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

Oct 8, 2023 – 09:34 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 6EA5 |
| Title | : | Structure of BDBV GPcl in complex with the pan-ebolavirus mAb ADI-15878 |
| Authors | : | King, L.B.; West, B.R.; Moyer, C.L.; Fusco, M.L.; Milligan, J.C.; Hui, S.; Saphire, E.O. |
| Deposited on | : | 2018-08-02 |
| Resolution | : | 4.75 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:

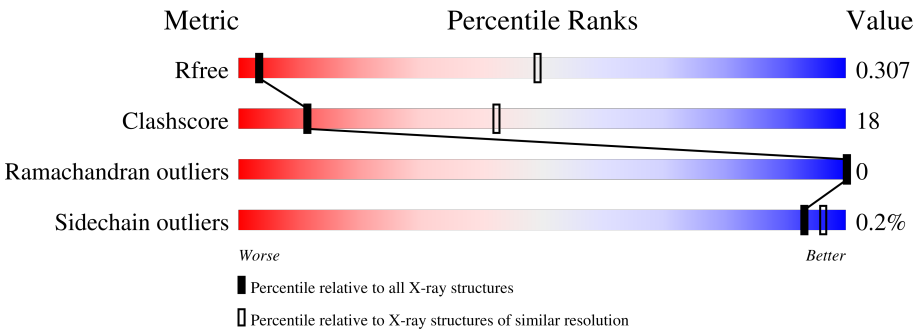
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (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 4.75 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 | 1089 (5.70-3.80) |
| Clashscore | 141614 | 1163 (5.70-3.80) |
| Ramachandran outliers | 138981 | 1098 (5.70-3.80) |
| Sidechain outliers | 138945 | 1078 (5.70-3.80) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 162 | 70% 30% |
| 1 | C | 162 | 59% 38% . |
| 1 | E | 162 | 61% 35% . |
| 2 | B | 111 | 44% 50% 6% |
| 2 | D | 111 | 59% 35% 6% |
| 2 | F | 111 | 63% 30% 7% |
| 3 | H | 233 | 66% 25% 9% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | M | 233 | 67% 26% 7% |
| 3 | Q | 233 | 65% 30% 5% |
| 4 | L | 213 | 77% 22% • |
| 4 | N | 213 | 76% 24% |
| 4 | R | 213 | 81% 18% • |
| 5 | G | 6 | 50% 50% |
| 6 | I | 5 | 60% 40% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 5 | NAG | G | 1 | - | - | X | - |
| 6 | BMA | I | 3 | - | - | X | - |

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 15944 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 Envelope glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 162 | 1251 | 798 | 213 | 235 | 5 | 0 | 0 | 0 |
| 1 | C | 158 | 1208 | 767 | 207 | 229 | 5 | 0 | 0 | 0 |
| 1 | E | 155 | 1187 | 755 | 204 | 223 | 5 | 0 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 64 | ALA | LYS | conflict | UNP B8XCN0 |
| C | 64 | ALA | LYS | conflict | UNP B8XCN0 |
| E | 64 | ALA | LYS | conflict | UNP B8XCN0 |

- Molecule 2 is a protein called Glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 2 | B | 104 | 813 | 518 | 142 | 147 | 6 | 0 | 0 | 0 |
| 2 | D | 104 | 813 | 518 | 142 | 147 | 6 | 0 | 0 | 0 |
| 2 | F | 103 | 808 | 515 | 141 | 146 | 6 | 0 | 0 | 0 |

- Molecule 3 is a protein called ADI-15878 Fab Heavy Chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | H | 213 | 1598 | 1016 | 269 | 307 | 6 | 0 | 0 | 0 |
| 3 | M | 217 | 1625 | 1031 | 274 | 314 | 6 | 0 | 0 | 0 |

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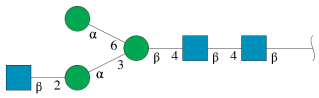
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 3 | Q | 222 | 1655 | 1047 | 280 | 322 | 6 | 0 | 0 | 0 |

- Molecule 4 is a protein called ADI-15878 Fab Light Chain.

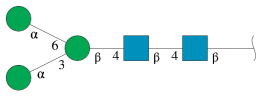
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 4 | L | 210 | 1597 | 999 | 261 | 333 | 4 | 0 | 0 | 0 |
| 4 | N | 212 | 1617 | 1011 | 267 | 335 | 4 | 0 | 0 | 0 |
| 4 | R | 211 | 1608 | 1006 | 266 | 332 | 4 | 0 | 0 | 0 |

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



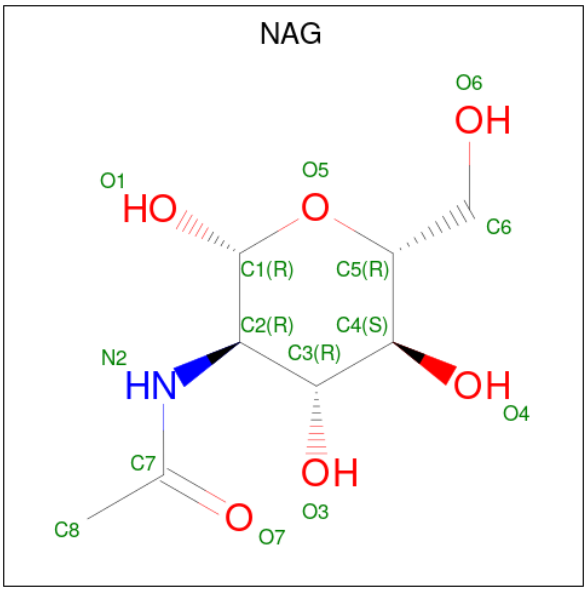

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 5 | G | 6 | 75 | 42 | 3 | 30 | 0 | 0 | 0 |

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | | |
| 6 | I | 5 | 61 | 34 | 2 | 25 | 0 | 0 | 0 |

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



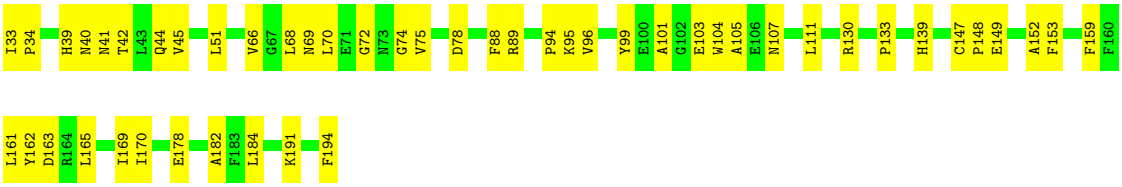

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 7 | A | 1 | 14 | 8 | 1 | 5 | 0 | 0 |
| | | | Total | C | N | O | | |
| 7 | B | 1 | 14 | 8 | 1 | 5 | 0 | 0 |

# 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. 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. 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.

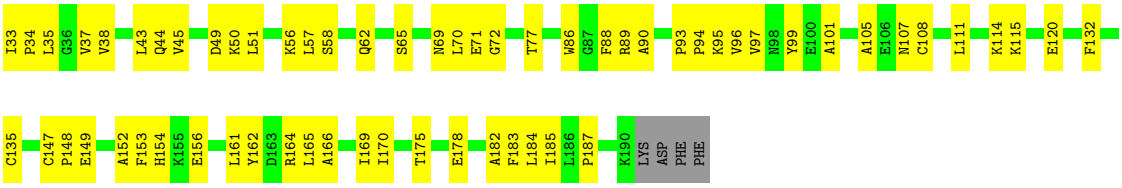
• Molecule 1: Envelope glycoprotein

Chain A:



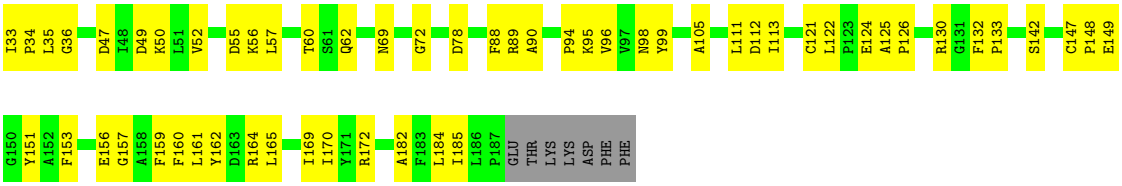

• Molecule 1: Envelope glycoprotein

Chain C:



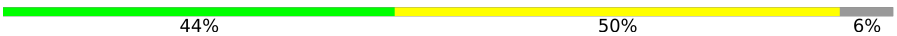

• Molecule 1: Envelope glycoprotein

Chain E:




• Molecule 2: Glycoprotein

Chain B:



L571 F572 L573 R574 A575 T576 T577 E578 L579 R580 T581 F582 R587 F592 L593 L594 Q595 R596 G599 T600 C601 H602 I603 I610 E611 P612

- Molecule 2: Glycoprotein

Chain D:

GLU ILE THR LEU ARG THR GLN A509 K510 C511 N512 P513 N514 L515 Q521 G524 I527 G528 L529 A530 W531 I532 F535 G536 P537 I542 L554 I555 C556 G557 L558 R559 Q560 L561 A562 N563 Q567 Q570 L573 R574 T577 E578 L579 R580 I584 L585 K588

L593 L594 Q595 R596 W597 C601 C609 P612

- Molecule 2: Glycoprotein

Chain F:

GLU ILE THR LEU ARG THR GLN ALA K510 H516 A526 I527 G528 L529 A530 W531 I532 P533 P537 I542 I547 L558 R559 Q560 L561 A562 N563 E564 T565 Q570 L571 F572 L573 R574 A575 T576 T577 R580 T581 F582 S583 I584 K588 L594 Q595 R596 W597 G598 G599 T600

