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

Feb 1, 2016 – 03:12 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 4BTY |
| Title | : | Crystal structure of human vascular adhesion protein-1 in complex with pyridazinone inhibitors |
| Authors | : | Bligt-Linden, E.; Pihlavisto, M.; Szatmari, I.; Otwinowski, Z.; Smith, D.J.; Lazar, L.; Fulop, F.; Salminen, T.A. |
| Deposited on | : | 2013-06-19 |
| Resolution | : | 3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

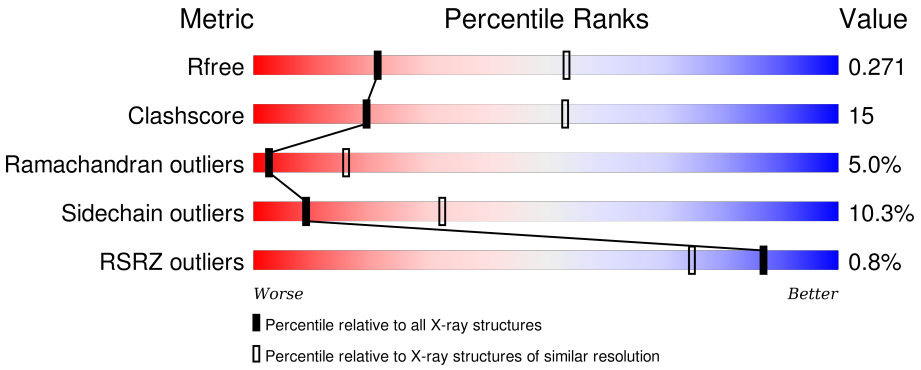
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 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 3.10 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 | 1114 (3.14-3.06) |
| Clashscore | 102246 | 1222 (3.14-3.06) |
| Ramachandran outliers | 100387 | 1174 (3.14-3.06) |
| Sidechain outliers | 100360 | 1174 (3.14-3.06) |
| RSRZ outliers | 91569 | 1119 (3.14-3.06) |

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 | 737 | 63% 28% 6% · |
| 1 | B | 737 | % 62% 28% 5% · · |

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 |
|---|---|---|---|---|---|---|---|
| 4 | NAG | B | 1771 | X | - | - | - |
| 5 | NAG | A | 1768 | X | - | - | - |
| 5 | NAG | A | 1770 | X | - | - | - |
| 7 | NAG | B | 1765 | X | - | - | - |
| 7 | BMA | B | 1767 | - | - | X | - |
| 7 | MAN | B | 1768 | X | - | - | - |
| 7 | MAN | B | 1769 | X | - | X | - |

# 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11484 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 MEMBRANE PRIMARY AMINE OXIDASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 711 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5604 | 3595 | 968 | 1021 | 20 | | | |
| 1 | B | 707 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5567 | 3574 | 957 | 1016 | 20 | | | |

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | B | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

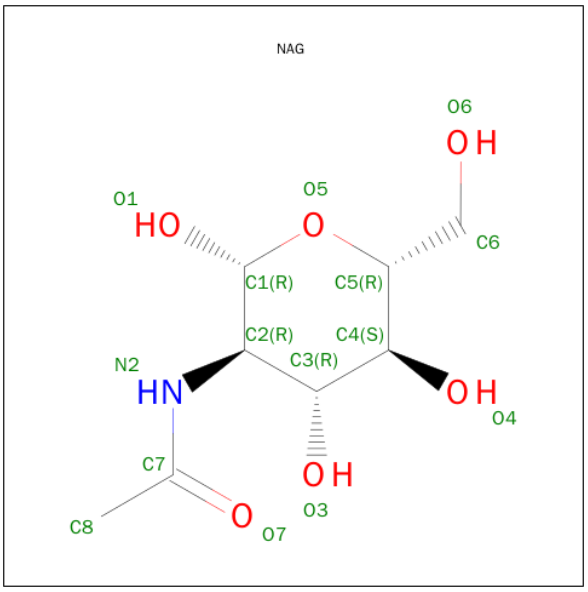
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | B | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | A | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

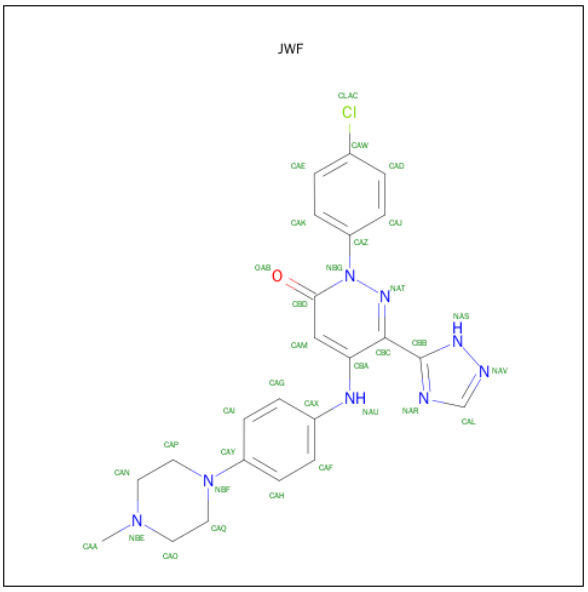
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | A | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |
| 4 | B | 2 | Total | C | N | O | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | |

- Molecule 5 is SUGAR (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 | B | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |
| 5 | B | 1 | Total C N O<br>14 8 1 5 | 0 | 0 |

- Molecule 6 is 5-[4-(4-METHYLPIPERAZIN-1-YL)PHENYLAMINO]-2-(4-CHLOROPHENYL)-6-(1H-1,2,4-TRIAZOL-5-YL)-3(2H)-PYRIDAZINONE (three-letter code: JWF) (formula: $C_{23}H_{23}ClN_8O$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 6 | A | 1 | Total C Cl N O<br>33 23 1 8 1 | 0 | 0 |
| 6 | B | 1 | Total C Cl N O<br>33 23 1 8 1 | 0 | 0 |

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 7 | B | 5 | Total C N O<br>61 34 2 25 | 0 | 0 |

- Molecule 8 is water.

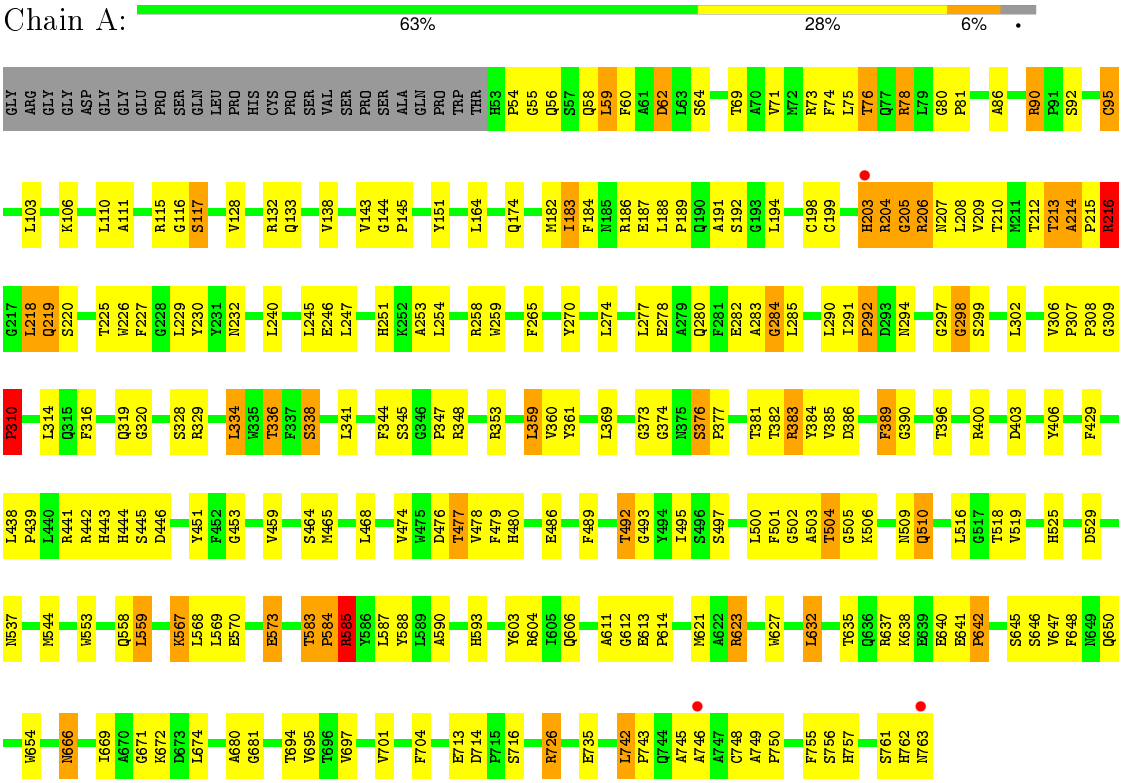
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 8 | A | 26 | Total O<br>26 26 | 0 | 0 |
| 8 | B | 14 | Total O<br>14 14 | 0 | 0 |

# 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.

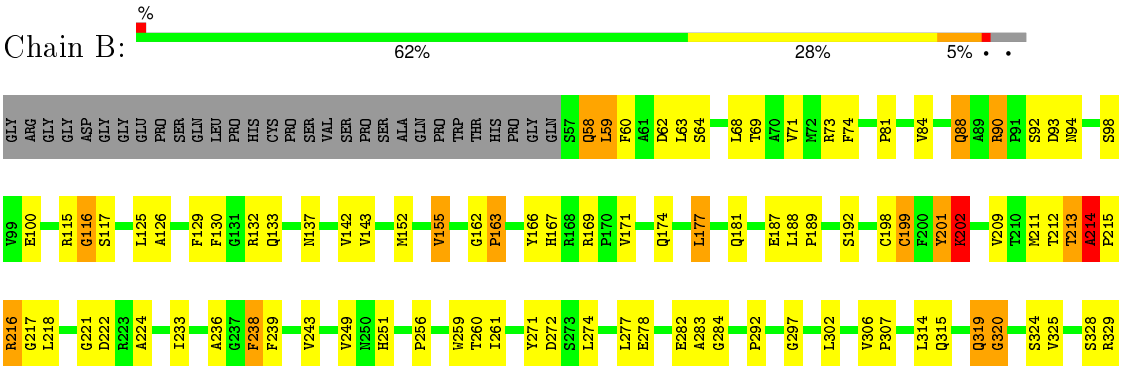
- Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

