| 2:I:1006:GLN:HG3 | 2:I:1022:SER:O | 2.17 | 0.45 |
| 1:G:445:SER:O | 1:G:631:PRO:HG2 | 2.16 | 0.45 |
| 1:M:597:LEU:HD11 | 1:M:619:TYR:CE1 | 2.52 | 0.45 |
| 2:U:59:TYR:HE2 | 2:U:69:ILE:HG13 | 1.81 | 0.45 |
| 2:K:6:GLN:HG3 | 2:K:110:GLY:N | 2.30 | 0.45 |
| 1:B:545:PRO:HB3 | 1:B:549:PHE:HE1 | 1.82 | 0.44 |
| 2:K:1049:TYR:O | 2:K:1053:ARG:HB2 | 2.17 | 0.44 |
| 2:Q:60:ASN:HB3 | 2:Q:63:PHE:HD1 | 1.82 | 0.44 |
| 1:T:613:LEU:HD22 | 1:T:619:TYR:HE2 | 1.81 | 0.44 |
| 2:E:1033:LEU:HB3 | 2:E:1051:THR:CG2 | 2.48 | 0.44 |
| 2:K:29:LEU:HD12 | 2:K:29:LEU:HA | 1.85 | 0.44 |
| 2:I:1049:TYR:O | 2:I:1053:ARG:HB2 | 2.17 | 0.44 |
| 1:G:504:PRO:HG3 | 1:G:521:TYR:CE1 | 2.52 | 0.44 |
| 1:G:524:LYS:HB3 | 1:G:540:ILE:HG12 | 2.00 | 0.44 |
| 2:O:92:ILE:HA | 2:O:112:SER:CB | 2.48 | 0.44 |
| 1:M:621:ALA:HB1 | 1:M:626:THR:HA | 1.99 | 0.44 |
| 1:T:438:GLY:HA2 | 1:T:487:LYS:HB2 | 1.99 | 0.44 |
| 2:E:67:LEU:HD11 | 2:E:80:PHE:CE1 | 2.52 | 0.44 |
| 1:S:560:ARG:HD2 | 1:T:558:PHE:O | 2.18 | 0.44 |
| 1:T:467:LEU:CD2 | 1:T:553:CYS:HA | 2.47 | 0.44 |
| 1:B:462:ASN:OD1 | 1:B:462:ASN:N | 2.47 | 0.44 |
| 2:I:38:ARG:HG3 | 2:I:93:TYR:CE1 | 2.53 | 0.44 |
| 2:E:60:ASN:OD1 | 2:E:61:ALA:N | 2.49 | 0.44 |
| 2:C:4:LEU:HD23 | 2:C:22:CYS:SG | 2.58 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:E:38:ARG:HG2 | 2:E:48:LEU:HD21 | 1.99 | 0.44 |
| 2:Q:1049:TYR:CE2 | 2:Q:1053:ARG:HD2 | 2.52 | 0.44 |
| 2:O:99:TYR:O | 2:O:100:TYR:HB2 | 2.18 | 0.44 |
| 1:M:452:LEU:O | 1:M:555:MET:HA | 2.16 | 0.44 |
| 1:A:433:VAL:HG11 | 1:A:522:PHE:CE1 | 2.53 | 0.44 |
| 1:G:560:ARG:HD2 | 1:G:569:ALA:O | 2.18 | 0.44 |
| 1:N:560:ARG:HD2 | 1:M:558:PHE:O | 2.17 | 0.44 |
| 1:M:467:LEU:HD13 | 1:M:479:ILE:HG23 | 2.00 | 0.44 |
| 2:U:102:ASN:ND2 | 2:U:1096:PRO:HG3 | 2.32 | 0.44 |
| 1:M:514:ILE:HG13 | 1:M:514:ILE:O | 2.18 | 0.44 |
| 1:M:613:LEU:HD22 | 1:M:619:TYR:HE2 | 1.83 | 0.44 |
| 1:S:626:THR:O | 1:T:626:THR:OG1 | 2.36 | 0.44 |
| 1:B:593:THR:HG21 | 1:B:628:PHE:HE2 | 1.83 | 0.43 |
| 1:B:621:ALA:HB1 | 1:B:626:THR:HA | 2.00 | 0.43 |
| 2:W:36:TRP:CZ3 | 2:W:95:CYS:HB3 | 2.53 | 0.43 |
| 1:G:473:ASP:O | 1:G:474:LEU:HB3 | 2.18 | 0.43 |
| 1:N:504:PRO:HG3 | 1:N:521:TYR:CE1 | 2.53 | 0.43 |
| 2:C:11:LEU:HD12 | 2:C:11:LEU:O | 2.18 | 0.43 |
| 2:C:36:TRP:CZ2 | 2:C:80:PHE:HB2 | 2.53 | 0.43 |
| 2:C:1089:GLN:HB2 | 2:C:1098:PHE:CE2 | 2.53 | 0.43 |
| 2:E:1037:GLN:O | 2:E:1044:VAL:HA | 2.18 | 0.43 |
| 1:G:621:ALA:HB1 | 1:G:626:THR:HA | 2.00 | 0.43 |
| 1:M:458:ALA:HA | 1:M:554:TYR:CE2 | 2.53 | 0.43 |
| 2:I:76:SER:O | 2:I:76:SER:OG | 2.36 | 0.43 |
| 2:W:5:LYS:N | 2:W:23:THR:O | 2.52 | 0.43 |
| 2:U:18:LEU:O | 2:U:81:LYS:HA | 2.18 | 0.43 |
| 2:C:38:ARG:HB3 | 2:C:48:LEU:HD11 | 2.00 | 0.43 |
| 1:A:548:ASP:OD1 | 1:A:586:VAL:N | 2.49 | 0.43 |
| 1:B:461:THR:HG22 | 1:B:462:ASN:N | 2.33 | 0.43 |
| 1:H:540:ILE:HG22 | 1:H:593:THR:HG22 | 2.01 | 0.43 |
| 2:K:1089:GLN:HG3 | 2:K:1098:PHE:CE1 | 2.54 | 0.43 |
| 2:I:39:GLN:OE1 | 2:I:1038:GLN:NE2 | 2.43 | 0.43 |
| 2:I:67:LEU:HD11 | 2:I:80:PHE:CE1 | 2.54 | 0.43 |
| 1:B:451:TRP:CE3 | 1:B:555:MET:HB3 | 2.54 | 0.43 |
| 1:G:533:ASN:OD1 | 1:G:534:ARG:N | 2.51 | 0.43 |
| 1:N:493:THR:HG23 | 1:N:495:ASP:N | 2.30 | 0.43 |
| 2:Q:22:CYS:HB2 | 2:Q:36:TRP:CH2 | 2.54 | 0.43 |
| 2:O:1048:ILE:HA | 2:O:1053:ARG:O | 2.19 | 0.43 |
| 1:A:476:HIS:HB3 | 1:A:608:TRP:CG | 2.54 | 0.43 |