C601 P612

- Molecule 3: ADI-15878 Fab Heavy Chain

Chain H:

GLN V2 Q3 L4 V5 Q6 T10 L11 V12 Q13 P14 G15 G16 S17 L18 A23 F27 S30 S35 W36 A40 K43 I51 S52 G56 A61 V64 F68 R72 D73 N74 L79 M83 L86 T91 Y94 Y95 V102 W103 G106

F109 D110 Y111 W112 V118 T119 V120 S121 S122 P128 P135 SER SER LYS SER THR SER GLY GLY T144 L147 V151 Y154 F155 P156 E157 P158 V159 T160 V161 N164 A167 S189 T202 N208 K215 K219 V220 E221 P222 LYS SER CYS ASP LEU GLU

VAL ASP ASP ASP ASP

- Molecule 3: ADI-15878 Fab Heavy Chain

Chain M:

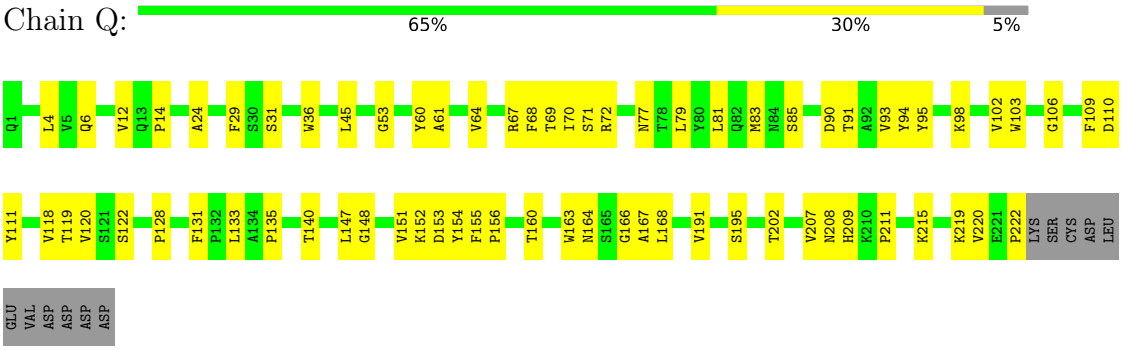
GLN V2 Q3 L4 V5 Q6 T10 L11 V12 Q13 P14 S17 L18 A24 S25 G26 F29 W36 L54 G55 G56 S57 S63 V64 K65 G66 R67 F68 R72 D73 N74 L81 Q82 M83 N84 S85 L86 T91 Y94 D99 H100 R101 V102 W103 H108 F109 D110

Y111 A116 L117 V118 T119 S122 T125 P128 F131 A134 P135 S136 S137 LYS SER THR SER GLY GLY T144 L147 V151 Y154 F155 P156 T160 V178 S186 S195 L198 T202 N208 K219 P222 K223 S224 CYS ASP LEU GLU VAL ASP

ASP ASP ASP

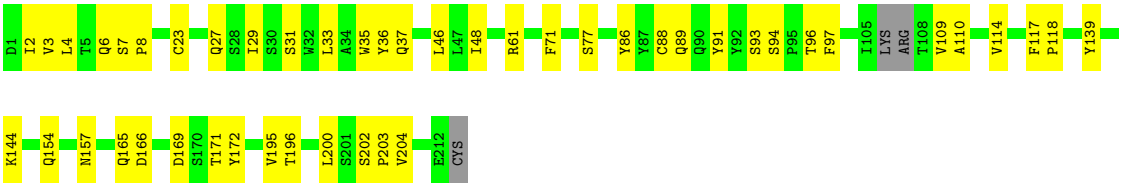
- Molecule 3: ADI-15878 Fab Heavy Chain

Chain Q:



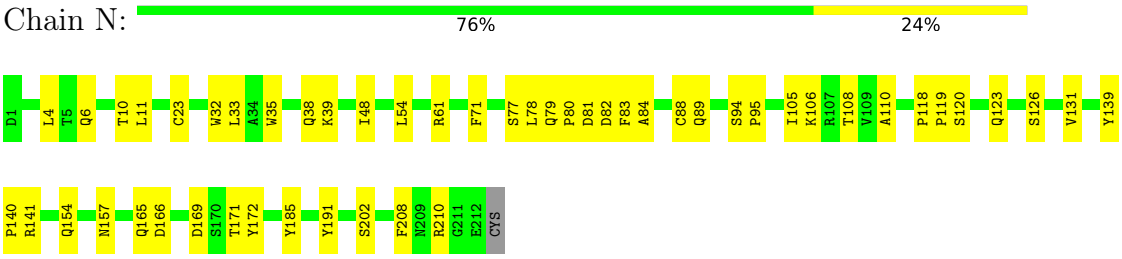

• Molecule 4: ADI-15878 Fab Light Chain

Chain L:



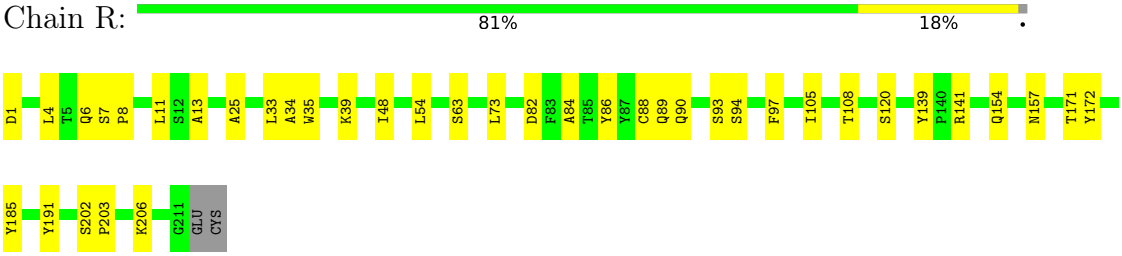

• Molecule 4: ADI-15878 Fab Light Chain

Chain N:




• Molecule 4: ADI-15878 Fab Light Chain

Chain R:




• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 31 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 151.62Å 151.62Å 247.10Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 41.26 – 4.75<br>43.77 – 4.75 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.4 (41.26-4.75)<br>99.4 (43.77-4.75) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.21 (at 4.85Å) | Xtriage |
| Refinement program | PHENIX DEV_1539 | Depositor |
| R, $R_{free}$ | 0.295 , 0.305<br>0.304 , 0.307 | Depositor<br>DCC |
| $R_{free}$ test set | 848 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 259.4 | Xtriage |
| Anisotropy | 0.392 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.24 , 161.9 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.43$, $< L^2 > = 0.25$ | Xtriage |
| Estimated twinning fraction | 0.075 for -h,-k,l | Xtriage |
| $F_o$,$F_c$ correlation | 0.86 | EDS |
| Total number of atoms | 15944 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 203.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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, MAN, BMA

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 | 0.40 | 0/1282 | 0.64 | 0/1741 |
| 1 | C | 0.38 | 0/1237 | 0.71 | 0/1683 |
| 1 | E | 0.37 | 0/1216 | 0.60 | 0/1654 |
| 2 | B | 0.36 | 0/833 | 0.65 | 0/1134 |
| 2 | D | 0.36 | 0/833 | 0.65 | 0/1134 |
| 2 | F | 0.38 | 0/828 | 0.63 | 0/1127 |
| 3 | H | 0.29 | 0/1639 | 0.52 | 0/2236 |
| 3 | M | 0.32 | 0/1666 | 0.52 | 0/2271 |
| 3 | Q | 0.30 | 0/1697 | 0.52 | 0/2314 |
| 4 | L | 0.31 | 0/1631 | 0.51 | 0/2218 |
| 4 | N | 0.31 | 0/1652 | 0.53 | 0/2246 |
| 4 | R | 0.30 | 0/1643 | 0.52 | 0/2234 |
| All | All | 0.33 | 0/16157 | 0.57 | 0/21992 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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 | 1251 | 0 | 1223 | 55 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | C | 1208 | 0 | 1180 | 72 | 0 |
| 1 | E | 1187 | 0 | 1163 | 68 | 0 |
| 2 | B | 813 | 0 | 790 | 73 | 0 |
| 2 | D | 813 | 0 | 790 | 62 | 1 |
| 2 | F | 808 | 0 | 785 | 56 | 0 |
| 3 | H | 1598 | 0 | 1560 | 50 | 0 |
| 3 | M | 1625 | 0 | 1588 | 64 | 0 |
| 3 | Q | 1655 | 0 | 1618 | 56 | 0 |
| 4 | L | 1597 | 0 | 1537 | 35 | 0 |
| 4 | N | 1617 | 0 | 1564 | 57 | 0 |
| 4 | R | 1608 | 0 | 1558 | 29 | 1 |
| 5 | G | 75 | 0 | 64 | 11 | 0 |
| 6 | I | 61 | 0 | 52 | 11 | 0 |
| 7 | A | 14 | 0 | 13 | 6 | 0 |
| 7 | B | 14 | 0 | 13 | 4 | 0 |
| All | All | 15944 | 0 | 15498 | 560 | 1 |

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 18.