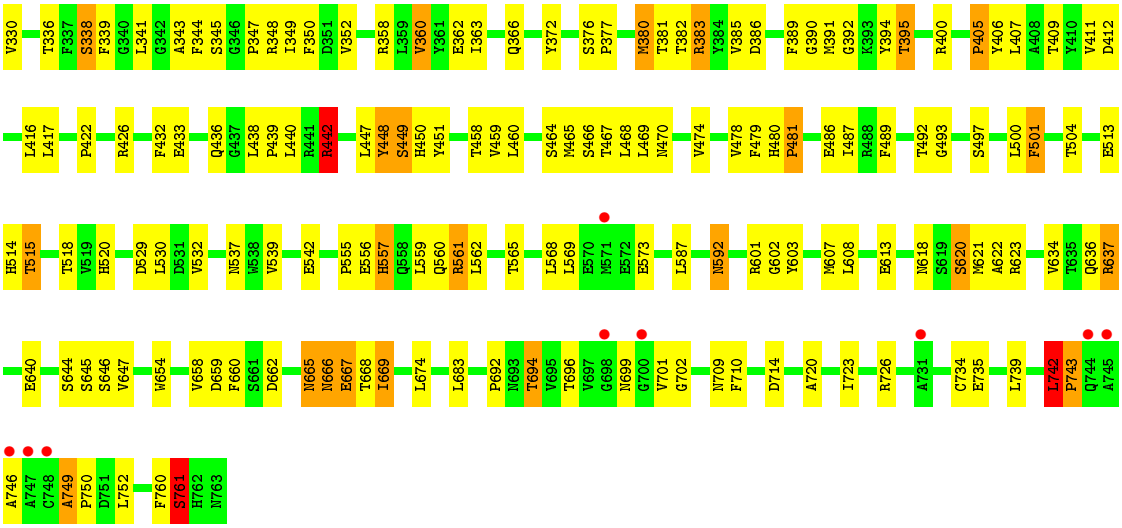
Chain A:




- Molecule 1: MEMBRANE PRIMARY AMINE OXIDASE

Chain B:




V330 T336 F337 S338 F339 G340 L341 G342 A343 F344 S345 G346 P347 R348 I349 F350 D351 V352 R358 L359 V360 Y361 E362 I363 Q366 Y372 S376 P377 M380 T381 T382 R383 Y384 V385 D386 F389 G390 M391 G392 K393 Y394 T395 R400 P405 Y406 L407 A408 T409 Y410 V411 D412
L416 L417 P422 R426 F432 E433 Q436 G437 L438 P439 L440 R441 R442 L447 Y448 S449 H450 Y451 T458 V459 L460 S464 M465 S466 T467 L468 L469 N470 V474 V478 F479 H480 P481 E486 I487 R488 F489 T492 G493 S497 L500 F501 T504 E513
H514 T515 T518 V519 H520 D529 L530 D531 V532 N537 W538 V539 E542 P555 E556 H557 Q558 L559 Q560 R561 L562 T565 L568 L569 E570 M571 E572 E573 L587 N592 R601 G602 Y603 M607 L608 E613 N618 S619 S620 M621 A622 R623 V634 T635 Q636 R637
E640 S644 S645 S646 V647 W654 V658 D659 F660 S661 D662 N665 N666 E667 T668 I669 L674 L683 P692 N693 T694 V695 T696 V697 G698 N699 G700 V701 G702 N709 F710 D714 A720 I723 R726 A731 C734 E735 L739 L742 P743 Q744 A745
A746 A747 C748 A749 P750 D751 L752 F760 S761 H762 N763

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 65 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 226.74Å 226.74Å 218.16Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 49.20 – 3.10<br>49.15 – 3.10 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 76.2 (49.20-3.10)<br>76.2 (49.15-3.10) | Depositor<br>EDS |
| $R_{merge}$ | 0.29 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.71 (at 3.12Å) | Xtriage |
| Refinement program | REFMAC 5.7.0032 | Depositor |
| R, $R_{free}$ | 0.184 , 0.246<br>0.217 , 0.271 | Depositor<br>DCC |
| $R_{free}$ test set | 2314 reflections (5.33%) | DCC |
| Wilson B-factor (Å$^2$) | 88.2 | Xtriage |
| Anisotropy | 0.183 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 78.8 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Outliers | 1 of 45763 reflections (0.002%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 11484 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 86.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, CA, JWF, TPQ, CU, 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 | 0.67 | 1/5769 (0.0%) | 0.89 | 5/7867 (0.1%) |
| 1 | B | 0.66 | 1/5730 (0.0%) | 0.88 | 1/7815 (0.0%) |
| All | All | 0.66 | 2/11499 (0.0%) | 0.88 | 6/15682 (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 | A | 0 | 2 |
| 1 | B | 0 | 7 |
| 4 | B | 1 | 0 |
| 7 | B | 3 | 0 |
| All | All | 4 | 9 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 666 | ASN | CG-ND2 | 6.88 | 1.50 | 1.32 |
| 1 | B | 592 | ASN | CG-ND2 | 5.50 | 1.46 | 1.32 |

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 585 | ARG | NE-CZ-NH1 | 8.69 | 124.65 | 120.30 |
| 1 | A | 529 | ASP | CB-CG-OD2 | -7.20 | 111.82 | 118.30 |
| 1 | B | 529 | ASP | CB-CG-OD2 | -6.92 | 112.07 | 118.30 |
| 1 | A | 258 | ARG | NE-CZ-NH1 | 6.56 | 123.58 | 120.30 |
| 1 | A | 585 | ARG | NE-CZ-NH2 | -5.69 | 117.46 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 216 | ARG | N-CA-C | -5.19 | 96.99 | 111.00 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 7 | B | 1765 | NAG | C1 |
| 7 | B | 1768 | MAN | C1 |
| 7 | B | 1769 | MAN | C1 |
| 4 | B | 1771 | NAG | C1 |

All (9) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 292 | PRO | Peptide |
| 1 | A | 438 | LEU | Peptide |
| 1 | B | 162 | GLY | Peptide |
| 1 | B | 202 | LYS | Peptide |
| 1 | B | 213 | THR | Peptide |
| 1 | B | 214 | ALA | Peptide |
| 1 | B | 480 | HIS | Peptide |
| 1 | B | 742 | LEU | Peptide |
| 1 | B | 761 | SER | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 5604 | 0 | 5335 | 169 | 0 |
| 1 | B | 5567 | 0 | 5299 | 182 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 2 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 28 | 0 | 25 | 1 | 0 |
| 4 | B | 28 | 0 | 25 | 1 | 0 |
| 5 | A | 56 | 0 | 52 | 1 | 0 |
| 5 | B | 28 | 0 | 26 | 4 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 6 | A | 33 | 0 | 23 | 5 | 0 |
| 6 | B | 33 | 0 | 23 | 3 | 0 |
| 7 | B | 61 | 0 | 52 | 9 | 0 |
| 8 | A | 26 | 0 | 0 | 2 | 0 |
| 8 | B | 14 | 0 | 0 | 4 | 0 |
| All | All | 11484 | 0 | 10860 | 337 | 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 15.