| 2:E:1054:LEU:HD21 | 2:E:1062:PHE:O | 2.19 | 0.43 |
| 1:M:459:PRO:HD3 | 1:M:554:TYR:CE2 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:556:SER:OG | 1:A:574:ARG:HB3 | 2.19 | 0.42 |
| 2:C:34:VAL:HG21 | 2:C:78:VAL:HG21 | 2.01 | 0.42 |
| 2:C:1046:LEU:HD23 | 2:C:1055:HIS:CD2 | 2.54 | 0.42 |
| 1:B:437:VAL:HG21 | 1:B:632:PRO:HB2 | 2.00 | 0.42 |
| 1:N:525:GLN:HG3 | 1:N:606:TRP:CZ3 | 2.54 | 0.42 |
| 2:K:1033:LEU:HD13 | 2:K:1071:TYR:CG | 2.54 | 0.42 |
| 1:G:452:LEU:O | 1:G:555:MET:HA | 2.18 | 0.42 |
| 1:G:476:HIS:HB3 | 1:G:608:TRP:CG | 2.54 | 0.42 |
| 2:U:1033:LEU:HB3 | 2:U:1051:THR:CG2 | 2.48 | 0.42 |
| 1:T:552:GLN:HG3 | 1:T:580:GLU:C | 2.39 | 0.42 |
| 2:C:1023:CYS:SG | 2:C:1033:LEU:HD11 | 2.60 | 0.42 |
| 2:E:1033:LEU:HD23 | 2:E:1034:ASN:N | 2.33 | 0.42 |
| 2:E:1035:TRP:HD1 | 2:E:1048:ILE:HB | 1.84 | 0.42 |
| 2:K:1:ASP:OD1 | 2:K:2:VAL:N | 2.52 | 0.42 |
| 2:I:99:TYR:HB2 | 2:I:105:ASP:HB3 | 2.00 | 0.42 |
| 1:M:504:PRO:HG3 | 1:M:521:TYR:CE1 | 2.54 | 0.42 |
| 2:W:28:SER:HB2 | 2:W:30:ILE:HG22 | 2.01 | 0.42 |
| 2:W:1034:ASN:N | 2:W:1089:GLN:O | 2.35 | 0.42 |
| 2:W:1051:THR:HG23 | 2:W:1052:SER:N | 2.33 | 0.42 |
| 2:U:1038:GLN:O | 2:U:1084:ALA:HB1 | 2.18 | 0.42 |
| 1:T:452:LEU:O | 1:T:555:MET:HA | 2.19 | 0.42 |
| 1:H:441:MET:HG3 | 1:H:485:HIS:HB2 | 2.02 | 0.42 |
| 2:K:16:GLN:O | 2:K:17:SER:OG | 2.27 | 0.42 |
| 2:K:28:SER:OG | 2:K:30:ILE:HG12 | 2.19 | 0.42 |
| 2:U:100:TYR:CD1 | 1:T:552:GLN:HB3 | 2.54 | 0.42 |
| 2:E:1085:THR:HG22 | 2:E:1103:LYS:HA | 2.02 | 0.42 |
| 1:N:514:ILE:HG13 | 1:N:514:ILE:O | 2.20 | 0.42 |
| 1:N:632:PRO:HA | 1:N:633:PRO:HD3 | 1.93 | 0.42 |
| 2:O:111:THR:O | 2:O:111:THR:HG22 | 2.19 | 0.42 |
| 2:E:18:LEU:N | 2:E:82:MET:O | 2.39 | 0.42 |
| 1:H:459:PRO:HA | 1:H:460:GLY:HA2 | 1.67 | 0.42 |
| 1:H:541:PHE:O | 1:H:591:LEU:HD12 | 2.20 | 0.42 |
| 2:K:1018:ARG:NH2 | 2:K:1074:THR:HG21 | 2.35 | 0.42 |
| 1:N:458:ALA:HA | 1:N:554:TYR:CE2 | 2.55 | 0.42 |
| 2:O:6:GLN:HE22 | 2:O:109:GLN:H | 1.67 | 0.42 |
| 1:S:447:ASP:OD1 | 1:S:448:ARG:N | 2.52 | 0.42 |
| 1:S:514:ILE:HG13 | 1:S:514:ILE:O | 2.20 | 0.42 |
| 1:T:545:PRO:HD2 | 1:T:588:GLU:O | 2.20 | 0.42 |
| 2:C:1089:GLN:HB2 | 2:C:1098:PHE:CD2 | 2.54 | 0.42 |
| 2:E:114:THR:HG21 | 1:M:477:TYR:CE1 | 2.54 | 0.42 |
| 1:B:472:HIS:HB2 | 1:B:508:MET:SD | 2.59 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:474:LEU:HD12 | 1:H:474:LEU:H | 1.85 | 0.42 |
| 1:A:508:MET:HG3 | 1:A:523:MET:SD | 2.59 | 0.42 |
| 2:C:29:LEU:HA | 2:C:29:LEU:HD23 | 1.76 | 0.42 |
| 1:A:596:THR:HG23 | 1:A:611:VAL:HB | 2.02 | 0.42 |
| 1:H:430:GLU:HA | 1:H:643:ASN:HA | 2.02 | 0.42 |
| 1:G:541:PHE:O | 1:G:591:LEU:HD12 | 2.20 | 0.42 |
| 1:M:484:MET:HB3 | 1:M:591:LEU:HB3 | 2.02 | 0.42 |
| 1:B:523:MET:HB3 | 1:B:606:TRP:CZ3 | 2.54 | 0.42 |
| 1:H:511:MET:HG2 | 1:H:516:LYS:HA | 2.00 | 0.42 |
| 2:K:6:GLN:HE22 | 2:K:95:CYS:N | 2.18 | 0.42 |
| 2:O:97:ARG:NH2 | 2:O:105:ASP:OD2 | 2.38 | 0.42 |
| 1:S:540:ILE:HG22 | 1:S:593:THR:HG22 | 2.02 | 0.42 |
| 1:M:435:LEU:HD13 | 1:M:486:ILE:HD12 | 2.02 | 0.41 |
| 1:A:432:ARG:HD3 | 1:A:496:PHE:CZ | 2.55 | 0.41 |
| 2:E:99:TYR:HB2 | 2:E:105:ASP:HB2 | 2.01 | 0.41 |
| 1:H:565:ASN:O | 1:G:574:ARG:NH1 | 2.49 | 0.41 |
| 2:I:1089:GLN:HB2 | 2:I:1098:PHE:CE2 | 2.55 | 0.41 |
| 2:O:1035:TRP:HD1 | 2:O:1048:ILE:HB | 1.85 | 0.41 |
| 2:O:1038:GLN:O | 2:O:1084:ALA:HB1 | 2.19 | 0.41 |
| 1:H:479:ILE:HG12 | 1:H:610:ARG:HD2 | 2.01 | 0.41 |