All (560) 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:A:41:ASN:HB2 | 7:A:201:NAG:C8 | 1.57 | 1.32 |
| 1:E:57:LEU:HD12 | 1:E:62:GLN:NE2 | 1.50 | 1.26 |
| 2:F:563:ASN:HD21 | 5:G:1:NAG:C1 | 1.50 | 1.23 |
| 1:A:41:ASN:HB2 | 7:A:201:NAG:H81 | 1.23 | 1.11 |
| 3:M:12:VAL:HG12 | 3:M:13:GLN:H | 1.16 | 1.09 |
| 3:M:12:VAL:HG12 | 3:M:13:GLN:N | 1.69 | 1.05 |
| 3:H:12:VAL:HG12 | 3:H:13:GLN:H | 1.21 | 1.04 |
| 3:M:12:VAL:CG1 | 3:M:13:GLN:H | 1.70 | 1.04 |
| 1:A:41:ASN:HB2 | 7:A:201:NAG:H82 | 1.37 | 1.02 |
| 2:F:563:ASN:OD1 | 5:G:1:NAG:C7 | 2.11 | 0.99 |
| 3:H:12:VAL:HG12 | 3:H:13:GLN:N | 1.76 | 0.95 |
| 1:E:124:GLU:HG3 | 1:E:172:ARG:NH1 | 1.81 | 0.94 |
| 1:E:57:LEU:HD12 | 1:E:62:GLN:HE21 | 1.05 | 0.94 |
| 3:H:12:VAL:CG1 | 3:H:13:GLN:H | 1.81 | 0.92 |
| 1:C:77:THR:HB | 1:C:107:ASN:HD22 | 1.32 | 0.92 |
| 2:F:563:ASN:ND2 | 5:G:1:NAG:C1 | 2.33 | 0.91 |
| 1:A:41:ASN:CB | 7:A:201:NAG:H81 | 1.99 | 0.91 |
| 1:C:164:ARG:HB2 | 2:F:577:THR:HG21 | 1.52 | 0.90 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:563:ASN:OD1 | 5:G:1:NAG:H82 | 1.73 | 0.89 |
| 4:R:7:SER:OG | 4:R:8:PRO:HD3 | 1.74 | 0.88 |
| 2:F:527:ILE:HG13 | 4:L:94:SER:H | 1.39 | 0.87 |
| 2:D:531:TRP:CZ3 | 2:D:532:ILE:HG22 | 2.10 | 0.87 |
| 1:E:124:GLU:HG3 | 1:E:172:ARG:HH12 | 1.36 | 0.87 |
| 1:E:57:LEU:CD1 | 1:E:62:GLN:HE21 | 1.86 | 0.86 |
| 1:E:72:GLY:HA3 | 2:F:559:ARG:NH2 | 1.91 | 0.85 |
| 1:E:124:GLU:CG | 1:E:172:ARG:HH12 | 1.88 | 0.85 |
| 1:C:94:PRO:HB3 | 1:C:169:ILE:HD12 | 1.59 | 0.85 |
| 2:F:563:ASN:OD1 | 5:G:1:NAG:C8 | 2.26 | 0.84 |
| 4:N:39:LYS:HE2 | 4:N:81:ASP:OD1 | 1.79 | 0.83 |
| 1:E:57:LEU:HA | 1:E:62:GLN:HE22 | 1.43 | 0.82 |
| 2:B:592:PHE:CZ | 2:B:596:ARG:NH1 | 2.49 | 0.81 |
| 3:Q:120:VAL:HG12 | 3:Q:120:VAL:O | 1.79 | 0.81 |
| 1:E:47:ASP:HB3 | 1:E:50:LYS:HG2 | 1.63 | 0.80 |
| 3:H:128:PRO:HB3 | 3:H:154:TYR:HB3 | 1.62 | 0.80 |
| 2:B:551:GLN:HG2 | 2:B:554:LEU:HD12 | 1.64 | 0.80 |
| 1:C:72:GLY:HA3 | 2:D:559:ARG:NH2 | 1.97 | 0.80 |
| 1:A:34:PRO:HD2 | 2:B:565:THR:HG23 | 1.65 | 0.79 |
| 2:B:599:GLY:HA3 | 1:E:56:LYS:NZ | 1.97 | 0.79 |
| 1:C:184:LEU:HD11 | 2:D:561:LEU:HD23 | 1.65 | 0.79 |
| 1:A:88:PHE:HB3 | 1:A:149:GLU:HB2 | 1.62 | 0.78 |
| 4:N:39:LYS:CE | 4:N:81:ASP:OD1 | 2.31 | 0.78 |
| 1:E:94:PRO:HB3 | 1:E:169:ILE:HD12 | 1.65 | 0.78 |
| 1:E:184:LEU:HD11 | 2:F:558:LEU:HD13 | 1.63 | 0.78 |
| 1:E:50:LYS:O | 2:F:595:GLN:NE2 | 2.16 | 0.78 |
| 1:E:72:GLY:HA3 | 2:F:559:ARG:HH22 | 1.44 | 0.78 |
| 4:N:33:LEU:HD22 | 4:N:71:PHE:CD2 | 2.16 | 0.78 |
| 2:D:531:TRP:HZ3 | 1:E:157:GLY:HA3 | 1.49 | 0.78 |
| 2:D:560:GLN:O | 2:D:563:ASN:HB3 | 1.83 | 0.78 |
| 4:R:6:GLN:NE2 | 4:R:88:CYS:SG | 2.57 | 0.78 |
| 2:B:557:GLY:O | 2:B:560:GLN:HB2 | 1.83 | 0.77 |
| 1:E:124:GLU:CG | 1:E:172:ARG:NH1 | 2.49 | 0.76 |
| 4:N:33:LEU:CD2 | 4:N:71:PHE:CG | 2.69 | 0.75 |
| 1:A:41:ASN:CB | 7:A:201:NAG:C8 | 2.52 | 0.75 |
| 1:C:43:LEU:O | 1:C:43:LEU:HD12 | 1.85 | 0.75 |
| 3:H:10:THR:HB | 3:H:18:LEU:HD21 | 1.66 | 0.75 |
| 3:Q:128:PRO:HB3 | 3:Q:154:TYR:HB3 | 1.69 | 0.75 |
| 2:D:532:ILE:HD11 | 2:D:535:PHE:HB2 | 1.69 | 0.75 |
| 1:C:164:ARG:HB2 | 2:F:577:THR:CG2 | 2.17 | 0.75 |
| 1:C:99:TYR:OH | 1:C:162:TYR:O | 2.04 | 0.74 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:113:ILE:HG23 | 1:E:121:CYS:HB2 | 1.69 | 0.74 |
| 4:N:154:GLN:HB3 | 4:N:157:ASN:HD21 | 1.52 | 0.74 |
| 4:N:108:THR:HB | 4:N:139:TYR:CE2 | 2.22 | 0.74 |
| 1:A:42:THR:HG22 | 1:A:44:GLN:NE2 | 2.03 | 0.73 |
| 3:Q:53:GLY:O | 3:Q:72:ARG:NH2 | 2.21 | 0.73 |
| 2:F:563:ASN:O | 5:G:1:NAG:H82 | 1.89 | 0.73 |
| 4:L:110:ALA:H | 4:L:139:TYR:HB2 | 1.54 | 0.72 |
| 1:A:51:LEU:HD21 | 2:B:596:ARG:HG2 | 1.71 | 0.72 |
| 3:H:61:ALA:HB3 | 3:H:64:VAL:HG22 | 1.70 | 0.72 |
| 2:B:592:PHE:CE1 | 2:B:596:ARG:NH1 | 2.58 | 0.71 |
| 1:C:58:SER:OG | 1:C:62:GLN:NE2 | 2.23 | 0.71 |
| 3:Q:67:ARG:NH2 | 3:Q:90:ASP:OD2 | 2.23 | 0.71 |
| 1:C:88:PHE:HB3 | 1:C:149:GLU:HB2 | 1.72 | 0.71 |
| 3:H:12:VAL:HG12 | 3:H:13:GLN:O | 1.91 | 0.70 |
| 2:D:521:GLN:NE2 | 2:D:524:GLY:HA3 | 2.06 | 0.70 |
| 1:C:77:THR:CB | 1:C:107:ASN:HD22 | 2.04 | 0.70 |
| 4:N:33:LEU:HD23 | 4:N:71:PHE:CD1 | 2.26 | 0.70 |
| 1:A:184:LEU:HD21 | 2:B:558:LEU:HD13 | 1.74 | 0.70 |
| 1:A:39:HIS:HB3 | 1:A:42:THR:HB | 1.72 | 0.70 |
| 2:F:527:ILE:HG13 | 4:L:94:SER:N | 2.05 | 0.70 |
| 4:R:35:TRP:HB2 | 4:R:48:ILE:HG22 | 1.73 | 0.70 |
| 3:H:2:VAL:N | 3:H:27:PHE:HB2 | 2.07 | 0.70 |
| 2:D:531:TRP:CH2 | 2:D:532:ILE:HG22 | 2.27 | 0.69 |
| 2:F:563:ASN:OD1 | 5:G:1:NAG:N2 | 2.25 | 0.69 |
| 4:L:89:GLN:OE1 | 4:L:97:PHE:CE1 | 2.46 | 0.69 |
| 4:L:144:LYS:HB3 | 4:L:196:THR:HB | 1.73 | 0.69 |
| 3:M:101:ARG:NH1 | 6:I:3:BMA:C6 | 2.57 | 0.68 |
| 4:N:105:ILE:HG13 | 4:N:165:GLN:OE1 | 1.94 | 0.68 |
| 1:E:99:TYR:OH | 1:E:162:TYR:O | 2.12 | 0.68 |
| 2:F:529:LEU:HD22 | 4:L:91:TYR:CE1 | 2.29 | 0.68 |