All (337) 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:B:592:ASN:ND2 | 5:B:1772:NAG:C1 | 1.90 | 1.35 |
| 1:B:592:ASN:ND2 | 5:B:1772:NAG:O5 | 1.62 | 1.32 |
| 7:B:1767:BMA:O4 | 7:B:1769:MAN:H2 | 1.33 | 1.25 |
| 7:B:1767:BMA:C4 | 7:B:1769:MAN:H2 | 1.79 | 1.13 |
| 1:B:592:ASN:HD22 | 5:B:1772:NAG:C1 | 1.59 | 1.00 |
| 1:B:58:GLN:HA | 1:B:58:GLN:HE21 | 1.26 | 0.99 |
| 1:B:592:ASN:HD21 | 5:B:1772:NAG:C1 | 1.70 | 0.96 |
| 7:B:1767:BMA:C4 | 7:B:1769:MAN:C2 | 2.48 | 0.92 |
| 1:B:492:THR:HG23 | 1:B:694:THR:O | 1.71 | 0.90 |
| 1:B:749:ALA:HB1 | 1:B:750:PRO:CD | 2.02 | 0.88 |
| 1:A:205:GLY:O | 1:A:207:ASN:N | 2.10 | 0.85 |
| 1:B:376:SER:O | 1:B:380:MET:HG2 | 1.79 | 0.82 |
| 1:B:749:ALA:HB1 | 1:B:750:PRO:HD2 | 1.60 | 0.82 |
| 1:A:389:PHE:CE2 | 6:A:2000:JWF:HAE | 2.20 | 0.77 |
| 1:A:204:ARG:HD3 | 1:A:206:ARG:N | 2.00 | 0.76 |
| 1:B:407:LEU:HD21 | 1:B:752:LEU:HD22 | 1.69 | 0.74 |
| 1:B:64:SER:O | 1:B:68:LEU:HG | 1.89 | 0.72 |
| 1:A:374:GLY:O | 1:B:561:ARG:NH2 | 2.23 | 0.72 |
| 1:A:495:ILE:N | 1:A:495:ILE:HD12 | 2.05 | 0.72 |
| 7:B:1767:BMA:H4 | 7:B:1769:MAN:O2 | 1.90 | 0.71 |
| 1:B:556:GLU:HB2 | 1:B:557:HIS:HB2 | 1.72 | 0.71 |
| 7:B:1767:BMA:H4 | 7:B:1769:MAN:C2 | 2.19 | 0.71 |
| 1:B:115:ARG:O | 1:B:117:SER:N | 2.23 | 0.71 |
| 7:B:1767:BMA:O4 | 7:B:1769:MAN:C2 | 2.28 | 0.70 |
| 1:B:163:PRO:HB3 | 7:B:1765:NAG:H82 | 1.74 | 0.70 |
| 1:A:265:PHE:HD2 | 1:A:270:TYR:CE1 | 2.12 | 0.68 |
| 1:B:400:ARG:NH1 | 1:B:406:TYR:O | 2.26 | 0.67 |
| 1:A:214:ALA:HB2 | 1:A:382:THR:HG23 | 1.77 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:319:GLN:O | 1:B:320:GLY:O | 2.11 | 0.66 |
| 1:A:749:ALA:H | 1:B:749:ALA:HB2 | 1.60 | 0.66 |
| 1:A:58:GLN:O | 1:A:60:PHE:N | 2.23 | 0.66 |
| 1:A:519:VAL:HG13 | 1:B:562:LEU:HD23 | 1.76 | 0.66 |
| 1:B:58:GLN:HA | 1:B:58:GLN:NE2 | 1.98 | 0.66 |
| 1:A:251:HIS:HA | 1:A:259:TRP:CD1 | 2.31 | 0.66 |
| 1:A:204:ARG:HD3 | 1:A:206:ARG:H | 1.60 | 0.65 |
| 1:B:360:VAL:HG13 | 1:B:530:LEU:HD23 | 1.77 | 0.65 |
| 1:A:504:THR:OG1 | 1:A:505:GLY:N | 2.30 | 0.65 |
| 1:A:640:GLU:OE1 | 1:A:640:GLU:N | 2.26 | 0.65 |
| 1:A:441:ARG:HA | 1:B:492:THR:HG21 | 1.79 | 0.65 |
| 1:A:214:ALA:CB | 1:A:215:PRO:CD | 2.76 | 0.64 |
| 1:B:71:VAL:HG13 | 1:B:143:VAL:HG11 | 1.80 | 0.64 |
| 1:B:561:ARG:HH11 | 1:B:561:ARG:HG3 | 1.62 | 0.63 |
| 1:A:573:GLU:OE2 | 1:A:666:ASN:HA | 1.98 | 0.63 |
| 1:B:381:THR:HG21 | 8:B:2003:HOH:O | 1.97 | 0.63 |
| 1:B:256:PRO:HA | 1:B:259:TRP:CE2 | 2.34 | 0.63 |
| 1:A:695:VAL:HG13 | 1:B:440:LEU:HG | 1.81 | 0.62 |
| 1:B:665:ASN:O | 1:B:667:GLU:N | 2.32 | 0.62 |
| 1:A:214:ALA:CB | 1:A:215:PRO:HD2 | 2.30 | 0.62 |
| 1:A:115:ARG:O | 1:A:117:SER:N | 2.32 | 0.62 |
| 1:B:637:ARG:HG2 | 1:B:637:ARG:HH11 | 1.63 | 0.62 |
| 1:A:214:ALA:HB1 | 1:A:215:PRO:CD | 2.30 | 0.61 |
| 1:B:59:LEU:H | 1:B:59:LEU:HD12 | 1.65 | 0.61 |
| 1:B:381:THR:CG2 | 8:B:2003:HOH:O | 2.47 | 0.61 |
| 1:A:377:PRO:O | 1:A:381:THR:HG22 | 2.00 | 0.61 |
| 1:B:556:GLU:N | 1:B:557:HIS:HB2 | 2.15 | 0.61 |
| 1:B:343:ALA:HA | 1:B:392:GLY:HA3 | 1.83 | 0.61 |
| 1:A:680:ALA:HB1 | 1:A:701:VAL:HG13 | 1.82 | 0.60 |
| 1:B:63:LEU:HB2 | 1:B:68:LEU:HD21 | 1.83 | 0.60 |
| 1:B:447:LEU:O | 1:B:449:SER:N | 2.34 | 0.60 |
| 1:A:588:TYR:HB3 | 1:A:604:ARG:HA | 1.83 | 0.59 |
| 1:B:501:PHE:O | 1:B:501:PHE:CD2 | 2.55 | 0.59 |
| 1:A:585:ARG:HG2 | 1:A:585:ARG:HH11 | 1.67 | 0.59 |
| 7:B:1767:BMA:C5 | 7:B:1769:MAN:C2 | 2.80 | 0.59 |
| 1:A:373:GLY:HA3 | 1:B:562:LEU:HB3 | 1.85 | 0.59 |
| 1:A:477:THR:HG22 | 1:A:479:PHE:CE1 | 2.38 | 0.58 |
| 1:B:212:THR:HG22 | 1:B:213:THR:N | 2.17 | 0.58 |
| 1:B:58:GLN:CA | 1:B:58:GLN:HE21 | 2.08 | 0.57 |
| 1:B:129:PHE:CZ | 1:B:169:ARG:HB2 | 2.39 | 0.57 |
| 1:B:214:ALA:HB1 | 1:B:215:PRO:HD2 | 1.86 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:762:HIS:CE1 | 6:A:2000:JWF:HAA1 | 2.40 | 0.57 |
| 7:B:1767:BMA:C5 | 7:B:1769:MAN:H2 | 2.35 | 0.57 |
| 1:B:556:GLU:CB | 1:B:557:HIS:HB2 | 2.35 | 0.57 |
| 1:A:735:GLU:H | 1:A:735:GLU:CD | 2.09 | 0.57 |
| 1:A:585:ARG:CG | 1:A:585:ARG:HH11 | 2.19 | 0.56 |
| 1:A:74:PHE:O | 1:A:78:ARG:NH1 | 2.38 | 0.56 |
| 1:B:352:VAL:HB | 1:B:360:VAL:HG23 | 1.87 | 0.56 |
| 1:B:749:ALA:CB | 1:B:750:PRO:CD | 2.81 | 0.56 |
| 1:B:251:HIS:HA | 1:B:259:TRP:CD1 | 2.41 | 0.56 |
| 1:B:696:THR:O | 1:B:699:ASN:HB2 | 2.06 | 0.56 |
| 1:B:212:THR:CG2 | 1:B:216:ARG:NH2 | 2.68 | 0.56 |
| 1:B:214:ALA:HB2 | 1:B:382:THR:HA | 1.89 | 0.55 |
| 1:A:306:VAL:HG23 | 1:A:307:PRO:HD2 | 1.86 | 0.55 |
| 1:B:201:TYR:O | 1:B:202:LYS:O | 2.24 | 0.55 |
| 1:A:209:VAL:CG1 | 1:B:448:TYR:CE2 | 2.90 | 0.55 |
| 1:B:669:ILE:HG22 | 1:B:674:LEU:HD22 | 1.88 | 0.55 |
| 1:A:389:PHE:CD2 | 6:A:2000:JWF:HAE | 2.41 | 0.54 |
| 1:B:352:VAL:HB | 1:B:360:VAL:CG2 | 2.37 | 0.54 |
| 1:A:492:THR:OG1 | 1:A:493:GLY:N | 2.34 | 0.54 |
| 1:B:556:GLU:CA | 1:B:557:HIS:HB2 | 2.38 | 0.54 |
| 1:B:63:LEU:CB | 1:B:68:LEU:HD21 | 2.38 | 0.54 |
| 1:A:58:GLN:C | 1:A:59:LEU:HD23 | 2.28 | 0.54 |
| 1:B:487:ILE:O | 1:B:702:GLY:HA3 | 2.07 | 0.54 |
| 4:B:1770:NAG:O6 | 4:B:1771:NAG:C1 | 2.56 | 0.54 |
| 1:A:640:GLU:C | 1:A:642:PRO:HD3 | 2.28 | 0.54 |
| 1:B:385:VAL:HG12 | 1:B:385:VAL:O | 2.07 | 0.53 |
| 1:B:386:ASP:HB3 | 1:B:468:LEU:CD1 | 2.38 | 0.53 |
| 1:A:78:ARG:HB2 | 1:A:78:ARG:HH11 | 1.73 | 0.53 |
| 1:A:569:LEU:HD12 | 1:A:569:LEU:N | 2.23 | 0.53 |
| 1:A:369:LEU:HD12 | 1:A:384:TYR:O | 2.09 | 0.53 |
| 1:A:132:ARG:HB2 | 1:A:132:ARG:CZ | 2.39 | 0.53 |
| 1:A:213:THR:HG22 | 1:A:225:THR:HG23 | 1.90 | 0.53 |
| 1:B:451:TYR:HA | 1:B:726:ARG:HA | 1.90 | 0.53 |
| 1:B:587:LEU:C | 1:B:587:LEU:HD23 | 2.29 | 0.53 |
| 1:A:245:LEU:HD12 | 1:A:265:PHE:O | 2.09 | 0.53 |
| 1:B:214:ALA:HB1 | 1:B:215:PRO:CD | 2.39 | 0.52 |
| 1:B:636:GLN:NE2 | 1:B:668:THR:O | 2.42 | 0.52 |
| 1:A:191:ALA:HA | 1:A:278:GLU:CG | 2.39 | 0.52 |
| 1:B:637:ARG:CG | 1:B:637:ARG:HH11 | 2.20 | 0.52 |
| 1:B:735:GLU:N | 1:B:735:GLU:OE1 | 2.42 | 0.52 |
| 1:A:183:ILE:HG22 | 1:A:184:PHE:N | 2.25 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:58:GLN:OE1 | 1:B:329:ARG:NH1 | 2.43 | 0.52 |
| 1:A:623:ARG:HA | 1:A:623:ARG:CZ | 2.39 | 0.52 |
| 1:B:349:ILE:HD11 | 1:B:363:ILE:HB | 1.91 | 0.52 |
| 1:A:314:LEU:HD12 | 8:A:2009:HOH:O | 2.10 | 0.52 |
| 1:B:459:VAL:HG11 | 1:B:478:VAL:CG1 | 2.40 | 0.52 |
| 1:B:314:LEU:HD12 | 1:B:315:GLN:N | 2.25 | 0.52 |
| 1:B:660:PHE:O | 1:B:662:ASP:N | 2.43 | 0.52 |
| 1:B:167:HIS:CE1 | 1:B:221:GLY:HA2 | 2.45 | 0.52 |
| 1:A:214:ALA:HB3 | 1:A:215:PRO:HD2 | 1.92 | 0.51 |
| 1:A:133:GLN:OE1 | 4:A:1765:NAG:O6 | 2.28 | 0.51 |
| 1:A:632:LEU:C | 1:A:632:LEU:HD23 | 2.30 | 0.51 |
| 1:A:62:ASP:OD1 | 1:A:348:ARG:NH2 | 2.42 | 0.51 |
| 1:B:623:ARG:HD3 | 1:B:659:ASP:OD2 | 2.10 | 0.51 |
| 1:B:142:VAL:HG23 | 1:B:155:VAL:CG2 | 2.40 | 0.51 |
| 1:A:749:ALA:N | 1:B:749:ALA:HB2 | 2.26 | 0.51 |
| 1:B:187:GLU:HB3 | 1:B:274:LEU:CD1 | 2.40 | 0.51 |
| 1:A:309:GLY:O | 1:A:310:PRO:O | 2.28 | 0.51 |
| 1:B:478:VAL:HB | 1:B:486:GLU:HB3 | 1.91 | 0.51 |
| 1:B:239:PHE:CD1 | 1:B:470:ASN:HB3 | 2.46 | 0.51 |
| 1:B:640:GLU:N | 1:B:640:GLU:OE1 | 2.41 | 0.51 |
| 1:A:400:ARG:NH1 | 1:A:406:TYR:O | 2.42 | 0.51 |
| 1:B:602:GLY:O | 1:B:710:PHE:HB2 | 2.10 | 0.51 |
| 1:A:306:VAL:CG2 | 1:A:307:PRO:HD2 | 2.41 | 0.51 |
| 1:A:309:GLY:H | 1:B:720:ALA:HB1 | 1.76 | 0.51 |
| 1:A:465:MET:HG2 | 1:A:474:VAL:HG22 | 1.93 | 0.50 |
| 1:B:742:LEU:O | 1:B:743:PRO:C | 2.50 | 0.50 |
| 1:B:601:ARG:HA | 1:B:709:ASN:O | 2.11 | 0.50 |
| 1:A:218:LEU:O | 1:A:219:GLN:CB | 2.59 | 0.50 |
| 1:A:214:ALA:HB3 | 1:A:382:THR:HA | 1.93 | 0.50 |
| 1:A:544:MET:HE2 | 1:B:683:LEU:HD13 | 1.94 | 0.50 |
| 1:B:94:ASN:HA | 1:B:129:PHE:O | 2.11 | 0.50 |
| 1:B:497:SER:HB2 | 1:B:515:THR:HG22 | 1.94 | 0.50 |
| 1:A:669:ILE:O | 1:A:674:LEU:HD11 | 2.13 | 0.49 |
| 1:A:75:LEU:O | 1:A:76:THR:C | 2.50 | 0.49 |
| 1:A:204:ARG:NE | 1:A:206:ARG:HB3 | 2.28 | 0.49 |
| 1:A:382:THR:C | 1:A:383:ARG:HD3 | 2.33 | 0.49 |
| 1:A:396:THR:OG1 | 1:B:442:ARG:NH2 | 2.44 | 0.49 |
| 1:B:556:GLU:N | 1:B:557:HIS:CB | 2.76 | 0.49 |
| 1:A:78:ARG:HB2 | 1:A:78:ARG:NH1 | 2.27 | 0.49 |
| 1:A:583:THR:HG23 | 1:A:583:THR:O | 2.12 | 0.49 |
| 1:B:58:GLN:HG2 | 1:B:329:ARG:HD3 | 1.95 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:360:VAL:CG1 | 1:B:530:LEU:HD23 | 2.42 | 0.48 |
| 1:A:403:ASP:OD2 | 1:B:442:ARG:NH1 | 2.44 | 0.48 |
| 1:A:218:LEU:HD12 | 1:B:557:HIS:ND1 | 2.28 | 0.48 |
| 1:A:213:THR:HB | 1:A:226:TRP:O | 2.11 | 0.48 |
| 1:A:671:GLY:C | 1:A:672:LYS:HD2 | 2.34 | 0.48 |
| 1:A:334:LEU:HD12 | 1:A:334:LEU:N | 2.28 | 0.48 |
| 1:A:328:SER:O | 1:A:338:SER:HA | 2.13 | 0.48 |
| 1:B:224:ALA:HA | 1:B:249:VAL:O | 2.13 | 0.48 |
| 1:A:95:CYS:O | 1:A:128:VAL:HA | 2.13 | 0.48 |
| 1:B:328:SER:O | 1:B:338:SER:HA | 2.13 | 0.48 |
| 1:A:443:HIS:HB2 | 1:B:493:GLY:HA2 | 1.95 | 0.48 |
| 1:A:187:GLU:HB3 | 1:A:274:LEU:HD12 | 1.96 | 0.48 |
| 1:B:171:VAL:HG23 | 1:B:216:ARG:NH1 | 2.29 | 0.48 |
| 1:B:214:ALA:CB | 1:B:382:THR:HA | 2.43 | 0.48 |
| 1:B:669:ILE:HG22 | 1:B:674:LEU:CD2 | 2.43 | 0.48 |
| 1:A:86:ALA:HA | 1:A:95:CYS:SG | 2.54 | 0.47 |
| 1:B:565:THR:O | 1:B:565:THR:HG22 | 2.15 | 0.47 |
| 1:A:106:LYS:HG3 | 1:A:361:TYR:CZ | 2.49 | 0.47 |
| 1:A:218:LEU:O | 1:A:219:GLN:HB2 | 2.13 | 0.47 |
| 1:A:385:VAL:HG12 | 1:A:385:VAL:O | 2.14 | 0.47 |
| 1:A:537:ASN:HA | 1:A:590:ALA:O | 2.14 | 0.47 |
| 1:A:453:GLY:HA3 | 1:B:302:LEU:HD13 | 1.96 | 0.47 |
| 1:A:480:HIS:NE2 | 1:A:486:GLU:OE1 | 2.48 | 0.47 |
| 1:B:344:PHE:HA | 1:B:390:GLY:HA2 | 1.97 | 0.47 |
| 1:B:62:ASP:OD1 | 1:B:348:ARG:NH2 | 2.46 | 0.47 |
| 1:B:59:LEU:CD1 | 1:B:60:PHE:CD2 | 2.97 | 0.47 |
| 1:A:383:ARG:CD | 1:A:383:ARG:N | 2.78 | 0.47 |
| 1:B:59:LEU:HD11 | 1:B:60:PHE:CE2 | 2.50 | 0.47 |
| 1:B:212:THR:HG23 | 1:B:216:ARG:HH21 | 1.80 | 0.47 |
| 1:B:256:PRO:HA | 1:B:259:TRP:CD2 | 2.50 | 0.47 |
| 1:A:106:LYS:HB2 | 1:A:637:ARG:NH2 | 2.30 | 0.47 |
| 1:A:726:ARG:CZ | 1:A:726:ARG:HB2 | 2.45 | 0.47 |
| 1:B:433:GLU:HA | 1:B:459:VAL:O | 2.15 | 0.46 |
| 1:A:745:ALA:O | 1:A:746:ALA:HB3 | 2.15 | 0.46 |
| 1:B:90:ARG:N | 1:B:90:ARG:HD2 | 2.29 | 0.46 |
| 1:B:520:HIS:CE1 | 8:B:2006:HOH:O | 2.68 | 0.46 |
| 1:B:395:THR:HA | 1:B:466:SER:HA | 1.97 | 0.46 |
| 1:A:611:ALA:HA | 1:A:681:GLY:O | 2.15 | 0.46 |
| 1:A:194:LEU:HD12 | 1:A:277:LEU:HG | 1.98 | 0.46 |
| 1:A:525:HIS:HB2 | 1:A:627:TRP:CE3 | 2.50 | 0.46 |
| 1:A:495:ILE:CD1 | 1:A:495:ILE:N | 2.73 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:381:THR:HG23 | 8:A:2006:HOH:O | 2.14 | 0.46 |
| 1:A:341:LEU:HB2 | 1:A:429:PHE:HZ | 1.81 | 0.46 |
| 1:B:556:GLU:H | 1:B:557:HIS:CB | 2.28 | 0.46 |
| 1:B:238:PHE:C | 1:B:238:PHE:CD1 | 2.89 | 0.46 |
| 1:A:214:ALA:HB1 | 1:A:215:PRO:HD2 | 1.95 | 0.46 |
| 1:B:243:VAL:CG1 | 1:B:243:VAL:O | 2.64 | 0.46 |
| 1:B:447:LEU:HG | 1:B:448:TYR:CD2 | 2.51 | 0.46 |
| 1:B:233:ILE:HG21 | 1:B:236:ALA:HB3 | 1.97 | 0.46 |
| 1:A:641:GLU:N | 1:A:642:PRO:HD3 | 2.29 | 0.45 |
| 1:B:130:PHE:HB2 | 1:B:137:ASN:O | 2.16 | 0.45 |
| 1:A:138:VAL:HB | 1:A:164:LEU:HB2 | 1.98 | 0.45 |
| 1:B:465:MET:HG2 | 1:B:474:VAL:HG22 | 1.98 | 0.45 |
| 1:A:389:PHE:CD2 | 6:A:2000:JWF:CAE | 3.00 | 0.45 |
| 1:B:500:LEU:O | 1:B:501:PHE:HB3 | 2.16 | 0.45 |
| 1:A:90:ARG:HA | 1:A:90:ARG:HH11 | 1.81 | 0.45 |
| 1:B:438:LEU:HD23 | 1:B:439:PRO:HD2 | 1.98 | 0.45 |
| 1:A:182:MET:HA | 1:A:186:ARG:HD3 | 1.98 | 0.45 |
| 1:B:116:GLY:O | 1:B:117:SER:C | 2.55 | 0.45 |
| 1:B:646:SER:HB3 | 1:B:658:VAL:HG23 | 1.99 | 0.45 |
| 1:A:444:HIS:O | 1:B:467:THR:HG21 | 2.17 | 0.45 |
| 1:A:492:THR:HB | 1:A:694:THR:O | 2.16 | 0.44 |
| 1:A:478:VAL:HB | 1:A:486:GLU:HB3 | 1.98 | 0.44 |
| 1:A:567:LYS:HE2 | 1:A:568:LEU:N | 2.33 | 0.44 |
| 1:B:59:LEU:CD1 | 1:B:60:PHE:CE2 | 3.00 | 0.44 |
| 1:A:588:TYR:HB2 | 1:A:603:TYR:O | 2.18 | 0.44 |
| 1:B:142:VAL:O | 1:B:152:MET:HA | 2.17 | 0.44 |
| 1:A:583:THR:HA | 1:A:584:PRO:HD2 | 1.54 | 0.44 |
| 1:A:204:ARG:CD | 1:A:205:GLY:H | 2.31 | 0.44 |
| 1:B:561:ARG:HH11 | 1:B:561:ARG:CG | 2.31 | 0.44 |
| 1:A:297:GLY:O | 1:A:298:GLY:C | 2.56 | 0.44 |
| 1:A:294:ASN:OD1 | 5:A:1768:NAG:H61 | 2.17 | 0.44 |
| 1:B:306:VAL:HG13 | 1:B:307:PRO:HD2 | 1.99 | 0.44 |
| 1:A:389:PHE:HE1 | 1:A:650:GLN:HE21 | 1.64 | 0.44 |
| 1:B:187:GLU:HB3 | 1:B:274:LEU:HD11 | 1.99 | 0.44 |
| 1:B:532:VAL:HB | 1:B:537:ASN:OD1 | 2.16 | 0.44 |
| 1:A:442:ARG:CD | 1:B:465:MET:SD | 3.07 | 0.43 |
| 1:B:350:PHE:CE1 | 1:B:362:GLU:HG3 | 2.53 | 0.43 |
| 1:A:500:LEU:HD21 | 1:A:510:GLN:HG3 | 1.99 | 0.43 |
| 1:B:513:GLU:O | 1:B:514:HIS:HB2 | 2.17 | 0.43 |
| 1:B:349:ILE:O | 1:B:349:ILE:HD12 | 2.19 | 0.43 |
| 1:A:92:SER:O | 1:A:132:ARG:N | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:372:TYR:CD2 | 1:B:520:HIS:HB3 | 2.53 | 0.43 |
| 1:A:567:LYS:HE2 | 1:A:568:LEU:H | 1.83 | 0.43 |
| 1:A:198:CYS:SG | 1:A:199:CYS:N | 2.91 | 0.43 |
| 1:B:416:LEU:O | 1:B:417:LEU:HD23 | 2.19 | 0.43 |
| 1:B:88:GLN:HA | 1:B:174:GLN:HB2 | 2.00 | 0.43 |
| 1:A:646:SER:O | 1:A:648:PHE:N | 2.50 | 0.43 |
| 1:A:501:PHE:O | 1:A:503:ALA:N | 2.51 | 0.43 |
| 1:A:714:ASP:OD2 | 1:A:716:SER:OG | 2.36 | 0.43 |
| 1:A:632:LEU:O | 1:A:632:LEU:HD23 | 2.19 | 0.43 |
| 1:B:492:THR:HG22 | 1:B:493:GLY:N | 2.33 | 0.43 |
| 1:B:212:THR:CG2 | 1:B:216:ARG:HH21 | 2.31 | 0.43 |
| 1:B:542:GLU:HA | 1:B:565:THR:O | 2.17 | 0.43 |
| 1:A:209:VAL:HG11 | 1:B:448:TYR:CD2 | 2.53 | 0.43 |
| 1:B:487:ILE:HD12 | 1:B:487:ILE:N | 2.34 | 0.43 |
| 1:A:671:GLY:O | 1:A:672:LYS:HD2 | 2.19 | 0.43 |
| 1:A:106:LYS:HG3 | 1:A:361:TYR:CE1 | 2.54 | 0.43 |
| 1:B:416:LEU:C | 1:B:416:LEU:HD23 | 2.39 | 0.43 |
| 1:A:755:PHE:CE2 | 1:A:757:HIS:HB2 | 2.54 | 0.43 |
| 1:A:316:PHE:CD2 | 1:A:750:PRO:HD3 | 2.54 | 0.43 |
| 1:B:739:LEU:HD23 | 1:B:742:LEU:HD11 | 2.01 | 0.43 |
| 1:B:125:LEU:HD23 | 1:B:126:ALA:N | 2.34 | 0.43 |
| 1:B:217:GLY:HA3 | 1:B:222:ASP:CB | 2.48 | 0.43 |
| 1:A:336:THR:HG23 | 1:A:353:ARG:HB2 | 2.01 | 0.43 |
| 1:A:445:SER:HB3 | 1:A:451:TYR:CE2 | 2.54 | 0.43 |
| 1:A:650:GLN:HA | 1:A:650:GLN:OE1 | 2.19 | 0.42 |
| 1:A:403:ASP:HB3 | 1:A:465:MET:CE | 2.49 | 0.42 |
| 1:B:411:VAL:HG12 | 1:B:412:ASP:N | 2.34 | 0.42 |
| 1:A:613:GLU:HG3 | 1:A:614:PRO:CD | 2.48 | 0.42 |
| 1:A:748:CYS:H | 1:B:749:ALA:HB3 | 1.84 | 0.42 |
| 1:A:465:MET:SD | 1:B:442:ARG:CD | 3.07 | 0.42 |
| 1:A:459:VAL:HG23 | 1:A:480:HIS:HA | 2.01 | 0.42 |
| 1:A:553:TRP:CZ3 | 1:B:377:PRO:HB3 | 2.55 | 0.42 |
| 1:A:559:LEU:O | 1:A:559:LEU:HD23 | 2.18 | 0.42 |
| 1:B:187:GLU:HB3 | 1:B:274:LEU:HD12 | 2.01 | 0.42 |
| 1:B:382:THR:C | 1:B:383:ARG:HD3 | 2.40 | 0.42 |
| 1:B:568:LEU:HG | 1:B:569:LEU:N | 2.34 | 0.42 |
| 1:B:405:PRO:HG2 | 1:B:432:PHE:CD1 | 2.55 | 0.42 |
| 1:A:500:LEU:CD2 | 1:A:510:GLN:HG3 | 2.49 | 0.42 |
| 1:B:389:PHE:CE1 | 6:B:2000:JWF:HAD | 2.54 | 0.42 |
| 1:A:282:GLU:C | 1:A:284:GLY:H | 2.22 | 0.42 |
| 1:B:282:GLU:C | 1:B:284:GLY:H | 2.22 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:359:LEU:HD23 | 1:A:359:LEU:N | 2.35 | 0.42 |
| 1:A:585:ARG:NH1 | 1:A:585:ARG:CG | 2.82 | 0.42 |
| 1:B:539:VAL:HG13 | 1:B:569:LEU:HB2 | 2.02 | 0.42 |
| 1:A:203:HIS:O | 1:A:204:ARG:HB2 | 2.19 | 0.42 |
| 1:B:187:GLU:HG3 | 1:B:261:ILE:HD11 | 2.02 | 0.42 |
| 1:B:620:SER:OG | 1:B:654:TRP:HD1 | 2.03 | 0.42 |
| 1:B:271:TYR:CE1 | 1:B:277:LEU:HD13 | 2.55 | 0.42 |
| 1:B:723:ILE:HD11 | 1:B:739:LEU:HG | 2.01 | 0.42 |
| 6:B:2000:JWF:HAU | 6:B:2000:JWF:HAS | 1.66 | 0.42 |
| 1:B:188:LEU:N | 1:B:189:PRO:CD | 2.83 | 0.42 |
| 1:A:212:THR:OG1 | 1:A:216:ARG:NH2 | 2.49 | 0.42 |
| 1:B:382:THR:O | 1:B:383:ARG:HD3 | 2.19 | 0.42 |
| 1:B:339:PHE:HB3 | 1:B:349:ILE:HG22 | 2.01 | 0.42 |
| 1:B:389:PHE:HB3 | 1:B:394:TYR:CE2 | 2.54 | 0.42 |
| 1:A:220:SER:HB2 | 1:A:654:TRP:HB2 | 2.02 | 0.42 |
| 1:A:383:ARG:NH2 | 1:B:560:GLN:O | 2.44 | 0.41 |
| 1:B:166:TYR:O | 1:B:169:ARG:HD3 | 2.19 | 0.41 |
| 1:A:735:GLU:N | 1:A:735:GLU:CD | 2.73 | 0.41 |
| 1:A:606:GLN:HB3 | 1:A:704:PHE:HB2 | 2.02 | 0.41 |
| 1:A:445:SER:CB | 1:A:451:TYR:CE2 | 3.03 | 0.41 |
| 1:B:177:LEU:HD12 | 6:B:2000:JWF:CAI | 2.50 | 0.41 |
| 1:B:278:GLU:O | 1:B:282:GLU:HG3 | 2.20 | 0.41 |
| 1:A:386:ASP:HB3 | 1:A:468:LEU:CD2 | 2.50 | 0.41 |
| 1:A:509:ASN:O | 1:A:516:LEU:HD12 | 2.20 | 0.41 |
| 1:B:750:PRO:HB3 | 1:B:752:LEU:HD21 | 2.03 | 0.41 |
| 1:A:383:ARG:HD3 | 1:A:383:ARG:N | 2.35 | 0.41 |
| 1:A:225:THR:HB | 1:A:227:PHE:CE2 | 2.54 | 0.41 |
| 1:B:69:THR:HG23 | 1:B:422:PRO:HG3 | 2.02 | 0.41 |
| 1:B:366:GLN:HG3 | 1:B:644:SER:OG | 2.21 | 0.41 |
| 1:A:144:GLY:C | 1:A:151:TYR:CE1 | 2.94 | 0.41 |
| 1:B:212:THR:HG21 | 1:B:216:ARG:NH2 | 2.34 | 0.41 |
| 1:B:460:LEU:HB3 | 1:B:479:PHE:HB2 | 2.02 | 0.41 |
| 1:A:110:LEU:O | 1:A:111:ALA:C | 2.59 | 0.41 |
| 1:A:246:GLU:OE1 | 1:A:376:SER:HB2 | 2.21 | 0.41 |
| 1:A:73:ARG:O | 1:A:76:THR:HB | 2.20 | 0.41 |
| 1:B:469:LEU:HD23 | 1:B:469:LEU:HA | 1.90 | 0.41 |
| 1:A:188:LEU:HB2 | 1:A:189:PRO:HD2 | 2.02 | 0.41 |
| 1:A:638:LYS:HD2 | 1:A:641:GLU:CD | 2.41 | 0.41 |
| 1:A:359:LEU:HD13 | 1:A:603:TYR:CZ | 2.56 | 0.41 |
| 1:A:476:ASP:O | 1:A:477:THR:CB | 2.69 | 0.41 |
| 1:A:308:PRO:HA | 1:B:720:ALA:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:246:GLU:C | 1:A:247:LEU:HD12 | 2.40 | 0.41 |
| 1:A:465:MET:SD | 1:B:442:ARG:HD2 | 2.61 | 0.41 |
| 1:B:436:GLN:HB2 | 1:B:438:LEU:HB2 | 2.02 | 0.41 |
| 1:B:74:PHE:C | 1:B:74:PHE:CD1 | 2.94 | 0.41 |
| 1:B:211:MET:HA | 8:B:2002:HOH:O | 2.21 | 0.41 |
| 1:A:695:VAL:CG1 | 1:B:440:LEU:HG | 2.50 | 0.40 |
| 1:B:174:GLN:NE2 | 1:B:174:GLN:HA | 2.35 | 0.40 |
| 1:A:144:GLY:O | 1:A:151:TYR:CD1 | 2.74 | 0.40 |
| 1:A:71:VAL:HG13 | 1:A:143:VAL:HG11 | 2.03 | 0.40 |
| 1:A:344:PHE:HA | 1:A:390:GLY:HA2 | 2.03 | 0.40 |
| 1:B:341:LEU:HD12 | 1:B:347:PRO:N | 2.35 | 0.40 |
| 1:A:245:LEU:HG | 1:A:247:LEU:CD1 | 2.52 | 0.40 |
| 1:A:344:PHE:HA | 1:A:390:GLY:CA | 2.51 | 0.40 |
| 1:B:84:VAL:HG21 | 1:B:93:ASP:HB3 | 2.03 | 0.40 |
| 6:A:2000:JWF:HAH | 6:A:2000:JWF:HAQ2 | 1.94 | 0.40 |
| 1:A:208:LEU:C | 1:A:209:VAL:HG23 | 2.41 | 0.40 |
| 1:A:213:THR:HG21 | 1:A:226:TRP:H | 1.87 | 0.40 |
| 1:B:260:THR:HG22 | 1:B:261:ILE:N | 2.36 | 0.40 |
| 1:A:341:LEU:HB2 | 1:A:429:PHE:CZ | 2.56 | 0.40 |
| 1:B:325:VAL:HG22 | 1:B:330:VAL:HG22 | 2.03 | 0.40 |
| 1:A:476:ASP:O | 1:A:477:THR:OG1 | 2.34 | 0.40 |
| 1:B:760:PHE:O | 1:B:761:SER:C | 2.60 | 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 | 708/737 (96%) | 596 (84%) | 73 (10%) | 39 (6%) | 2 13 |
| 1 | B | 704/737 (96%) | 593 (84%) | 79 (11%) | 32 (4%) | 3 17 |
| All | All | 1412/1474 (96%) | 1189 (84%) | 152 (11%) | 71 (5%) | 3 16 |