| 1:H:593:THR:HG1 | 1:H:628:PHE:HE2 | 1.67 | 0.41 |
| 1:S:438:GLY:HA2 | 1:S:487:LYS:HB2 | 2.01 | 0.41 |
| 1:S:456:LEU:HD13 | 1:S:610:ARG:HG2 | 2.02 | 0.41 |
| 2:W:1029:ILE:HD13 | 2:W:1090:GLN:HB2 | 2.02 | 0.41 |
| 2:I:1029:ILE:CD1 | 2:I:1033:LEU:HG | 2.50 | 0.41 |
| 2:U:37:VAL:HG23 | 2:U:94:TYR:HB2 | 2.02 | 0.41 |
| 1:H:564:ASP:HB3 | 1:G:576:MET:HE1 | 2.03 | 0.41 |
| 2:O:1029:ILE:HD11 | 2:O:1091:GLY:H | 1.85 | 0.41 |
| 2:U:1049:TYR:CE2 | 2:U:1053:ARG:HD2 | 2.55 | 0.41 |
| 1:T:551:VAL:HG23 | 1:T:553:CYS:SG | 2.61 | 0.41 |
| 2:C:60:ASN:O | 2:C:64:ILE:HG13 | 2.20 | 0.41 |
| 1:H:596:THR:HG23 | 1:H:611:VAL:HB | 2.03 | 0.41 |
| 1:H:625:LEU:HD23 | 1:H:628:PHE:HD2 | 1.86 | 0.41 |
| 2:K:1015:LEU:HD23 | 2:K:1015:LEU:HA | 1.90 | 0.41 |
| 1:G:447:ASP:OD1 | 1:G:448:ARG:N | 2.54 | 0.41 |
| 2:O:92:ILE:HG12 | 2:O:112:SER:OG | 2.21 | 0.41 |
| 1:S:522:PHE:HE2 | 1:S:540:ILE:HD11 | 1.86 | 0.41 |
| 1:T:453:ASN:HB3 | 1:T:480:MET:O | 2.21 | 0.41 |
| 2:K:58:ASP:OD1 | 2:K:58:ASP:N | 2.54 | 0.41 |
| 1:A:555:MET:O | 1:A:577:THR:HA | 2.21 | 0.41 |
| 1:H:555:MET:HE3 | 1:H:582:ILE:HD11 | 2.01 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:1025:ALA:HB2 | 2:K:1029:ILE:HD11 | 2.03 | 0.41 |
| 1:G:571:LEU:HD12 | 1:G:619:TYR:O | 2.20 | 0.41 |
| 2:Q:28:SER:OG | 2:Q:30:ILE:HG22 | 2.21 | 0.41 |
| 2:Q:35:HIS:CD2 | 2:Q:98:PRO:HB3 | 2.55 | 0.41 |
| 1:M:468:VAL:HG13 | 1:M:510:VAL:HG13 | 2.02 | 0.41 |
| 2:U:90:THR:HG23 | 2:U:113:VAL:O | 2.21 | 0.41 |
| 1:N:548:ASP:OD1 | 1:N:586:VAL:N | 2.48 | 0.41 |
| 2:W:22:CYS:HB2 | 2:W:36:TRP:CH2 | 2.55 | 0.41 |
| 2:C:1075:ILE:HD11 | 2:C:1086:TYR:HE2 | 1.85 | 0.41 |
| 2:E:48:LEU:O | 2:E:60:ASN:N | 2.52 | 0.41 |
| 1:H:450:VAL:HB | 1:H:628:PHE:O | 2.20 | 0.41 |
| 1:H:454:LYS:NZ | 1:H:575:SER:O | 2.54 | 0.41 |
| 1:H:545:PRO:HB3 | 1:H:549:PHE:HE1 | 1.86 | 0.41 |
| 2:O:4:LEU:HG | 2:O:24:VAL:HG12 | 2.03 | 0.41 |
| 2:O:1049:TYR:O | 2:O:1053:ARG:HB2 | 2.21 | 0.41 |
| 1:M:523:MET:HB3 | 1:M:606:TRP:CZ3 | 2.56 | 0.41 |
| 2:U:1029:ILE:HA | 2:U:1092:ASN:ND2 | 2.36 | 0.41 |
| 1:A:537:ILE:HD11 | 1:A:602:LEU:HD22 | 2.03 | 0.40 |
| 2:K:1086:TYR:C | 2:K:1087:PHE:HD1 | 2.24 | 0.40 |
| 1:A:626:THR:OG1 | 1:B:626:THR:O | 2.39 | 0.40 |
| 2:E:6:GLN:NE2 | 2:E:95:CYS:H | 2.19 | 0.40 |
| 1:H:545:PRO:HD2 | 1:H:588:GLU:O | 2.21 | 0.40 |
| 2:O:1091:GLY:O | 1:M:460:GLY:HA3 | 2.21 | 0.40 |
| 1:N:459:PRO:HD3 | 1:N:554:TYR:CE2 | 2.57 | 0.40 |
| 2:K:1062:PHE:N | 2:K:1062:PHE:CD1 | 2.90 | 0.40 |
| 2:I:117:SER:O | 2:I:117:SER:OG | 2.33 | 0.40 |
| 2:U:28:SER:OG | 2:U:30:ILE:HG22 | 2.22 | 0.40 |
| 1:B:524:LYS:HB3 | 1:B:540:ILE:HG12 | 2.04 | 0.40 |
| 1:N:626:THR:O | 1:M:626:THR:OG1 | 2.39 | 0.40 |
| 2:O:1083:ILE:HG23 | 2:O:1104:LEU:O | 2.20 | 0.40 |
| 1:S:514:ILE:CG1 | 2:W:30:ILE:HD11 | 2.51 | 0.40 |
| 2:U:36:TRP:CZ3 | 2:U:95:CYS:HB3 | 2.57 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

of similar resolution.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 214/228 (94%) | 206 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | B | 216/228 (95%) | 205 (95%) | 11 (5%) | 0 | 100 | 100 |
| 1 | G | 217/228 (95%) | 207 (95%) | 10 (5%) | 0 | 100 | 100 |
| 1 | H | 214/228 (94%) | 206 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | M | 214/228 (94%) | 204 (95%) | 10 (5%) | 0 | 100 | 100 |