| 3:Q:163:TRP:O | 3:Q:166:GLY:N | 2.26 | 0.67 |
| 2:B:599:GLY:HA3 | 1:E:56:LYS:HZ3 | 1.58 | 0.67 |
| 1:E:122:LEU:HB2 | 1:E:172:ARG:HG3 | 1.76 | 0.67 |
| 3:M:12:VAL:HG11 | 3:M:86:LEU:HD12 | 1.77 | 0.66 |
| 4:L:35:TRP:HB2 | 4:L:48:ILE:HG22 | 1.77 | 0.66 |
| 1:A:40:ASN:O | 7:A:201:NAG:H82 | 1.96 | 0.66 |
| 4:L:4:LEU:HD12 | 4:L:4:LEU:C | 2.16 | 0.66 |
| 3:M:72:ARG:NH1 | 3:M:74:ASN:OD1 | 2.29 | 0.66 |
| 2:F:529:LEU:HD11 | 3:H:106:GLY:HA2 | 1.78 | 0.65 |
| 3:H:102:VAL:HG11 | 3:H:106:GLY:HA3 | 1.77 | 0.65 |
| 1:C:51:LEU:HD22 | 2:D:595:GLN:HG3 | 1.78 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:90:ASP:O | 3:Q:94:TYR:OH | 2.14 | 0.65 |
| 2:D:532:ILE:CD1 | 2:D:535:PHE:HB2 | 2.27 | 0.65 |
| 2:D:531:TRP:CZ3 | 1:E:157:GLY:HA3 | 2.31 | 0.64 |
| 4:N:106:LYS:HB2 | 4:N:139:TYR:HB2 | 1.78 | 0.64 |
| 2:D:593:LEU:HD21 | 2:F:594:LEU:HD23 | 1.79 | 0.64 |
| 4:N:119:PRO:HD3 | 4:N:131:VAL:HG22 | 1.79 | 0.64 |
| 1:C:69:ASN:ND2 | 1:C:105:ALA:HB2 | 2.13 | 0.64 |
| 1:C:152:ALA:O | 1:C:169:ILE:HA | 1.97 | 0.64 |
| 1:E:147:CYS:N | 1:E:148:PRO:HD3 | 2.12 | 0.64 |
| 2:D:554:LEU:C | 2:D:554:LEU:HD23 | 2.17 | 0.64 |
| 2:B:533:PRO:HB2 | 1:C:153:PHE:CD2 | 2.33 | 0.63 |
| 3:M:135:PRO:HG3 | 3:M:147:LEU:HB3 | 1.80 | 0.63 |
| 1:C:43:LEU:HD21 | 2:D:557:GLY:HA3 | 1.80 | 0.63 |
| 1:E:52:VAL:O | 2:F:596:ARG:NH2 | 2.30 | 0.63 |
| 4:R:108:THR:H | 4:R:139:TYR:HE2 | 1.45 | 0.63 |
| 1:E:111:LEU:HD12 | 1:E:170:ILE:HG21 | 1.81 | 0.63 |
| 1:C:45:VAL:HG21 | 3:M:54:LEU:HG | 1.80 | 0.63 |
| 1:C:71:GLU:OE2 | 1:C:107:ASN:N | 2.21 | 0.63 |
| 3:M:36:TRP:CE2 | 3:M:81:LEU:HB2 | 2.34 | 0.63 |
| 3:H:10:THR:CB | 3:H:18:LEU:HD21 | 2.29 | 0.62 |
| 3:H:83:MET:HB3 | 3:H:86:LEU:HD21 | 1.81 | 0.62 |
| 1:A:66:VAL:HG22 | 1:A:101:ALA:HB3 | 1.81 | 0.62 |
| 4:N:33:LEU:HD22 | 4:N:71:PHE:CG | 2.32 | 0.62 |
| 1:A:45:VAL:HG21 | 3:H:56:GLY:CA | 2.29 | 0.62 |
| 2:B:576:THR:HG21 | 2:B:581:THR:HG21 | 1.79 | 0.62 |
| 7:B:701:NAG:H83 | 2:F:531:TRP:HH2 | 1.62 | 0.62 |
| 2:F:563:ASN:CG | 5:G:1:NAG:C7 | 2.66 | 0.62 |
| 3:Q:140:THR:HG23 | 3:Q:140:THR:O | 1.99 | 0.62 |
| 2:D:537:PRO:HG2 | 2:D:542:ILE:HG22 | 1.82 | 0.61 |
| 3:M:144:THR:N | 3:M:195:SER:HG | 1.98 | 0.61 |
| 1:A:99:TYR:OH | 1:A:162:TYR:O | 2.12 | 0.61 |
| 1:A:99:TYR:CZ | 1:A:161:LEU:HD22 | 2.37 | 0.60 |
| 2:B:536:GLY:O | 1:C:89:ARG:NH2 | 2.31 | 0.60 |
| 1:A:40:ASN:O | 1:A:40:ASN:OD1 | 2.20 | 0.60 |
| 3:H:147:LEU:HB2 | 3:H:220:VAL:HG11 | 1.84 | 0.60 |
| 1:A:182:ALA:HB2 | 2:B:562:ALA:HB2 | 1.83 | 0.60 |
| 4:L:4:LEU:HD12 | 4:L:4:LEU:O | 2.02 | 0.60 |
| 4:N:105:ILE:HG13 | 4:N:105:ILE:O | 2.01 | 0.60 |
| 2:F:558:LEU:HD12 | 2:F:558:LEU:O | 2.01 | 0.60 |
| 3:M:101:ARG:HH12 | 6:I:3:BMA:H62 | 1.68 | 0.59 |
| 1:E:55:ASP:OD1 | 2:F:596:ARG:NH2 | 2.35 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:R:4:LEU:HA | 4:R:25:ALA:HA | 1.85 | 0.59 |
| 1:A:103:GLU:HA | 2:B:517:TYR:HA | 1.84 | 0.59 |
| 2:B:563:ASN:HD21 | 7:B:701:NAG:C1 | 2.14 | 0.59 |
| 3:Q:120:VAL:O | 3:Q:120:VAL:CG1 | 2.50 | 0.59 |
| 2:D:532:ILE:HD12 | 2:D:535:PHE:HD2 | 1.67 | 0.58 |
| 2:D:561:LEU:HD13 | 3:M:54:LEU:HD23 | 1.85 | 0.58 |
| 1:C:97:VAL:HG23 | 2:D:584:ILE:HD12 | 1.84 | 0.58 |
| 3:M:125:THR:HG22 | 3:M:156:PRO:HD3 | 1.86 | 0.58 |
| 3:M:101:ARG:NH1 | 6:I:3:BMA:H62 | 2.19 | 0.58 |
| 4:N:35:TRP:HB2 | 4:N:48:ILE:HG22 | 1.85 | 0.57 |
| 3:M:103:TRP:HB3 | 6:I:1:NAG:H62 | 1.86 | 0.57 |
| 1:A:107:ASN:OD1 | 1:A:139:HIS:NE2 | 2.36 | 0.57 |
| 4:N:106:LYS:HD2 | 4:N:141:ARG:H | 1.68 | 0.57 |
| 1:C:69:ASN:HD22 | 1:C:105:ALA:HB2 | 1.69 | 0.57 |
| 2:F:576:THR:HG23 | 2:F:576:THR:O | 2.05 | 0.57 |
| 1:A:130:ARG:NH2 | 2:D:577:THR:OG1 | 2.38 | 0.57 |
| 1:E:57:LEU:HD12 | 1:E:62:GLN:HE22 | 1.61 | 0.57 |
| 1:E:89:ARG:HB3 | 1:E:153:PHE:CD1 | 2.39 | 0.57 |
| 3:H:102:VAL:HB | 3:H:106:GLY:H | 1.70 | 0.57 |
| 2:B:551:GLN:HG2 | 2:B:554:LEU:CD1 | 2.34 | 0.56 |
| 2:F:516:HIS:HA | 2:F:547:ILE:HG22 | 1.87 | 0.56 |
| 3:M:135:PRO:HD2 | 3:M:222:PRO:HB3 | 1.87 | 0.56 |
| 2:B:528:GLY:O | 2:B:531:TRP:NE1 | 2.38 | 0.56 |
| 2:B:539:ALA:HB2 | 1:C:93:PRO:HD3 | 1.87 | 0.56 |
| 2:B:548:MET:HG3 | 2:B:555:ILE:HD11 | 1.88 | 0.56 |
| 4:R:1:ASP:HB2 | 4:R:94:SER:CB | 2.35 | 0.56 |
| 1:C:154:HIS:CD2 | 1:C:156:GLU:HB2 | 2.41 | 0.56 |
| 1:C:51:LEU:HD11 | 2:D:596:ARG:CZ | 2.35 | 0.56 |
| 2:D:532:ILE:HG13 | 2:D:532:ILE:O | 2.06 | 0.56 |
| 1:E:88:PHE:HB3 | 1:E:149:GLU:HB2 | 1.88 | 0.56 |
| 1:E:96:VAL:HB | 2:F:580:ARG:HG2 | 1.87 | 0.56 |
| 4:N:105:ILE:CG1 | 4:N:165:GLN:OE1 | 2.53 | 0.56 |
| 1:A:152:ALA:O | 1:A:169:ILE:HA | 2.06 | 0.56 |
| 3:Q:168:LEU:HD21 | 3:Q:191:VAL:HG21 | 1.88 | 0.56 |
| 1:C:115:LYS:HD3 | 1:C:147:CYS:H | 1.70 | 0.55 |
| 2:B:582:PHE:CE2 | 2:D:578:GLU:HG2 | 2.40 | 0.55 |
| 1:E:57:LEU:HA | 1:E:62:GLN:NE2 | 2.17 | 0.55 |
| 4:R:1:ASP:HB2 | 4:R:94:SER:HB2 | 1.89 | 0.55 |