All (71) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 59 | LEU |
| 1 | A | 116 | GLY |
| 1 | A | 203 | HIS |
| 1 | A | 204 | ARG |
| 1 | A | 206 | ARG |
| 1 | A | 214 | ALA |
| 1 | A | 219 | GLN |
| 1 | A | 310 | PRO |
| 1 | A | 477 | THR |
| 1 | A | 642 | PRO |
| 1 | B | 116 | GLY |
| 1 | B | 181 | GLN |
| 1 | B | 201 | TYR |
| 1 | B | 202 | LYS |
| 1 | B | 214 | ALA |
| 1 | B | 297 | GLY |
| 1 | B | 320 | GLY |
| 1 | B | 481 | PRO |
| 1 | B | 504 | THR |
| 1 | B | 618 | ASN |
| 1 | B | 622 | ALA |
| 1 | B | 667 | GLU |
| 1 | B | 742 | LEU |
| 1 | A | 81 | PRO |
| 1 | A | 253 | ALA |
| 1 | A | 284 | GLY |
| 1 | A | 298 | GLY |
| 1 | A | 320 | GLY |
| 1 | A | 593 | HIS |
| 1 | B | 133 | GLN |
| 1 | B | 501 | PHE |
| 1 | B | 749 | ALA |
| 1 | A | 283 | ALA |
| 1 | A | 292 | PRO |
| 1 | A | 347 | PRO |
| 1 | A | 502 | GLY |
| 1 | A | 584 | PRO |
| 1 | B | 283 | ALA |
| 1 | B | 448 | TYR |
| 1 | B | 557 | HIS |
| 1 | B | 743 | PRO |
| 1 | B | 761 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 55 | GLY |
| 1 | A | 76 | THR |
| 1 | A | 183 | ILE |
| 1 | A | 439 | PRO |
| 1 | A | 504 | THR |
| 1 | A | 623 | ARG |
| 1 | A | 647 | VAL |
| 1 | A | 761 | SER |
| 1 | B | 81 | PRO |
| 1 | B | 132 | ARG |
| 1 | B | 199 | CYS |
| 1 | B | 442 | ARG |
| 1 | B | 555 | PRO |
| 1 | B | 665 | ASN |
| 1 | A | 232 | ASN |
| 1 | A | 280 | GLN |
| 1 | A | 697 | VAL |
| 1 | A | 743 | PRO |
| 1 | B | 405 | PRO |
| 1 | B | 746 | ALA |
| 1 | A | 612 | GLY |
| 1 | A | 742 | LEU |
| 1 | B | 666 | ASN |
| 1 | A | 54 | PRO |
| 1 | A | 80 | GLY |
| 1 | A | 205 | GLY |
| 1 | B | 163 | PRO |
| 1 | A | 145 | PRO |
| 1 | B | 692 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 588/610 (96%) | 527 (90%) | 61 (10%) | 9 32 |
| 1 | B | 584/610 (96%) | 524 (90%) | 60 (10%) | 9 32 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| All | All | 1172/1220 (96%) | 1051 (90%) | 121 (10%) | 9 32 |