| 1 | N | 215/228 (94%) | 201 (94%) | 14 (6%) | 0 | 100 | 100 |
| 1 | S | 216/228 (95%) | 204 (94%) | 12 (6%) | 0 | 100 | 100 |
| 1 | T | 214/228 (94%) | 202 (94%) | 12 (6%) | 0 | 100 | 100 |
| 2 | C | 219/251 (87%) | 213 (97%) | 6 (3%) | 0 | 100 | 100 |
| 2 | E | 220/251 (88%) | 211 (96%) | 9 (4%) | 0 | 100 | 100 |
| 2 | I | 221/251 (88%) | 212 (96%) | 9 (4%) | 0 | 100 | 100 |
| 2 | K | 219/251 (87%) | 209 (95%) | 10 (5%) | 0 | 100 | 100 |
| 2 | O | 202/251 (80%) | 194 (96%) | 8 (4%) | 0 | 100 | 100 |
| 2 | Q | 81/251 (32%) | 69 (85%) | 12 (15%) | 0 | 100 | 100 |
| 2 | U | 218/251 (87%) | 209 (96%) | 9 (4%) | 0 | 100 | 100 |
| 2 | W | 91/251 (36%) | 84 (92%) | 7 (8%) | 0 | 100 | 100 |
| All | All | 3191/3832 (83%) | 3036 (95%) | 155 (5%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 197/204 (97%) | 196 (100%) | 1 (0%) | 88 | 94 |
| 1 | B | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | G | 197/204 (97%) | 196 (100%) | 1 (0%) | 88 | 94 |
| 1 | H | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |
| 1 | M | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |
| 1 | N | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |
| 1 | S | 197/204 (97%) | 197 (100%) | 0 | 100 | 100 |
| 1 | T | 197/204 (97%) | 196 (100%) | 1 (0%) | 88 | 94 |
| 2 | C | 193/206 (94%) | 193 (100%) | 0 | 100 | 100 |
| 2 | E | 194/206 (94%) | 193 (100%) | 1 (0%) | 88 | 94 |
| 2 | I | 195/206 (95%) | 194 (100%) | 1 (0%) | 88 | 94 |
| 2 | K | 193/206 (94%) | 193 (100%) | 0 | 100 | 100 |
| 2 | O | 185/206 (90%) | 184 (100%) | 1 (0%) | 88 | 94 |
| 2 | Q | 82/206 (40%) | 82 (100%) | 0 | 100 | 100 |
| 2 | U | 192/206 (93%) | 191 (100%) | 1 (0%) | 88 | 94 |
| 2 | W | 93/206 (45%) | 93 (100%) | 0 | 100 | 100 |
| All | All | 2903/3280 (88%) | 2896 (100%) | 7 (0%) | 93 | 97 |

All (7) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 522 | PHE |
| 2 | E | 100 | TYR |
| 2 | I | 1092 | ASN |
| 1 | G | 571 | LEU |
| 2 | O | 1050 | TYR |
| 2 | U | 1050 | TYR |
| 1 | T | 444 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | K | 6 | GLN |
| 2 | I | 1034 | ASN |
| 1 | G | 513 | ASN |
| 2 | O | 6 | GLN |
| 1 | T | 552 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

4 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 | $\#\|Z\| > 2$ |
| 3 | NAG | C | 1201 | 2 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | NAG | K | 1201 | 2 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.44 | 0 |
| 3 | NAG | I | 1201 | 2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.51 | 0 |
| 3 | NAG | E | 1201 | 2 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.57 | 0 |

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 |
|---|---|---|---|---|---|---|---|
| 3 | NAG | C | 1201 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | K | 1201 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | I | 1201 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | NAG | E | 1201 | 2 | - | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 3 | I | 1201 | NAG | O5-C5-C6-O6 |
| 3 | K | 1201 | NAG | O5-C5-C6-O6 |
| 3 | C | 1201 | NAG | O5-C5-C6-O6 |
| 3 | I | 1201 | NAG | C4-C5-C6-O6 |
| 3 | C | 1201 | NAG | C4-C5-C6-O6 |
| 3 | K | 1201 | NAG | C4-C5-C6-O6 |
| 3 | E | 1201 | NAG | C4-C5-C6-O6 |
| 3 | E | 1201 | NAG | O5-C5-C6-O6 |

There are no ring outliers.