| 1:C:162:TYR:HB2 | 1:C:165:LEU:O | 2.05 | 0.55 |
| 4:L:29:ILE:HD11 | 4:L:33:LEU:HD12 | 1.88 | 0.55 |
| 3:Q:147:LEU:HB2 | 3:Q:220:VAL:HG11 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:164:ASN:CB | 3:Q:167:ALA:HB3 | 2.36 | 0.55 |
| 1:A:42:THR:CG2 | 1:A:44:GLN:NE2 | 2.70 | 0.55 |
| 4:N:106:LYS:HA | 4:N:139:TYR:CD2 | 2.42 | 0.55 |
| 2:B:599:GLY:HA3 | 1:E:56:LYS:HZ2 | 1.72 | 0.55 |
| 1:E:159:PHE:CZ | 2:F:570:GLN:NE2 | 2.75 | 0.54 |
| 3:M:91:THR:HG23 | 3:M:119:THR:HA | 1.90 | 0.54 |
| 2:D:521:GLN:NE2 | 2:D:524:GLY:CA | 2.69 | 0.54 |
| 2:D:531:TRP:CH2 | 2:D:532:ILE:CG2 | 2.90 | 0.54 |
| 1:A:70:LEU:HD21 | 1:A:75:VAL:HG11 | 1.88 | 0.54 |
| 2:F:560:GLN:O | 2:F:563:ASN:HB3 | 2.08 | 0.54 |
| 3:M:110:ASP:OD1 | 3:M:111:TYR:N | 2.40 | 0.54 |
| 1:E:36:GLY:HA3 | 2:F:561:LEU:HD21 | 1.89 | 0.54 |
| 4:R:33:LEU:HD22 | 4:R:89:GLN:O | 2.08 | 0.54 |
| 3:M:36:TRP:CZ2 | 3:M:81:LEU:HB2 | 2.43 | 0.54 |
| 1:A:111:LEU:HD12 | 1:A:170:ILE:HG21 | 1.90 | 0.54 |
| 2:D:521:GLN:HB3 | 2:D:524:GLY:HA3 | 1.90 | 0.53 |
| 3:H:110:ASP:OD1 | 3:H:111:TYR:N | 2.40 | 0.53 |
| 3:M:2:VAL:O | 3:M:2:VAL:HG13 | 2.08 | 0.53 |
| 3:Q:94:TYR:HE2 | 3:Q:118:VAL:HB | 1.73 | 0.53 |
| 2:B:599:GLY:O | 2:B:600:THR:C | 2.46 | 0.53 |
| 3:M:6:GLN:HB3 | 3:M:116:ALA:HB2 | 1.89 | 0.53 |
| 3:M:198:LEU:HD21 | 3:M:222:PRO:HG3 | 1.90 | 0.53 |
| 4:R:154:GLN:HB3 | 4:R:157:ASN:HD21 | 1.74 | 0.53 |
| 1:A:45:VAL:HG21 | 3:H:56:GLY:HA3 | 1.90 | 0.53 |
| 4:N:202:SER:HB3 | 4:R:11:LEU:HD13 | 1.91 | 0.53 |
| 2:B:531:TRP:CD1 | 2:D:567:GLN:HG3 | 2.44 | 0.53 |
| 3:M:4:LEU:CD2 | 3:M:24:ALA:HA | 2.39 | 0.53 |
| 1:E:112:ASP:O | 1:E:142:SER:HA | 2.08 | 0.53 |
| 4:N:48:ILE:HG13 | 4:N:54:LEU:HD23 | 1.91 | 0.53 |
| 1:A:94:PRO:HB3 | 1:A:169:ILE:HD13 | 1.90 | 0.52 |
| 1:A:130:ARG:HH11 | 1:C:93:PRO:CB | 2.21 | 0.52 |
| 1:A:95:LYS:NZ | 2:B:574:ARG:HA | 2.24 | 0.52 |
| 3:H:30:SER:HB3 | 3:H:74:ASN:HB3 | 1.90 | 0.52 |
| 1:C:96:VAL:HB | 2:D:580:ARG:HA | 1.91 | 0.52 |
| 3:Q:6:GLN:OE1 | 3:Q:6:GLN:HA | 2.08 | 0.52 |
| 1:A:159:PHE:CE2 | 2:B:566:THR:HG23 | 2.43 | 0.52 |
| 2:B:531:TRP:HE3 | 2:D:570:GLN:HG3 | 1.74 | 0.52 |
| 1:A:78:ASP:OD1 | 1:A:78:ASP:N | 2.43 | 0.52 |
| 2:D:597:TRP:CE2 | 2:F:597:TRP:HB3 | 2.44 | 0.52 |
| 1:C:77:THR:CB | 1:C:107:ASN:ND2 | 2.73 | 0.52 |
| 3:H:95:TYR:HB3 | 3:H:112:TRP:HE3 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:L:36:TYR:CZ | 4:L:46:LEU:HD23 | 2.45 | 0.52 |
| 3:M:202:THR:HB | 3:M:219:LYS:HE3 | 1.90 | 0.52 |
| 1:E:151:TYR:CG | 1:E:169:ILE:HD13 | 2.45 | 0.52 |
| 4:R:1:ASP:HB2 | 4:R:94:SER:OG | 2.09 | 0.52 |
| 3:H:160:THR:OG1 | 3:H:208:ASN:HB3 | 2.10 | 0.52 |
| 2:D:521:GLN:NE2 | 2:D:524:GLY:C | 2.64 | 0.51 |
| 2:D:531:TRP:CH2 | 1:E:156:GLU:O | 2.63 | 0.51 |
| 4:N:185:TYR:HA | 4:N:191:TYR:OH | 2.10 | 0.51 |
| 4:R:185:TYR:HA | 4:R:191:TYR:OH | 2.10 | 0.51 |
| 3:Q:93:VAL:HG11 | 3:Q:95:TYR:OH | 2.09 | 0.51 |
| 3:Q:164:ASN:HB2 | 3:Q:167:ALA:HB3 | 1.92 | 0.51 |
| 1:A:72:GLY:O | 2:B:512:ASN:HB2 | 2.10 | 0.51 |
| 3:H:12:VAL:CG1 | 3:H:16:GLY:HA3 | 2.39 | 0.51 |
| 3:H:35:SER:HB3 | 3:H:109:PHE:CZ | 2.46 | 0.51 |
| 3:Q:12:VAL:HG23 | 3:Q:120:VAL:HA | 1.92 | 0.51 |
| 2:B:563:ASN:ND2 | 7:B:701:NAG:C1 | 2.73 | 0.51 |
| 1:E:113:ILE:HG12 | 1:E:121:CYS:SG | 2.50 | 0.51 |
| 4:N:108:THR:HB | 4:N:139:TYR:CZ | 2.45 | 0.51 |
| 1:A:104:TRP:N | 2:B:516:HIS:O | 2.37 | 0.51 |
| 3:M:64:VAL:HB | 3:M:68:PHE:CD2 | 2.46 | 0.51 |
| 4:N:165:GLN:HB2 | 4:N:172:TYR:CZ | 2.46 | 0.51 |
| 2:F:510:LYS:HE3 | 5:G:2:NAG:H82 | 1.92 | 0.51 |
| 4:N:39:LYS:HE3 | 4:N:81:ASP:OD1 | 2.08 | 0.51 |
| 4:L:169:ASP:OD2 | 4:L:171:THR:OG1 | 2.21 | 0.51 |
| 4:R:82:ASP:O | 4:R:86:TYR:OH | 2.24 | 0.51 |
| 1:C:95:LYS:NZ | 2:D:574:ARG:HA | 2.26 | 0.51 |
| 3:M:14:PRO:HD3 | 3:M:122:SER:HB2 | 1.93 | 0.51 |
| 1:E:33:ILE:HB | 2:F:588:LYS:CE | 2.41 | 0.51 |
| 4:N:11:LEU:HD13 | 4:R:202:SER:HB3 | 1.93 | 0.50 |
| 2:D:515:LEU:CB | 2:D:555:ILE:HD12 | 2.42 | 0.50 |
| 3:Q:110:ASP:OD1 | 3:Q:111:TYR:N | 2.44 | 0.50 |
| 3:Q:93:VAL:CG1 | 3:Q:95:TYR:CZ | 2.94 | 0.50 |
| 1:A:39:HIS:HB2 | 1:A:44:GLN:OE1 | 2.12 | 0.50 |
| 4:N:6:GLN:NE2 | 4:N:88:CYS:SG | 2.85 | 0.50 |
| 4:L:6:GLN:NE2 | 4:L:88:CYS:SG | 2.84 | 0.50 |
| 4:L:31:SER:HA | 4:L:71:PHE:HZ | 1.76 | 0.50 |
| 3:M:94:TYR:HE2 | 3:M:118:VAL:HB | 1.76 | 0.50 |
| 2:B:544:THR:HG22 | 2:B:545:GLU:N | 2.26 | 0.50 |
| 1:C:77:THR:HB | 1:C:107:ASN:ND2 | 2.14 | 0.50 |
| 3:M:99:ASP:HA | 3:M:108:HIS:O | 2.12 | 0.50 |
| 1:C:34:PRO:HG3 | 3:M:57:SER:OG | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:182:ALA:HB2 | 2:F:562:ALA:HB2 | 1.93 | 0.50 |
| 3:Q:202:THR:HB | 3:Q:219:LYS:HE3 | 1.94 | 0.50 |
| 1:C:182:ALA:HB2 | 2:D:562:ALA:HA | 1.94 | 0.49 |
| 3:M:12:VAL:CG1 | 3:M:13:GLN:N | 2.34 | 0.49 |
| 2:B:603:ILE:HG12 | 2:B:610:ILE:HG21 | 1.94 | 0.49 |
| 2:D:528:GLY:O | 2:D:529:LEU:HB3 | 2.12 | 0.49 |