All (121) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 56 | GLN |
| 1 | A | 62 | ASP |
| 1 | A | 64 | SER |
| 1 | A | 69 | THR |
| 1 | A | 78 | ARG |
| 1 | A | 90 | ARG |
| 1 | A | 95 | CYS |
| 1 | A | 103 | LEU |
| 1 | A | 117 | SER |
| 1 | A | 174 | GLN |
| 1 | A | 192 | SER |
| 1 | A | 210 | THR |
| 1 | A | 213 | THR |
| 1 | A | 216 | ARG |
| 1 | A | 218 | LEU |
| 1 | A | 229 | LEU |
| 1 | A | 230 | TYR |
| 1 | A | 240 | LEU |
| 1 | A | 254 | LEU |
| 1 | A | 285 | LEU |
| 1 | A | 290 | LEU |
| 1 | A | 291 | ILE |
| 1 | A | 299 | SER |
| 1 | A | 302 | LEU |
| 1 | A | 310 | PRO |
| 1 | A | 319 | GLN |
| 1 | A | 329 | ARG |
| 1 | A | 334 | LEU |
| 1 | A | 336 | THR |
| 1 | A | 338 | SER |
| 1 | A | 345 | SER |
| 1 | A | 359 | LEU |
| 1 | A | 360 | VAL |
| 1 | A | 376 | SER |
| 1 | A | 383 | ARG |
| 1 | A | 389 | PHE |
| 1 | A | 446 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 464 | SER |
| 1 | A | 489 | PHE |
| 1 | A | 492 | THR |
| 1 | A | 497 | SER |
| 1 | A | 506 | LYS |
| 1 | A | 510 | GLN |
| 1 | A | 518 | THR |
| 1 | A | 558 | GLN |
| 1 | A | 559 | LEU |
| 1 | A | 567 | LYS |
| 1 | A | 570 | GLU |
| 1 | A | 573 | GLU |
| 1 | A | 583 | THR |
| 1 | A | 585 | ARG |
| 1 | A | 587 | LEU |
| 1 | A | 621 | MET |
| 1 | A | 632 | LEU |
| 1 | A | 635 | THR |
| 1 | A | 645 | SER |
| 1 | A | 713 | GLU |
| 1 | A | 726 | ARG |
| 1 | A | 742 | LEU |
| 1 | A | 756 | SER |
| 1 | A | 763 | ASN |
| 1 | B | 58 | GLN |
| 1 | B | 59 | LEU |
| 1 | B | 73 | ARG |
| 1 | B | 88 | GLN |
| 1 | B | 90 | ARG |
| 1 | B | 92 | SER |
| 1 | B | 98 | SER |
| 1 | B | 100 | GLU |
| 1 | B | 155 | VAL |
| 1 | B | 177 | LEU |
| 1 | B | 192 | SER |
| 1 | B | 198 | CYS |
| 1 | B | 199 | CYS |
| 1 | B | 209 | VAL |
| 1 | B | 216 | ARG |
| 1 | B | 218 | LEU |
| 1 | B | 238 | PHE |
| 1 | B | 272 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 292 | PRO |
| 1 | B | 319 | GLN |
| 1 | B | 324 | SER |
| 1 | B | 336 | THR |
| 1 | B | 338 | SER |
| 1 | B | 345 | SER |
| 1 | B | 358 | ARG |
| 1 | B | 360 | VAL |
| 1 | B | 380 | MET |
| 1 | B | 383 | ARG |
| 1 | B | 391 | MET |
| 1 | B | 395 | THR |
| 1 | B | 409 | THR |
| 1 | B | 426 | ARG |
| 1 | B | 442 | ARG |
| 1 | B | 449 | SER |
| 1 | B | 450 | HIS |
| 1 | B | 458 | THR |
| 1 | B | 464 | SER |
| 1 | B | 481 | PRO |
| 1 | B | 489 | PHE |
| 1 | B | 515 | THR |
| 1 | B | 518 | THR |
| 1 | B | 559 | LEU |
| 1 | B | 561 | ARG |
| 1 | B | 573 | GLU |
| 1 | B | 603 | TYR |
| 1 | B | 607 | MET |
| 1 | B | 608 | LEU |
| 1 | B | 613 | GLU |
| 1 | B | 620 | SER |
| 1 | B | 621 | MET |
| 1 | B | 634 | VAL |
| 1 | B | 637 | ARG |
| 1 | B | 645 | SER |
| 1 | B | 647 | VAL |
| 1 | B | 666 | ASN |
| 1 | B | 669 | ILE |
| 1 | B | 694 | THR |
| 1 | B | 701 | VAL |
| 1 | B | 714 | ASP |
| 1 | B | 734 | CYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 592 | ASN |
| 1 | B | 593 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