2 monomers are involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | C | 1201 | NAG | 1 | 0 |
| 3 | K | 1201 | NAG | 1 | 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 (i)

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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 216/228 (94%) | 0.62 | 11 (5%) | 28 | 18 | 50, 81, 124, 168 | 0 |
| 1 | B | 218/228 (95%) | 0.73 | 22 (10%) | 7 | 5 | 59, 106, 136, 152 | 0 |
| 1 | G | 219/228 (96%) | 0.83 | 29 (13%) | 3 | 2 | 64, 108, 146, 163 | 0 |
| 1 | H | 216/228 (94%) | 0.59 | 13 (6%) | 21 | 14 | 52, 82, 127, 165 | 0 |
| 1 | M | 216/228 (94%) | 0.91 | 24 (11%) | 5 | 4 | 66, 103, 135, 151 | 0 |
| 1 | N | 217/228 (95%) | 0.55 | 11 (5%) | 28 | 18 | 59, 91, 129, 147 | 0 |
| 1 | S | 218/228 (95%) | 0.60 | 19 (8%) | 10 | 7 | 58, 92, 131, 149 | 0 |
| 1 | T | 216/228 (94%) | 0.90 | 32 (14%) | 2 | 2 | 70, 103, 138, 164 | 0 |
| 2 | C | 223/251 (88%) | 0.54 | 11 (4%) | 29 | 19 | 48, 70, 122, 147 | 3 (1%) |
| 2 | E | 224/251 (89%) | 0.81 | 23 (10%) | 6 | 5 | 86, 121, 149, 166 | 3 (1%) |
| 2 | I | 225/251 (89%) | 0.90 | 37 (16%) | 1 | 1 | 93, 126, 157, 175 | 3 (1%) |
| 2 | K | 223/251 (88%) | 0.67 | 12 (5%) | 25 | 16 | 46, 72, 125, 146 | 3 (1%) |
| 2 | O | 212/251 (84%) | 0.70 | 24 (11%) | 5 | 4 | 97, 131, 155, 167 | 3 (1%) |
| 2 | Q | 93/251 (37%) | 1.02 | 21 (22%) | 0 | 1 | 120, 145, 163, 172 | 0 |
| 2 | U | 222/251 (88%) | 0.83 | 25 (11%) | 5 | 4 | 96, 129, 166, 193 | 3 (1%) |
| 2 | W | 105/251 (41%) | 1.36 | 34 (32%) | 0 | 0 | 114, 145, 162, 173 | 0 |
| All | All | 3263/3832 (85%) | 0.76 | 348 (10%) | 6 | 4 | 46, 107, 151, 193 | 18 (0%) |

All (348) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | I | 37 | VAL | 6.0 |
| 2 | W | 69 | ILE | 6.0 |
| 1 | M | 468 | VAL | 5.9 |
| 2 | W | 1027 | GLN | 5.6 |
| 1 | B | 608 | TRP | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | I | 1106 | ILE | 5.5 |
| 2 | W | 47 | TRP | 5.5 |
| 2 | U | 11 | LEU | 5.4 |
| 2 | Q | 80 | PHE | 5.3 |
| 2 | W | 63 | PHE | 5.3 |
| 2 | E | 34 | VAL | 5.2 |
| 2 | W | 33 | GLY | 5.0 |
| 2 | U | 23 | THR | 4.9 |
| 2 | U | 96 | GLY | 4.8 |
| 2 | E | 82 | MET | 4.8 |
| 2 | W | 67 | LEU | 4.7 |
| 2 | I | 1011 | LEU | 4.7 |
| 2 | W | 25 | SER | 4.6 |
| 1 | G | 596 | THR | 4.5 |
| 2 | O | 1011 | LEU | 4.5 |
| 2 | W | 34 | VAL | 4.5 |
| 2 | O | 1094 | PHE | 4.5 |
| 2 | W | 46 | GLU | 4.4 |
| 1 | G | 522 | PHE | 4.4 |
| 2 | W | 70 | SER | 4.4 |
| 1 | T | 429 | GLY | 4.4 |
| 2 | U | 4 | LEU | 4.3 |
| 2 | Q | 1046 | LEU | 4.3 |
| 2 | U | 21 | THR | 4.3 |
| 2 | I | 1080 | GLN | 4.3 |
| 1 | M | 456 | LEU | 4.3 |
| 2 | O | 1092 | ASN | 4.2 |
| 2 | E | 77 | GLN | 4.2 |
| 1 | M | 452 | LEU | 4.1 |
| 2 | U | 12 | VAL | 4.1 |
| 1 | M | 455 | THR | 4.0 |
| 1 | B | 510 | VAL | 4.0 |
| 2 | W | 94 | TYR | 3.9 |
| 2 | E | 75 | LYS | 3.9 |
| 2 | E | 1104 | LEU | 3.9 |
| 2 | Q | 93 | TYR | 3.8 |
| 1 | N | 558 | PHE | 3.8 |
| 2 | U | 102 | ASN | 3.8 |
| 1 | T | 598 | LYS | 3.8 |
| 1 | T | 543 | ILE | 3.8 |
| 1 | G | 584 | PHE | 3.8 |