| 2:B:594:LEU:HD22 | 1:E:57:LEU:HB3 | 1.93 | 0.49 |
| 4:L:3:VAL:HG23 | 4:L:96:THR:HG21 | 1.93 | 0.49 |
| 1:A:45:VAL:CG2 | 3:H:56:GLY:CA | 2.90 | 0.49 |
| 4:N:38:GLN:O | 4:N:84:ALA:HB1 | 2.12 | 0.49 |
| 2:B:593:LEU:HD21 | 2:D:594:LEU:HD23 | 1.94 | 0.49 |
| 1:C:97:VAL:HG13 | 1:C:166:ALA:HB3 | 1.95 | 0.49 |
| 3:M:10:THR:OG1 | 3:M:117:LEU:O | 2.27 | 0.49 |
| 3:M:12:VAL:HG13 | 3:M:13:GLN:H | 1.71 | 0.49 |
| 2:B:513:PRO:O | 2:B:555:ILE:HG21 | 2.13 | 0.49 |
| 1:C:183:PHE:C | 1:C:184:LEU:HD12 | 2.33 | 0.49 |
| 3:Q:93:VAL:HG12 | 3:Q:95:TYR:CZ | 2.47 | 0.49 |
| 3:Q:207:VAL:O | 3:Q:215:LYS:HA | 2.13 | 0.49 |
| 3:H:10:THR:HB | 3:H:18:LEU:CD2 | 2.39 | 0.49 |
| 4:L:109:VAL:HA | 4:L:139:TYR:HB2 | 1.95 | 0.49 |
| 3:Q:12:VAL:CG2 | 3:Q:120:VAL:HG22 | 2.42 | 0.49 |
| 4:R:1:ASP:CB | 4:R:94:SER:OG | 2.61 | 0.49 |
| 2:B:527:ILE:HG12 | 4:N:94:SER:N | 2.28 | 0.48 |
| 1:C:38:VAL:O | 1:C:187:PRO:HG3 | 2.13 | 0.48 |
| 1:E:160:PHE:CE2 | 1:E:170:ILE:HG12 | 2.48 | 0.48 |
| 4:N:139:TYR:CE1 | 4:N:171:THR:HG22 | 2.48 | 0.48 |
| 1:A:184:LEU:HD21 | 2:B:558:LEU:CD1 | 2.42 | 0.48 |
| 2:B:529:LEU:HD21 | 4:N:32:TRP:CG | 2.47 | 0.48 |
| 3:M:100:HIS:HB3 | 3:M:108:HIS:HB3 | 1.95 | 0.48 |
| 3:Q:156:PRO:HD2 | 3:Q:211:PRO:HG2 | 1.94 | 0.48 |
| 2:D:531:TRP:CZ3 | 2:D:532:ILE:CG2 | 2.91 | 0.48 |
| 4:L:165:GLN:HG2 | 4:L:172:TYR:CE2 | 2.49 | 0.48 |
| 1:A:162:TYR:HB2 | 1:A:165:LEU:O | 2.14 | 0.48 |
| 1:C:33:ILE:HB | 2:D:588:LYS:CE | 2.43 | 0.48 |
| 3:M:67:ARG:HB2 | 3:M:85:SER:HB2 | 1.94 | 0.48 |
| 1:E:99:TYR:CZ | 1:E:161:LEU:HD22 | 2.49 | 0.48 |
| 4:L:2:ILE:CG2 | 4:L:27:GLN:CD | 2.82 | 0.48 |
| 3:M:83:MET:HB3 | 3:M:86:LEU:HD21 | 1.94 | 0.48 |
| 3:Q:91:THR:HG23 | 3:Q:119:THR:HA | 1.94 | 0.48 |
| 3:H:64:VAL:HB | 3:H:68:PHE:CD2 | 2.48 | 0.48 |
| 2:B:527:ILE:HG12 | 4:N:94:SER:HA | 1.96 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:F:572:PHE:CE2 | 2:F:584:ILE:HG12 | 2.48 | 0.48 |
| 4:N:108:THR:O | 4:N:139:TYR:CD2 | 2.66 | 0.48 |
| 3:Q:14:PRO:HD3 | 3:Q:122:SER:HB2 | 1.96 | 0.48 |
| 4:R:90:GLN:NE2 | 4:R:94:SER:O | 2.47 | 0.48 |
| 4:N:10:THR:O | 4:R:203:PRO:HD2 | 2.14 | 0.48 |
| 1:C:33:ILE:HB | 2:D:588:LYS:HE3 | 1.95 | 0.48 |
| 3:Q:147:LEU:HD13 | 3:Q:220:VAL:HG21 | 1.94 | 0.48 |
| 6:I:3:BMA:H62 | 6:I:5:MAN:H2 | 1.49 | 0.47 |
| 1:C:99:TYR:HD2 | 1:C:101:ALA:O | 1.97 | 0.47 |
| 3:Q:4:LEU:HD23 | 3:Q:24:ALA:HA | 1.95 | 0.47 |
| 1:A:165:LEU:HG | 2:D:577:THR:HG21 | 1.97 | 0.47 |
| 2:B:560:GLN:HG2 | 3:H:103:TRP:CZ2 | 2.49 | 0.47 |
| 2:B:563:ASN:ND2 | 3:H:103:TRP:CZ3 | 2.82 | 0.47 |
| 2:B:567:GLN:HA | 2:F:531:TRP:CD2 | 2.49 | 0.47 |
| 2:B:571:LEU:CD1 | 2:F:526:ALA:HB2 | 2.44 | 0.47 |
| 1:A:130:ARG:HD3 | 1:A:163:ASP:OD2 | 2.14 | 0.47 |
| 3:Q:135:PRO:HG2 | 3:Q:222:PRO:HB3 | 1.95 | 0.47 |
| 2:B:551:GLN:HG2 | 2:B:554:LEU:CG | 2.45 | 0.47 |
| 2:D:511:CYS:O | 2:D:513:PRO:HD3 | 2.15 | 0.47 |
| 1:E:98:ASN:HB3 | 2:F:582:PHE:CE2 | 2.50 | 0.47 |
| 3:H:4:LEU:HA | 3:H:23:ALA:O | 2.15 | 0.47 |
| 3:H:40:ALA:HB3 | 3:H:43:LYS:HB2 | 1.96 | 0.47 |
| 2:D:531:TRP:CZ3 | 1:E:156:GLU:O | 2.67 | 0.47 |
| 5:G:3:BMA:H62 | 5:G:6:MAN:H2 | 1.49 | 0.47 |
| 3:H:61:ALA:HB3 | 3:H:64:VAL:CG2 | 2.44 | 0.47 |
| 4:N:106:LYS:HD2 | 4:N:140:PRO:HA | 1.97 | 0.47 |
| 3:Q:60:TYR:CZ | 3:Q:70:ILE:HG22 | 2.49 | 0.47 |
| 1:E:89:ARG:HA | 1:E:149:GLU:HG3 | 1.97 | 0.47 |
| 3:M:63:SER:O | 3:M:67:ARG:NH1 | 2.47 | 0.47 |
| 4:L:200:LEU:HD13 | 4:L:204:VAL:HG23 | 1.97 | 0.46 |
| 3:M:131:PHE:HB3 | 4:N:120:SER:OG | 2.15 | 0.46 |
| 4:N:78:LEU:HD12 | 4:N:82:ASP:OD2 | 2.15 | 0.46 |
| 4:N:118:PRO:HB3 | 4:N:208:PHE:CE2 | 2.51 | 0.46 |
| 1:C:51:LEU:HD21 | 2:D:596:ARG:HG2 | 1.98 | 0.46 |
| 3:H:202:THR:HB | 3:H:219:LYS:HE3 | 1.96 | 0.46 |
| 3:M:101:ARG:CZ | 6:I:3:BMA:H61 | 2.46 | 0.46 |
| 1:A:69:ASN:ND2 | 1:A:105:ALA:HB2 | 2.30 | 0.46 |
| 2:B:570:GLN:HB2 | 2:F:531:TRP:HB2 | 1.97 | 0.46 |
| 1:C:65:SER:HB3 | 2:D:585:LEU:HD21 | 1.96 | 0.46 |
| 2:D:554:LEU:HD23 | 2:D:554:LEU:O | 2.16 | 0.46 |
| 1:E:57:LEU:CD1 | 1:E:62:GLN:NE2 | 2.45 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:M:101:ARG:NH1 | 6:I:3:BMA:C5 | 2.78 | 0.46 |
| 4:N:110:ALA:N | 4:N:139:TYR:O | 2.43 | 0.46 |
| 1:C:111:LEU:HD12 | 1:C:170:ILE:HG21 | 1.97 | 0.46 |
| 1:E:35:LEU:HD21 | 1:E:185:ILE:HD11 | 1.97 | 0.46 |
| 3:H:51:ILE:HD13 | 3:H:72:ARG:HG2 | 1.97 | 0.46 |
| 3:M:14:PRO:HD3 | 3:M:122:SER:CB | 2.46 | 0.46 |
| 3:Q:29:PHE:CD2 | 3:Q:77:ASN:HA | 2.51 | 0.46 |
| 4:R:48:ILE:HG13 | 4:R:54:LEU:HD23 | 1.96 | 0.46 |
| 4:N:33:LEU:CD2 | 4:N:71:PHE:CD1 | 2.93 | 0.46 |
| 2:B:572:PHE:O | 2:B:576:THR:HG22 | 2.16 | 0.46 |
| 4:R:141:ARG:HB2 | 4:R:172:TYR:CE1 | 2.50 | 0.46 |
| 2:B:570:GLN:HG3 | 2:F:531:TRP:HE3 | 1.80 | 0.46 |
| 2:F:588:LYS:HA | 2:F:588:LYS:HD3 | 1.74 | 0.46 |
| 3:H:128:PRO:HB2 | 3:H:151:VAL:HG13 | 1.98 | 0.46 |