2 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 | $\#\|Z\| > 2$ |
| 1 | TPQ | A | 471 | 1 | 13,14,15 | 1.30 | 3 (23%) | 15,19,21 | 1.67 | 3 (20%) |
| 1 | TPQ | B | 471 | 1 | 13,14,15 | 1.30 | 1 (7%) | 15,19,21 | 1.72 | 2 (13%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | TPQ | A | 471 | 1 | - | 0/4/22/24 | 0/1/1/1 |
| 1 | TPQ | B | 471 | 1 | - | 0/4/22/24 | 0/1/1/1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 471 | TPQ | C6-C5 | -2.24 | 1.38 | 1.44 |
| 1 | A | 471 | TPQ | C6-C1 | 2.01 | 1.39 | 1.34 |
| 1 | A | 471 | TPQ | C3-C4 | 2.42 | 1.39 | 1.35 |
| 1 | B | 471 | TPQ | C3-C4 | 2.70 | 1.40 | 1.35 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 471 | TPQ | C1-C6-C5 | -2.83 | 121.25 | 122.97 |
| 1 | B | 471 | TPQ | O5-C5-C4 | 2.38 | 122.97 | 119.16 |
| 1 | A | 471 | TPQ | O5-C5-C4 | 2.77 | 123.60 | 119.16 |
| 1 | A | 471 | TPQ | C6-C1-C2 | 4.08 | 121.32 | 118.44 |
| 1 | B | 471 | TPQ | C6-C1-C2 | 4.72 | 121.78 | 118.44 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