| 2 | U | 73 | ASN | 3.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | O | 1087 | PHE | 3.8 |
| 1 | M | 644 | THR | 3.7 |
| 1 | B | 552 | GLN | 3.7 |
| 2 | E | 85 | LEU | 3.7 |
| 2 | I | 102 | ASN | 3.7 |
| 2 | W | 107 | TRP | 3.7 |
| 1 | T | 522 | PHE | 3.6 |
| 1 | M | 542 | LEU | 3.6 |
| 2 | I | 27 | PHE | 3.6 |
| 1 | B | 582 | ILE | 3.6 |
| 1 | T | 455 | THR | 3.6 |
| 2 | Q | 1029 | ILE | 3.6 |
| 1 | B | 522 | PHE | 3.6 |
| 2 | I | 1012 | SER | 3.5 |
| 2 | Q | 100 | TYR | 3.5 |
| 2 | O | 1100 | GLY | 3.5 |
| 1 | M | 619 | TYR | 3.5 |
| 1 | B | 607 | VAL | 3.5 |
| 1 | G | 608 | TRP | 3.5 |
| 2 | E | 2 | VAL | 3.4 |
| 1 | T | 518 | ALA | 3.4 |
| 2 | W | 102 | ASN | 3.4 |
| 1 | M | 478 | LEU | 3.3 |
| 1 | T | 640 | PHE | 3.3 |
| 1 | M | 474 | LEU | 3.3 |
| 1 | T | 541 | PHE | 3.3 |
| 2 | U | 1045 | LYS | 3.3 |
| 1 | N | 459 | PRO | 3.3 |
| 2 | W | 95 | CYS | 3.2 |
| 2 | E | 71 | LYS | 3.2 |
| 2 | W | 61 | ALA | 3.2 |
| 2 | O | 63 | PHE | 3.2 |
| 2 | Q | 59 | TYR | 3.2 |
| 2 | W | 35 | HIS | 3.2 |
| 2 | O | 34 | VAL | 3.2 |
| 1 | G | 602 | LEU | 3.2 |
| 1 | G | 478 | LEU | 3.2 |
| 2 | K | 11 | LEU | 3.2 |
| 1 | S | 630 | THR | 3.2 |
| 2 | Q | 105 | ASP | 3.1 |
| 1 | T | 625 | LEU | 3.1 |
| 2 | E | 105 | ASP | 3.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | C | 1104 | LEU | 3.1 |
| 1 | B | 508 | MET | 3.1 |
| 1 | G | 511 | MET | 3.1 |
| 1 | H | 521 | TYR | 3.1 |
| 1 | M | 522 | PHE | 3.1 |
| 1 | G | 468 | VAL | 3.1 |
| 2 | I | 1104 | LEU | 3.1 |
| 2 | I | 29 | LEU | 3.1 |
| 2 | U | 24 | VAL | 3.1 |
| 2 | I | 80 | PHE | 3.1 |
| 1 | N | 468 | VAL | 3.1 |
| 2 | Q | 67 | LEU | 3.1 |
| 1 | H | 619 | TYR | 3.1 |
| 1 | M | 512 | VAL | 3.1 |
| 2 | C | 74 | SER | 3.0 |
| 2 | I | 1021 | ILE | 3.0 |
| 1 | B | 584 | PHE | 3.0 |
| 1 | M | 624 | ALA | 3.0 |
| 1 | G | 510 | VAL | 3.0 |
| 2 | U | 1073 | LEU | 3.0 |
| 1 | T | 542 | LEU | 3.0 |
| 1 | H | 624 | ALA | 3.0 |
| 1 | H | 540 | ILE | 2.9 |
| 1 | T | 639 | LEU | 2.9 |
| 1 | B | 613 | LEU | 2.9 |
| 2 | W | 66 | ARG | 2.9 |
| 2 | U | 87 | ALA | 2.9 |
| 2 | W | 20 | ILE | 2.9 |
| 2 | E | 94 | TYR | 2.9 |
| 2 | Q | 26 | GLY | 2.9 |
| 2 | U | 1086 | TYR | 2.9 |
| 1 | T | 523 | MET | 2.8 |
| 1 | G | 635 | ASP | 2.8 |
| 1 | M | 543 | ILE | 2.8 |
| 2 | I | 1014 | SER | 2.8 |
| 2 | E | 1063 | SER | 2.8 |
| 2 | U | 100 | TYR | 2.8 |
| 1 | H | 629 | ILE | 2.8 |
| 2 | E | 80 | PHE | 2.8 |
| 1 | T | 555 | MET | 2.8 |
| 2 | I | 1047 | LEU | 2.8 |
| 2 | U | 45 | LEU | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | M | 604 | GLU | 2.7 |
| 2 | I | 11 | LEU | 2.7 |
| 1 | N | 571 | LEU | 2.7 |
| 1 | T | 599 | GLU | 2.7 |
| 1 | B | 542 | LEU | 2.7 |
| 1 | M | 592 | LEU | 2.7 |
| 1 | T | 456 | LEU | 2.7 |
| 1 | B | 555 | MET | 2.7 |
| 1 | S | 451 | TRP | 2.7 |
| 2 | E | 37 | VAL | 2.7 |
| 2 | I | 1033 | LEU | 2.7 |
| 2 | U | 5 | LYS | 2.7 |
| 1 | A | 543 | ILE | 2.7 |
| 1 | B | 478 | LEU | 2.7 |
| 1 | G | 508 | MET | 2.7 |
| 2 | C | 15 | SER | 2.7 |
| 2 | E | 67 | LEU | 2.7 |
| 1 | T | 573 | VAL | 2.7 |
| 2 | I | 34 | VAL | 2.7 |
| 1 | G | 461 | THR | 2.7 |