| 1:E:162:TYR:HB2 | 1:E:165:LEU:O | 2.15 | 0.46 |
| 3:H:91:THR:HG23 | 3:H:119:THR:HA | 1.97 | 0.46 |
| 3:Q:67:ARG:HD2 | 3:Q:85:SER:HB2 | 1.97 | 0.46 |
| 1:A:70:LEU:N | 1:A:178:GLU:O | 2.44 | 0.46 |
| 2:B:528:GLY:C | 2:B:531:TRP:HE1 | 2.19 | 0.46 |
| 4:L:109:VAL:HA | 4:L:139:TYR:CB | 2.46 | 0.46 |
| 1:E:113:ILE:CG2 | 1:E:121:CYS:HB2 | 2.44 | 0.45 |
| 1:C:182:ALA:HB2 | 2:D:562:ALA:CA | 2.46 | 0.45 |
| 3:Q:14:PRO:HD3 | 3:Q:122:SER:CB | 2.45 | 0.45 |
| 2:B:531:TRP:HB2 | 2:D:570:GLN:HB2 | 1.97 | 0.45 |
| 2:B:564:GLU:OE1 | 3:H:52:SER:HB2 | 2.17 | 0.45 |
| 2:F:537:PRO:HG2 | 2:F:542:ILE:HG22 | 1.97 | 0.45 |
| 3:Q:128:PRO:HB2 | 3:Q:151:VAL:HG13 | 1.99 | 0.45 |
| 3:Q:154:TYR:HB2 | 3:Q:209:HIS:CD2 | 2.52 | 0.45 |
| 1:E:34:PRO:HD2 | 2:F:565:THR:HG23 | 1.98 | 0.45 |
| 4:L:117:PHE:HA | 4:L:118:PRO:HD3 | 1.72 | 0.45 |
| 4:N:4:LEU:HD13 | 4:N:23:CYS:SG | 2.57 | 0.45 |
| 3:Q:164:ASN:HB3 | 3:Q:167:ALA:HB3 | 1.99 | 0.45 |
| 2:D:596:ARG:HD3 | 2:D:609:CYS:SG | 2.57 | 0.45 |
| 3:H:164:ASN:HB3 | 3:H:167:ALA:HB3 | 1.98 | 0.45 |
| 3:M:10:THR:HB | 3:M:18:LEU:HD21 | 1.99 | 0.45 |
| 4:N:33:LEU:HD12 | 4:N:89:GLN:O | 2.17 | 0.45 |
| 4:N:106:LYS:O | 4:N:106:LYS:HG3 | 2.17 | 0.45 |
| 3:Q:69:THR:O | 3:Q:81:LEU:HD12 | 2.17 | 0.45 |
| 1:C:86:TRP:CD1 | 1:C:154:HIS:ND1 | 2.85 | 0.45 |
| 1:A:34:PRO:HB2 | 2:B:561:LEU:HD11 | 1.99 | 0.45 |
| 2:B:551:GLN:HG2 | 2:B:554:LEU:HB2 | 1.97 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:587:ARG:HG3 | 1:E:60:THR:HG21 | 1.99 | 0.45 |
| 1:C:49:ASP:OD1 | 1:C:50:LYS:N | 2.50 | 0.45 |
| 3:H:94:TYR:HE1 | 3:H:118:VAL:HB | 1.81 | 0.45 |
| 3:M:67:ARG:HD2 | 3:M:85:SER:O | 2.17 | 0.45 |
| 1:C:70:LEU:HD12 | 1:C:178:GLU:OE1 | 2.17 | 0.45 |
| 3:M:128:PRO:HB2 | 3:M:151:VAL:HG13 | 1.98 | 0.45 |
| 3:M:178:VAL:HG22 | 3:M:186:SER:O | 2.16 | 0.45 |
| 1:C:132:PHE:HB3 | 1:C:135:CYS:SG | 2.57 | 0.45 |
| 2:D:531:TRP:CE2 | 2:D:532:ILE:HG23 | 2.51 | 0.45 |
| 1:A:133:PRO:HB3 | 2:B:543:TYR:CE2 | 2.52 | 0.44 |
| 3:M:2:VAL:N | 3:M:26:GLY:HA3 | 2.32 | 0.44 |
| 4:R:13:ALA:O | 4:R:105:ILE:HA | 2.17 | 0.44 |
| 1:C:37:VAL:HG22 | 1:C:44:GLN:O | 2.17 | 0.44 |
| 4:R:33:LEU:HD13 | 4:R:34:ALA:N | 2.33 | 0.44 |
| 3:M:6:GLN:HE22 | 3:M:36:TRP:HZ3 | 1.66 | 0.44 |
| 4:N:166:ASP:HB2 | 4:N:169:ASP:OD1 | 2.16 | 0.44 |
| 3:M:160:THR:OG1 | 3:M:208:ASN:HB3 | 2.17 | 0.44 |
| 3:Q:155:PHE:HA | 3:Q:156:PRO:HA | 1.76 | 0.44 |
| 4:R:63:SER:O | 4:R:73:LEU:HD12 | 2.18 | 0.44 |
| 2:B:578:GLU:HG3 | 2:F:582:PHE:CE1 | 2.52 | 0.44 |
| 2:D:515:LEU:HB2 | 2:D:555:ILE:HD12 | 1.98 | 0.44 |
| 1:E:130:ARG:HH21 | 1:E:164:ARG:HH11 | 1.65 | 0.44 |
| 4:N:33:LEU:HD23 | 4:N:71:PHE:CG | 2.46 | 0.44 |
| 4:N:139:TYR:HA | 4:N:140:PRO:C | 2.38 | 0.44 |
| 3:M:13:GLN:HB3 | 3:M:14:PRO:HD2 | 1.99 | 0.44 |
| 4:R:39:LYS:HG2 | 4:R:84:ALA:HB2 | 1.99 | 0.44 |
| 1:C:35:LEU:HD21 | 1:C:185:ILE:HD11 | 2.00 | 0.44 |
| 1:C:45:VAL:CG2 | 3:M:54:LEU:HG | 2.46 | 0.44 |
| 4:N:123:GLN:O | 4:N:126:SER:OG | 2.27 | 0.44 |
| 1:A:191:LYS:HE2 | 3:M:65:LYS:NZ | 2.32 | 0.44 |
| 2:B:539:ALA:O | 2:B:542:ILE:HG12 | 2.17 | 0.44 |
| 2:B:567:GLN:HG3 | 2:F:531:TRP:CD1 | 2.53 | 0.44 |
| 3:Q:152:LYS:HG2 | 3:Q:153:ASP:OD1 | 2.17 | 0.44 |
| 7:B:701:NAG:C8 | 2:F:531:TRP:HH2 | 2.30 | 0.44 |
| 1:C:94:PRO:CB | 1:C:169:ILE:HD12 | 2.39 | 0.44 |
| 4:L:166:ASP:HB2 | 4:L:169:ASP:OD1 | 2.17 | 0.44 |
| 3:Q:133:LEU:HD12 | 3:Q:148:GLY:HA3 | 2.00 | 0.44 |
| 3:Q:160:THR:HG23 | 3:Q:208:ASN:HB3 | 2.00 | 0.43 |
| 3:M:83:MET:HE1 | 3:M:118:VAL:HG21 | 2.00 | 0.43 |
| 3:Q:131:PHE:HB3 | 4:R:120:SER:OG | 2.17 | 0.43 |
| 4:R:206:LYS:HA | 4:R:206:LYS:HD3 | 1.83 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:98:LYS:O | 3:Q:109:PHE:HA | 2.19 | 0.43 |
| 1:C:99:TYR:CZ | 1:C:161:LEU:HD22 | 2.53 | 0.43 |
| 4:N:80:PRO:HA | 4:N:83:PHE:CE2 | 2.52 | 0.43 |
| 2:B:523:GLU:OE1 | 2:B:526:ALA:HB2 | 2.17 | 0.43 |
| 2:D:563:ASN:HD21 | 6:I:1:NAG:C1 | 2.32 | 0.43 |
| 4:L:61:ARG:HD2 | 4:L:77:SER:O | 2.19 | 0.43 |
| 3:M:17:SER:HA | 3:M:83:MET:O | 2.19 | 0.43 |
| 2:B:527:ILE:HG13 | 4:N:95:PRO:HD3 | 2.00 | 0.43 |
| 1:C:77:THR:OG1 | 1:C:107:ASN:ND2 | 2.52 | 0.43 |
| 1:E:78:ASP:N | 1:E:78:ASP:OD1 | 2.51 | 0.43 |
| 4:N:154:GLN:HB3 | 4:N:157:ASN:ND2 | 2.27 | 0.43 |
| 2:B:531:TRP:CD2 | 2:D:567:GLN:HA | 2.54 | 0.43 |
| 3:H:155:PHE:HA | 3:H:156:PRO:HA | 1.72 | 0.43 |
| 3:Q:12:VAL:HG21 | 3:Q:120:VAL:HG22 | 2.00 | 0.43 |
| 2:F:527:ILE:HG13 | 4:L:93:SER:HA | 2.01 | 0.43 |
| 1:A:68:LEU:HD11 | 2:B:558:LEU:HG | 2.01 | 0.43 |
| 4:L:4:LEU:C | 4:L:4:LEU:CD1 | 2.85 | 0.43 |
| 4:N:4:LEU:HD12 | 4:N:4:LEU:C | 2.39 | 0.43 |
| 4:R:202:SER:HA | 4:R:203:PRO:HD2 | 1.89 | 0.43 |
| 1:E:69:ASN:ND2 | 1:E:105:ALA:HB2 | 2.34 | 0.43 |
| 3:Q:31:SER:HG | 3:Q:103:TRP:HE1 | 1.67 | 0.43 |
| 1:A:74:GLY:HA3 | 2:B:510:LYS:HB2 | 2.00 | 0.42 |
| 1:C:156:GLU:HG2 | 6:I:2:NAG:H61 | 2.01 | 0.42 |