9 carbohydrates 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 | $\#\|Z\| > 2$ |
| 4 | NAG | A | 1765 | 1,4 | 14,14,15 | 0.56 | 0 | 15,19,21 | 1.54 | 3 (20%) |
| 4 | NAG | A | 1766 | 4 | 14,14,15 | 0.67 | 0 | 15,19,21 | 1.34 | 2 (13%) |
| 7 | NAG | B | 1765 | 1,7 | 14,14,15 | 0.68 | 0 | 15,19,21 | 2.15 | 6 (40%) |
| 7 | NAG | B | 1766 | 7 | 14,14,15 | 0.49 | 0 | 15,19,21 | 1.85 | 1 (6%) |
| 7 | BMA | B | 1767 | 7 | 11,11,12 | 1.28 | 2 (18%) | 14,15,17 | 2.53 | 7 (50%) |
| 7 | MAN | B | 1768 | 7 | 11,11,12 | 1.68 | 3 (27%) | 14,15,17 | 1.85 | 5 (35%) |
| 7 | MAN | B | 1769 | 7 | 11,11,12 | 0.26 | 0 | 14,15,17 | 0.61 | 0 |
| 4 | NAG | B | 1770 | 1,4 | 14,14,15 | 0.79 | 0 | 15,19,21 | 2.03 | 5 (33%) |
| 4 | NAG | B | 1771 | 4 | 14,14,15 | 0.68 | 0 | 15,19,21 | 2.44 | 4 (26%) |

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 |
|---|---|---|---|---|---|---|---|
| 4 | NAG | A | 1765 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | A | 1766 | 4 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | B | 1765 | 1,7 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 7 | NAG | B | 1766 | 7 | - | 0/6/23/26 | 0/1/1/1 |
| 7 | BMA | B | 1767 | 7 | - | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | B | 1768 | 7 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 7 | MAN | B | 1769 | 7 | 1/1/4/5 | 0/2/19/22 | 0/1/1/1 |
| 4 | NAG | B | 1770 | 1,4 | - | 0/6/23/26 | 0/1/1/1 |
| 4 | NAG | B | 1771 | 4 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 7 | B | 1767 | BMA | O6-C6 | 2.08 | 1.51 | 1.42 |
| 7 | B | 1768 | MAN | C4-C3 | 2.31 | 1.58 | 1.52 |
| 7 | B | 1767 | BMA | O3-C3 | 2.76 | 1.49 | 1.43 |
| 7 | B | 1768 | MAN | C1-C2 | 3.30 | 1.60 | 1.52 |
| 7 | B | 1768 | MAN | C2-C3 | 3.51 | 1.57 | 1.52 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 7 | B | 1765 | NAG | O4-C4-C3 | -4.68 | 99.80 | 110.34 |
| 4 | B | 1771 | NAG | O7-C7-C8 | -3.37 | 115.87 | 122.06 |
| 7 | B | 1765 | NAG | C3-C4-C5 | -3.31 | 104.43 | 110.20 |
| 7 | B | 1768 | MAN | C1-O5-C5 | -3.25 | 108.12 | 112.25 |
| 4 | B | 1770 | NAG | C4-C3-C2 | -2.54 | 107.28 | 111.23 |
| 7 | B | 1765 | NAG | O3-C3-C4 | -2.36 | 105.02 | 110.34 |
| 7 | B | 1765 | NAG | C2-N2-C7 | -2.28 | 120.11 | 123.04 |
| 4 | A | 1765 | NAG | C3-C2-N2 | -2.01 | 105.76 | 110.56 |
| 7 | B | 1768 | MAN | C1-C2-C3 | -2.00 | 107.17 | 109.54 |
| 7 | B | 1765 | NAG | O3-C3-C2 | 2.09 | 113.25 | 109.11 |
| 7 | B | 1767 | BMA | O3-C3-C4 | 2.13 | 115.13 | 110.34 |
| 4 | B | 1770 | NAG | O4-C4-C5 | 2.15 | 114.95 | 109.24 |
| 4 | A | 1766 | NAG | O4-C4-C5 | 2.29 | 115.30 | 109.24 |
| 7 | B | 1767 | BMA | O5-C1-C2 | 2.30 | 114.59 | 110.86 |
| 7 | B | 1767 | BMA | O6-C6-C5 | 2.35 | 119.11 | 111.33 |
| 7 | B | 1767 | BMA | O5-C5-C6 | 2.39 | 112.52 | 107.35 |
| 7 | B | 1765 | NAG | O4-C4-C5 | 2.45 | 115.73 | 109.24 |
| 7 | B | 1768 | MAN | O4-C4-C3 | 2.52 | 116.01 | 110.34 |
| 7 | B | 1767 | BMA | C3-C4-C5 | 2.55 | 114.64 | 110.20 |
| 7 | B | 1768 | MAN | O5-C5-C6 | 2.57 | 112.91 | 107.35 |
| 4 | B | 1771 | NAG | O3-C3-C2 | 2.63 | 114.33 | 109.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | A | 1765 | NAG | C1-O5-C5 | 2.76 | 115.75 | 112.25 |
| 7 | B | 1768 | MAN | O2-C2-C1 | 2.95 | 115.12 | 109.21 |
| 4 | A | 1765 | NAG | O3-C3-C2 | 3.08 | 115.22 | 109.11 |
| 4 | A | 1766 | NAG | C1-O5-C5 | 3.15 | 116.24 | 112.25 |
| 4 | B | 1770 | NAG | O3-C3-C2 | 3.32 | 115.70 | 109.11 |
| 4 | B | 1770 | NAG | C2-N2-C7 | 3.94 | 128.10 | 123.04 |
| 7 | B | 1767 | BMA | O2-C2-C1 | 4.22 | 117.67 | 109.21 |
| 4 | B | 1770 | NAG | C3-C2-N2 | 4.36 | 121.00 | 110.56 |
| 4 | B | 1771 | NAG | C2-N2-C7 | 4.48 | 128.79 | 123.04 |
| 7 | B | 1766 | NAG | C1-O5-C5 | 5.58 | 119.33 | 112.25 |
| 4 | B | 1771 | NAG | C1-O5-C5 | 5.94 | 119.78 | 112.25 |
| 7 | B | 1767 | BMA | O3-C3-C2 | 6.17 | 121.15 | 110.00 |

All (4) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 4 | B | 1771 | NAG | C1 |
| 7 | B | 1765 | NAG | C1 |
| 7 | B | 1769 | MAN | C1 |
| 7 | B | 1768 | MAN | C1 |

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 4 | A | 1765 | NAG | 1 | 0 |
| 7 | B | 1765 | NAG | 1 | 0 |
| 7 | B | 1767 | BMA | 8 | 0 |
| 7 | B | 1769 | MAN | 8 | 0 |
| 4 | B | 1770 | NAG | 1 | 0 |
| 4 | B | 1771 | NAG | 1 | 0 |

## 5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | NAG | A | 1767 | 1 | 14,14,15 | 0.81 | 0 | 15,19,21 | 2.35 | 7 (46%) |
| 5 | NAG | A | 1768 | 1 | 14,14,15 | 0.97 | 1 (7%) | 15,19,21 | 3.19 | 6 (40%) |
| 5 | NAG | A | 1769 | 1 | 14,14,15 | 0.75 | 0 | 15,19,21 | 2.29 | 5 (33%) |
| 5 | NAG | A | 1770 | 1 | 14,14,15 | 2.73 | 3 (21%) | 15,19,21 | 3.54 | 6 (40%) |
| 6 | JWF | A | 2000 | - | 32,37,37 | 2.57 | 9 (28%) | 36,52,52 | 2.32 | 7 (19%) |
| 5 | NAG | B | 1772 | - | 14,14,15 | 0.27 | 0 | 15,19,21 | 0.53 | 0 |
| 5 | NAG | B | 1773 | 1 | 14,14,15 | 1.64 | 2 (14%) | 15,19,21 | 2.77 | 3 (20%) |
| 6 | JWF | B | 2000 | - | 32,37,37 | 2.45 | 6 (18%) | 36,52,52 | 2.47 | 11 (30%) |

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 | 1767 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 1768 | 1 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 1769 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | A | 1770 | 1 | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 6 | JWF | A | 2000 | - | - | 0/13/26/26 | 0/5/5/5 |
| 5 | NAG | B | 1772 | - | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | B | 1773 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | JWF | B | 2000 | - | - | 0/13/26/26 | 0/5/5/5 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | A | 2000 | JWF | NAV-NAS | -8.90 | 1.18 | 1.37 |
| 6 | B | 2000 | JWF | CBC-CBB | -8.50 | 1.33 | 1.49 |
| 6 | B | 2000 | JWF | NAV-NAS | -7.46 | 1.21 | 1.37 |
| 6 | A | 2000 | JWF | CBC-CBB | -7.34 | 1.36 | 1.49 |
| 6 | A | 2000 | JWF | CAZ-NBG | -4.30 | 1.35 | 1.44 |
| 6 | B | 2000 | JWF | CAZ-NBG | -3.68 | 1.36 | 1.44 |
| 6 | A | 2000 | JWF | CAX-NAU | -2.58 | 1.35 | 1.40 |
| 6 | B | 2000 | JWF | CAX-NAU | -2.29 | 1.35 | 1.40 |
| 6 | A | 2000 | JWF | CBA-NAU | -2.19 | 1.34 | 1.39 |
| 6 | A | 2000 | JWF | CAJ-CAZ | 2.08 | 1.41 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | A | 1768 | NAG | C2-N2 | 2.18 | 1.50 | 1.46 |
| 6 | B | 2000 | JWF | CBC-NAT | 2.43 | 1.35 | 1.33 |
| 6 | A | 2000 | JWF | CBC-NAT | 2.43 | 1.35 | 1.33 |
| 5 | A | 1770 | NAG | C3-C2 | 2.46 | 1.58 | 1.52 |
| 6 | A | 2000 | JWF | CAQ-NBF | 3.00 | 1.51 | 1.46 |
| 6 | B | 2000 | JWF | CAW-CLAC | 3.01 | 1.81 | 1.74 |
| 6 | A | 2000 | JWF | CAP-NBF | 3.05 | 1.51 | 1.46 |
| 5 | B | 1773 | NAG | O5-C1 | 3.40 | 1.49 | 1.43 |
| 5 | A | 1770 | NAG | C2-N2 | 4.33 | 1.54 | 1.46 |
| 5 | B | 1773 | NAG | C1-C2 | 4.67 | 1.58 | 1.52 |
| 5 | A | 1770 | NAG | C1-C2 | 8.38 | 1.64 | 1.52 |