| 1 | T | 591 | LEU | 2.7 |
| 2 | K | 13 | GLN | 2.7 |
| 2 | W | 65 | SER | 2.6 |
| 2 | U | 65 | SER | 2.6 |
| 1 | G | 558 | PHE | 2.6 |
| 1 | B | 470 | ILE | 2.6 |
| 1 | B | 517 | LYS | 2.6 |
| 2 | U | 1046 | LEU | 2.6 |
| 2 | K | 40 | SER | 2.6 |
| 2 | I | 33 | GLY | 2.6 |
| 2 | I | 1019 | VAL | 2.6 |
| 1 | T | 572 | THR | 2.6 |
| 2 | I | 1102 | THR | 2.6 |
| 1 | G | 540 | ILE | 2.6 |
| 2 | O | 29 | LEU | 2.6 |
| 2 | E | 1006 | GLN | 2.6 |
| 1 | G | 591 | LEU | 2.6 |
| 2 | E | 18 | LEU | 2.6 |
| 2 | Q | 27 | PHE | 2.6 |
| 2 | I | 71 | LYS | 2.6 |
| 2 | Q | 29 | LEU | 2.6 |
| 2 | W | 27 | PHE | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | U | 93 | TYR | 2.6 |
| 2 | O | 1069 | THR | 2.6 |
| 1 | T | 489 | VAL | 2.6 |
| 2 | K | 12 | VAL | 2.6 |
| 1 | G | 542 | LEU | 2.6 |
| 2 | I | 18 | LEU | 2.6 |
| 1 | H | 627 | TYR | 2.6 |
| 1 | A | 489 | VAL | 2.6 |
| 1 | A | 610 | ARG | 2.6 |
| 2 | K | 41 | PRO | 2.6 |
| 1 | B | 592 | LEU | 2.6 |
| 2 | O | 1080 | GLN | 2.6 |
| 2 | I | 1024 | ARG | 2.6 |
| 2 | O | 1047 | LEU | 2.6 |
| 2 | I | 1086 | TYR | 2.5 |
| 1 | T | 628 | PHE | 2.5 |
| 1 | M | 470 | ILE | 2.5 |
| 1 | T | 627 | TYR | 2.5 |
| 1 | S | 456 | LEU | 2.5 |
| 1 | T | 480 | MET | 2.5 |
| 2 | C | 1062 | PHE | 2.5 |
| 1 | T | 596 | THR | 2.5 |
| 1 | A | 499 | SER | 2.5 |
| 1 | G | 610 | ARG | 2.5 |
| 1 | S | 549 | PHE | 2.5 |
| 2 | I | 106 | TYR | 2.5 |
| 1 | M | 560 | ARG | 2.5 |
| 2 | I | 1097 | THR | 2.5 |
| 2 | O | 1021 | ILE | 2.4 |
| 2 | I | 1048 | ILE | 2.4 |
| 2 | W | 78 | VAL | 2.4 |
| 2 | E | 92 | ILE | 2.4 |
| 1 | S | 484 | MET | 2.4 |
| 2 | U | 1032 | TYR | 2.4 |
| 1 | T | 457 | THR | 2.4 |
| 2 | U | 43 | LYS | 2.4 |
| 2 | K | 9 | PRO | 2.4 |
| 2 | Q | 63 | PHE | 2.4 |
| 2 | I | 4 | LEU | 2.4 |
| 1 | A | 553 | CYS | 2.4 |
| 1 | G | 553 | CYS | 2.4 |
| 2 | I | 77 | GLN | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 604 | GLU | 2.4 |
| 1 | T | 644 | THR | 2.4 |
| 2 | E | 113 | VAL | 2.4 |
| 1 | G | 453 | ASN | 2.4 |
| 2 | E | 93 | TYR | 2.4 |
| 1 | N | 467 | LEU | 2.4 |
| 1 | N | 591 | LEU | 2.4 |
| 2 | C | 10 | GLY | 2.4 |
| 2 | I | 8 | GLY | 2.4 |
| 2 | O | 1098 | PHE | 2.4 |
| 1 | S | 459 | PRO | 2.4 |
| 1 | S | 602 | LEU | 2.4 |
| 1 | M | 640 | PHE | 2.3 |
| 2 | I | 36 | TRP | 2.3 |
| 2 | W | 104 | MET | 2.3 |
| 1 | G | 629 | ILE | 2.3 |
| 2 | K | 69 | ILE | 2.3 |
| 2 | I | 99 | TYR | 2.3 |
| 2 | Q | 73 | ASN | 2.3 |
| 2 | W | 36 | TRP | 2.3 |
| 2 | W | 68 | THR | 2.3 |
| 2 | U | 83 | ASN | 2.3 |
| 1 | T | 517 | LYS | 2.3 |
| 2 | K | 102 | ASN | 2.3 |
| 1 | G | 594 | SER | 2.3 |
| 1 | H | 570 | ASN | 2.3 |
| 1 | M | 638 | ILE | 2.3 |
| 1 | S | 467 | LEU | 2.3 |
| 2 | O | 1027 | GLN | 2.3 |
| 2 | W | 80 | PHE | 2.3 |
| 1 | H | 435 | LEU | 2.3 |
| 2 | E | 45 | LEU | 2.3 |
| 2 | E | 1047 | LEU | 2.3 |
| 1 | M | 479 | ILE | 2.3 |
| 2 | I | 91 | GLY | 2.3 |
| 2 | K | 1096 | PRO | 2.3 |
| 2 | E | 111 | THR | 2.3 |
| 2 | I | 9 | PRO | 2.3 |
| 2 | I | 85 | LEU | 2.3 |
| 1 | T | 550 | LYS | 2.3 |
| 1 | T | 553 | CYS | 2.2 |