All (45) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | A | 2000 | JWF | NAR-CBB-NAS | -9.58 | 107.20 | 114.88 |
| 6 | B | 2000 | JWF | NAR-CBB-NAS | -8.46 | 108.09 | 114.88 |
| 5 | A | 1770 | NAG | O7-C7-C8 | -4.56 | 113.70 | 122.06 |
| 6 | A | 2000 | JWF | CBA-CBC-NAT | -4.36 | 115.86 | 121.12 |
| 5 | A | 1767 | NAG | C3-C4-C5 | -3.97 | 103.28 | 110.20 |
| 6 | A | 2000 | JWF | CAP-CAN-NBE | -3.15 | 107.46 | 110.79 |
| 6 | B | 2000 | JWF | CAP-CAN-NBE | -3.12 | 107.50 | 110.79 |
| 6 | B | 2000 | JWF | CBB-CBC-NAT | -3.01 | 113.44 | 117.47 |
| 5 | A | 1768 | NAG | C4-C3-C2 | -2.84 | 106.81 | 111.23 |
| 5 | A | 1768 | NAG | O7-C7-C8 | -2.81 | 116.90 | 122.06 |
| 5 | B | 1773 | NAG | C3-C4-C5 | -2.65 | 105.58 | 110.20 |
| 5 | A | 1769 | NAG | O7-C7-C8 | -2.56 | 117.36 | 122.06 |
| 6 | B | 2000 | JWF | CAK-CAZ-CAJ | -2.53 | 117.28 | 121.21 |
| 5 | A | 1767 | NAG | C4-C3-C2 | -2.25 | 107.74 | 111.23 |
| 6 | B | 2000 | JWF | CAI-CAY-NBF | -2.23 | 118.39 | 121.38 |
| 6 | B | 2000 | JWF | CAE-CAW-CAD | -2.01 | 118.39 | 121.26 |
| 5 | A | 1770 | NAG | C6-C5-C4 | 2.03 | 118.03 | 113.02 |
| 5 | A | 1769 | NAG | O7-C7-N2 | 2.14 | 126.23 | 121.86 |
| 6 | B | 2000 | JWF | CAD-CAW-CLAC | 2.30 | 123.12 | 119.35 |
| 5 | B | 1773 | NAG | O5-C5-C6 | 2.32 | 112.38 | 107.35 |
| 5 | A | 1768 | NAG | O3-C3-C2 | 2.42 | 113.90 | 109.11 |
| 6 | A | 2000 | JWF | CAO-NBE-CAN | 2.57 | 112.91 | 109.53 |
| 6 | A | 2000 | JWF | CAQ-NBF-CAP | 2.61 | 117.07 | 111.59 |
| 5 | A | 1769 | NAG | C2-N2-C7 | 2.67 | 126.47 | 123.04 |
| 6 | B | 2000 | JWF | CAH-CAY-NBF | 2.80 | 125.14 | 121.38 |
| 6 | B | 2000 | JWF | CAQ-NBF-CAY | 2.80 | 125.44 | 117.92 |
| 6 | A | 2000 | JWF | CAK-CAE-CAW | 2.85 | 122.39 | 119.23 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | A | 1769 | NAG | C3-C2-N2 | 2.87 | 117.44 | 110.56 |
| 6 | A | 2000 | JWF | CAJ-CAZ-NBG | 2.88 | 123.46 | 119.50 |
| 5 | A | 1767 | NAG | O3-C3-C2 | 3.13 | 115.31 | 109.11 |
| 5 | A | 1767 | NAG | O4-C4-C5 | 3.16 | 117.62 | 109.24 |
| 5 | A | 1767 | NAG | C2-N2-C7 | 3.17 | 127.11 | 123.04 |
| 5 | A | 1770 | NAG | O7-C7-N2 | 3.41 | 128.82 | 121.86 |
| 5 | A | 1767 | NAG | C3-C2-N2 | 3.46 | 118.85 | 110.56 |
| 6 | B | 2000 | JWF | CAE-CAK-CAZ | 3.60 | 122.89 | 119.23 |
| 5 | A | 1767 | NAG | O5-C5-C6 | 3.66 | 115.27 | 107.35 |
| 5 | A | 1768 | NAG | O5-C5-C6 | 3.92 | 115.84 | 107.35 |
| 5 | A | 1770 | NAG | O3-C3-C2 | 4.04 | 117.11 | 109.11 |
| 5 | A | 1770 | NAG | C1-O5-C5 | 5.94 | 119.78 | 112.25 |
| 6 | B | 2000 | JWF | CAO-NBE-CAN | 6.31 | 117.81 | 109.53 |
| 5 | A | 1769 | NAG | C1-O5-C5 | 6.64 | 120.68 | 112.25 |
| 5 | A | 1768 | NAG | C3-C2-N2 | 6.98 | 127.28 | 110.56 |
| 5 | A | 1768 | NAG | C2-N2-C7 | 7.10 | 132.16 | 123.04 |
| 5 | A | 1770 | NAG | C2-N2-C7 | 9.28 | 134.96 | 123.04 |
| 5 | B | 1773 | NAG | C1-O5-C5 | 9.58 | 124.41 | 112.25 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 5 | A | 1768 | NAG | C1 |
| 5 | A | 1770 | NAG | C1 |

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 5 | A | 1768 | NAG | 1 | 0 |
| 6 | A | 2000 | JWF | 5 | 0 |
| 5 | B | 1772 | NAG | 4 | 0 |
| 6 | B | 2000 | JWF | 3 | 0 |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 710/737 (96%) | -0.24 | 3 (0%) | 93 | 85 | 58, 83, 112, 163 | 0 |
| 1 | B | 706/737 (95%) | -0.14 | 9 (1%) | 79 | 62 | 63, 84, 115, 180 | 0 |
| All | All | 1416/1474 (96%) | -0.19 | 12 (0%) | 87 | 75 | 58, 83, 115, 180 | 0 |

All (12) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 746 | ALA | 4.1 |
| 1 | B | 744 | GLN | 4.0 |
| 1 | B | 745 | ALA | 4.0 |
| 1 | A | 203 | HIS | 3.5 |
| 1 | A | 763 | ASN | 3.3 |
| 1 | A | 746 | ALA | 3.1 |
| 1 | B | 748 | CYS | 2.9 |
| 1 | B | 731 | ALA | 2.7 |
| 1 | B | 747 | ALA | 2.6 |
| 1 | B | 698 | GLY | 2.6 |
| 1 | B | 700 | GLY | 2.0 |
| 1 | B | 571 | MET | 2.0 |

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

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 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | TPQ | A | 471 | 14/15 | 0.94 | 0.24 | - | 68,74,80,80 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 1 | TPQ | B | 471 | 14/15 | 0.97 | 0.31 | - | 68,76,90,94 | 0 |

## 6.3 Carbohydrates (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 |
|---|---|---|---|---|---|---|---|---|---|
| 4 | NAG | A | 1765 | 14/15 | 0.96 | 0.17 | 0.12 | 78,83,93,101 | 0 |
| 7 | NAG | B | 1765 | 14/15 | 0.90 | 0.16 | -1.02 | 74,82,91,94 | 0 |
| 4 | NAG | B | 1770 | 14/15 | 0.94 | 0.14 | -1.38 | 97,105,126,137 | 0 |
| 7 | NAG | B | 1766 | 14/15 | 0.94 | 0.17 | - | 100,110,119,123 | 0 |
| 7 | MAN | B | 1769 | 11/12 | 0.56 | 0.36 | - | 89,129,154,162 | 0 |
| 7 | BMA | B | 1767 | 11/12 | 0.80 | 0.30 | - | 113,133,158,163 | 0 |
| 4 | NAG | B | 1771 | 14/15 | 0.90 | 0.23 | - | 106,130,141,143 | 0 |
| 4 | NAG | A | 1766 | 14/15 | 0.85 | 0.24 | - | 101,123,145,157 | 0 |
| 7 | MAN | B | 1768 | 11/12 | 0.81 | 0.49 | - | 87,119,138,139 | 0 |

## 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 |
|---|---|---|---|---|---|---|---|---|---|
| 6 | JWF | B | 2000 | 33/33 | 0.91 | 0.21 | -0.11 | 71,78,101,108 | 0 |
| 5 | NAG | A | 1767 | 14/15 | 0.87 | 0.20 | -0.31 | 93,104,130,130 | 0 |
| 6 | JWF | A | 2000 | 33/33 | 0.96 | 0.18 | -0.31 | 71,90,120,127 | 0 |
| 3 | CA | B | 1763 | 1/1 | 0.95 | 0.05 | -2.14 | 72,72,72,72 | 0 |
| 3 | CA | A | 1764 | 1/1 | 0.77 | 0.13 | -2.48 | 94,94,94,94 | 0 |
| 3 | CA | B | 1764 | 1/1 | 0.93 | 0.11 | -2.55 | 81,81,81,81 | 0 |
| 3 | CA | A | 1763 | 1/1 | 0.96 | 0.05 | -2.73 | 71,71,71,71 | 0 |
| 5 | NAG | B | 1773 | 14/15 | 0.76 | 0.46 | - | 118,149,156,156 | 0 |
| 5 | NAG | A | 1769 | 14/15 | 0.63 | 0.56 | - | 127,148,167,183 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 5 | NAG | A | 1768 | 14/15 | 0.67 | 0.28 | - | 121,169,177,179 | 0 |
| 5 | NAG | A | 1770 | 14/15 | 0.54 | 0.61 | - | 114,149,166,170 | 0 |
| 5 | NAG | B | 1772 | 14/15 | 0.64 | 0.21 | - | 98,134,157,157 | 0 |
| 2 | CU | A | 1762 | 1/1 | 0.89 | 0.20 | - | 85,85,85,85 | 0 |
| 2 | CU | B | 1762 | 1/1 | 0.90 | 0.24 | - | 74,74,74,74 | 0 |

## 6.5 Other polymers

There are no such residues in this entry.