| 2 | Q | 1047 | LEU | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | U | 79 | PHE | 2.2 |
| 1 | A | 432 | ARG | 2.2 |
| 1 | H | 641 | GLU | 2.2 |
| 2 | O | 7 | SER | 2.2 |
| 1 | A | 522 | PHE | 2.2 |
| 2 | O | 1005 | THR | 2.2 |
| 2 | W | 1054 | LEU | 2.2 |
| 1 | S | 558 | PHE | 2.2 |
| 1 | B | 500 | ARG | 2.2 |
| 2 | W | 50 | VAL | 2.2 |
| 1 | M | 606 | TRP | 2.2 |
| 2 | W | 108 | GLY | 2.2 |
| 2 | O | 78 | VAL | 2.2 |
| 1 | M | 518 | ALA | 2.2 |
| 2 | E | 1078 | LEU | 2.2 |
| 2 | U | 1059 | PRO | 2.2 |
| 2 | I | 23 | THR | 2.2 |
| 1 | N | 546 | LEU | 2.2 |
| 2 | C | 1083 | ILE | 2.2 |
| 1 | G | 550 | LYS | 2.2 |
| 1 | S | 434 | LEU | 2.2 |
| 1 | A | 536 | GLN | 2.2 |
| 1 | H | 479 | ILE | 2.2 |
| 1 | S | 512 | VAL | 2.2 |
| 1 | T | 592 | LEU | 2.1 |
| 1 | H | 468 | VAL | 2.1 |
| 1 | S | 470 | ILE | 2.1 |
| 2 | Q | 78 | VAL | 2.1 |
| 1 | H | 491 | TRP | 2.1 |
| 2 | Q | 60 | ASN | 2.1 |
| 2 | Q | 1054 | LEU | 2.1 |
| 2 | W | 59 | TYR | 2.1 |
| 1 | G | 616 | ASP | 2.1 |
| 1 | G | 455 | THR | 2.1 |
| 1 | S | 440 | ILE | 2.1 |
| 2 | K | 55 | GLY | 2.1 |
| 1 | S | 517 | LYS | 2.1 |
| 2 | C | 75 | LYS | 2.1 |
| 2 | U | 46 | GLU | 2.1 |
| 1 | B | 438 | GLY | 2.1 |
| 1 | M | 625 | LEU | 2.1 |
| 2 | K | 1098 | PHE | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | O | 1062 | PHE | 2.1 |
| 1 | G | 486 | ILE | 2.1 |
| 1 | S | 449 | GLN | 2.1 |
| 2 | W | 1048 | ILE | 2.1 |
| 1 | S | 542 | LEU | 2.1 |
| 2 | K | 45 | LEU | 2.1 |
| 2 | Q | 62 | ALA | 2.1 |
| 1 | S | 520 | VAL | 2.1 |
| 2 | Q | 20 | ILE | 2.1 |
| 1 | G | 523 | MET | 2.1 |
| 2 | I | 78 | VAL | 2.1 |
| 2 | O | 1032 | TYR | 2.1 |
| 1 | N | 455 | THR | 2.1 |
| 2 | W | 60 | ASN | 2.1 |
| 1 | G | 557 | TYR | 2.1 |
| 1 | G | 642 | GLY | 2.1 |
| 1 | T | 536 | GLN | 2.1 |
| 2 | C | 1036 | TYR | 2.1 |
| 2 | Q | 61 | ALA | 2.1 |
| 2 | Q | 71 | LYS | 2.1 |
| 2 | W | 32 | TYR | 2.1 |
| 2 | O | 1078 | LEU | 2.1 |
| 1 | M | 558 | PHE | 2.1 |
| 2 | C | 80 | PHE | 2.1 |
| 1 | A | 602 | LEU | 2.0 |
| 1 | S | 478 | LEU | 2.0 |
| 1 | N | 583 | ARG | 2.0 |
| 1 | G | 518 | ALA | 2.0 |
| 2 | I | 22 | CYS | 2.0 |
| 1 | H | 455 | THR | 2.0 |
| 2 | O | 45 | LEU | 2.0 |
| 1 | S | 455 | THR | 2.0 |
| 2 | O | 96 | GLY | 2.0 |
| 1 | B | 561 | GLU | 2.0 |
| 2 | C | 40 | SER | 2.0 |
| 1 | T | 479 | ILE | 2.0 |
| 2 | C | 69 | ILE | 2.0 |
| 2 | O | 51 | ILE | 2.0 |
| 1 | N | 570 | ASN | 2.0 |
| 1 | A | 490 | GLU | 2.0 |
| 1 | A | 561 | GLU | 2.0 |
| 1 | B | 523 | MET | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | O | 1025 | ALA | 2.0 |
| 2 | W | 62 | ALA | 2.0 |
| 2 | W | 1049 | TYR | 2.0 |
| 1 | T | 498 | PRO | 2.0 |
| 1 | B | 484 | MET | 2.0 |
| 1 | B | 550 | LYS | 2.0 |
| 1 | B | 512 | VAL | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | NAG | C | 1201 | 14/15 | 0.65 | 0.42 | 146,163,170,174 | 0 |
| 3 | NAG | K | 1201 | 14/15 | 0.65 | 0.29 | 140,179,188,188 | 0 |
| 3 | NAG | I | 1201 | 14/15 | 0.79 | 0.19 | 133,147,156,157 | 0 |
| 3 | NAG | E | 1201 | 14/15 | 0.84 | 0.29 | 138,153,158,158 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.