| 2:D:521:GLN:HE21 | 2:D:524:GLY:HA3 | 1.82 | 0.42 |
| 1:E:33:ILE:HD11 | 2:F:572:PHE:CG | 2.52 | 0.42 |
| 4:L:7:SER:OG | 4:L:8:PRO:HD3 | 2.18 | 0.42 |
| 3:Q:68:PHE:CE1 | 3:Q:83:MET:HB3 | 2.53 | 0.42 |
| 2:B:517:TYR:CZ | 2:B:546:GLY:HA3 | 2.54 | 0.42 |
| 2:B:592:PHE:CE2 | 2:B:596:ARG:NH1 | 2.79 | 0.42 |
| 1:C:88:PHE:CB | 1:C:149:GLU:HB2 | 2.47 | 0.42 |
| 1:C:108:CYS:HB3 | 1:C:175:THR:CG2 | 2.50 | 0.42 |
| 3:Q:163:TRP:O | 3:Q:164:ASN:C | 2.55 | 0.42 |
| 2:B:577:THR:HG21 | 1:E:164:ARG:O | 2.19 | 0.42 |
| 1:E:49:ASP:OD1 | 1:E:50:LYS:N | 2.52 | 0.42 |
| 3:H:36:TRP:CZ2 | 3:H:79:LEU:HG | 2.55 | 0.42 |
| 3:Q:36:TRP:CE2 | 3:Q:81:LEU:HB2 | 2.54 | 0.42 |
| 1:A:39:HIS:CB | 1:A:44:GLN:HE22 | 2.32 | 0.42 |
| 4:N:61:ARG:HD2 | 4:N:77:SER:O | 2.20 | 0.42 |
| 2:F:532:ILE:HA | 2:F:533:PRO:HD3 | 1.86 | 0.42 |
| 3:H:157:GLU:HB3 | 3:H:158:PRO:HA | 2.01 | 0.42 |
| 3:Q:61:ALA:HB3 | 3:Q:64:VAL:HG22 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Q:91:THR:HG23 | 3:Q:118:VAL:O | 2.20 | 0.42 |
| 3:M:12:VAL:CG2 | 3:M:18:LEU:HD22 | 2.50 | 0.42 |
| 3:Q:60:TYR:OH | 3:Q:70:ILE:HG22 | 2.20 | 0.42 |
| 3:Q:140:THR:HB | 3:Q:195:SER:CB | 2.50 | 0.42 |
| 1:A:33:ILE:HA | 1:A:34:PRO:HD3 | 1.75 | 0.42 |
| 1:A:39:HIS:HB2 | 1:A:44:GLN:HE22 | 1.85 | 0.42 |
| 1:E:132:PHE:HA | 1:E:133:PRO:HD3 | 1.91 | 0.42 |
| 3:H:147:LEU:HD13 | 3:H:220:VAL:HG21 | 2.01 | 0.42 |
| 3:M:29:PHE:HE1 | 3:M:72:ARG:NH1 | 2.18 | 0.42 |
| 1:A:89:ARG:HB3 | 1:A:153:PHE:CD1 | 2.55 | 0.42 |
| 1:C:90:ALA:N | 1:C:149:GLU:HG2 | 2.35 | 0.42 |
| 1:C:114:LYS:HE3 | 1:C:120:GLU:OE2 | 2.20 | 0.42 |
| 1:A:45:VAL:CG2 | 3:H:56:GLY:HA3 | 2.50 | 0.42 |
| 1:E:147:CYS:N | 1:E:148:PRO:CD | 2.82 | 0.42 |
| 1:E:151:TYR:CB | 1:E:169:ILE:HD13 | 2.50 | 0.42 |
| 4:N:106:LYS:NZ | 4:N:140:PRO:HB3 | 2.35 | 0.42 |
| 4:R:139:TYR:CE1 | 4:R:171:THR:HG22 | 2.55 | 0.42 |
| 1:A:51:LEU:HD11 | 2:B:596:ARG:CG | 2.50 | 0.41 |
| 1:C:69:ASN:N | 1:C:69:ASN:OD1 | 2.53 | 0.41 |
| 1:C:165:LEU:HD21 | 2:F:577:THR:OG1 | 2.20 | 0.41 |
| 2:D:561:LEU:HD13 | 3:M:54:LEU:CD2 | 2.50 | 0.41 |
| 4:L:4:LEU:HD21 | 4:L:88:CYS:O | 2.19 | 0.41 |
| 4:L:139:TYR:CZ | 4:L:171:THR:HG22 | 2.55 | 0.41 |
| 2:B:525:ALA:HB1 | 2:B:527:ILE:HD13 | 2.02 | 0.41 |
| 1:C:156:GLU:OE2 | 6:I:1:NAG:O3 | 2.38 | 0.41 |
| 2:D:530:ALA:HB1 | 2:D:537:PRO:HD3 | 2.02 | 0.41 |
| 3:H:161:VAL:HG11 | 3:H:189:SER:CB | 2.51 | 0.41 |
| 4:N:78:LEU:HD11 | 4:N:82:ASP:HB2 | 2.02 | 0.41 |
| 1:C:45:VAL:HG11 | 3:M:56:GLY:CA | 2.51 | 0.41 |
| 3:M:2:VAL:O | 3:M:2:VAL:HG22 | 2.19 | 0.41 |
| 1:C:33:ILE:HA | 1:C:34:PRO:HD3 | 1.87 | 0.41 |
| 1:C:45:VAL:HG11 | 3:M:56:GLY:HA3 | 2.02 | 0.41 |
| 1:E:182:ALA:HB2 | 2:F:562:ALA:CB | 2.50 | 0.41 |
| 3:H:30:SER:HA | 3:H:72:ARG:NH2 | 2.36 | 0.41 |
| 5:G:5:NAG:O7 | 5:G:5:NAG:H3 | 2.20 | 0.41 |
| 2:B:531:TRP:HB2 | 2:D:570:GLN:CB | 2.49 | 0.41 |
| 2:B:551:GLN:CG | 2:B:554:LEU:HB2 | 2.50 | 0.41 |
| 1:E:151:TYR:HB3 | 1:E:169:ILE:HD13 | 2.02 | 0.41 |
| 3:H:86:LEU:CB | 3:H:120:VAL:HG11 | 2.51 | 0.41 |
| 4:N:61:ARG:CZ | 4:N:79:GLN:HG3 | 2.51 | 0.41 |
| 1:A:147:CYS:N | 1:A:148:PRO:CD | 2.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:89:ARG:NE | 1:E:90:ALA:O | 2.53 | 0.41 |
| 3:H:14:PRO:HD3 | 3:H:122:SER:HB2 | 2.03 | 0.41 |
| 3:M:134:ALA:HA | 3:M:135:PRO:HD3 | 1.75 | 0.41 |
| 1:A:96:VAL:HB | 2:B:580:ARG:HG2 | 2.02 | 0.41 |
| 2:D:532:ILE:HD12 | 2:D:535:PHE:CD2 | 2.52 | 0.41 |
| 2:D:554:LEU:C | 2:D:554:LEU:CD2 | 2.85 | 0.41 |
| 2:F:527:ILE:CG1 | 4:L:93:SER:HA | 2.51 | 0.41 |
| 3:H:208:ASN:OD1 | 3:H:215:LYS:HG2 | 2.21 | 0.41 |
| 1:E:33:ILE:HB | 2:F:588:LYS:HE3 | 2.01 | 0.41 |
| 1:E:95:LYS:NZ | 2:F:574:ARG:HA | 2.36 | 0.41 |
| 1:E:125:ALA:HA | 1:E:126:PRO:HD3 | 1.84 | 0.41 |
| 4:L:33:LEU:HD21 | 4:L:88:CYS:HB2 | 2.02 | 0.41 |
| 4:L:114:VAL:HG22 | 4:L:195:VAL:HG21 | 2.03 | 0.41 |
| 3:M:12:VAL:HG23 | 3:M:18:LEU:HD22 | 2.02 | 0.41 |
| 4:N:78:LEU:CD1 | 4:N:82:ASP:HB2 | 2.50 | 0.41 |
| 3:Q:45:LEU:HB2 | 4:R:97:PHE:CG | 2.56 | 0.41 |
| 4:R:82:ASP:N | 4:R:82:ASP:OD1 | 2.53 | 0.41 |
| 1:C:57:LEU:HD12 | 1:C:62:GLN:OE1 | 2.21 | 0.41 |
| 3:H:12:VAL:CG1 | 3:H:13:GLN:N | 2.43 | 0.41 |
| 4:L:4:LEU:HD22 | 4:L:23:CYS:SG | 2.61 | 0.41 |
| 4:L:37:GLN:HB2 | 4:L:86:TYR:HE1 | 1.86 | 0.41 |
| 3:M:12:VAL:HG12 | 3:M:13:GLN:O | 2.21 | 0.41 |
| 3:Q:64:VAL:HB | 3:Q:68:PHE:CD2 | 2.56 | 0.41 |
| 3:Q:102:VAL:HG21 | 3:Q:106:GLY:CA | 2.51 | 0.41 |
| 2:B:527:ILE:HG12 | 4:N:94:SER:CA | 2.51 | 0.40 |
| 1:C:72:GLY:HA3 | 2:D:559:ARG:HH22 | 1.79 | 0.40 |
| 1:C:94:PRO:O | 1:C:95:LYS:HD3 | 2.21 | 0.40 |
| 4:L:202:SER:HA | 4:L:203:PRO:HD2 | 1.89 | 0.40 |
| 4:N:39:LYS:HG2 | 4:N:84:ALA:HB2 | 2.03 | 0.40 |
| 4:N:106:LYS:HZ2 | 4:N:140:PRO:HB3 | 1.86 | 0.40 |
| 2:B:512:ASN:HA | 2:B:513:PRO:HD3 | 1.87 | 0.40 |
| 1:C:56:LYS:HG2 | 2:F:599:GLY:HA2 | 2.03 | 0.40 |
| 1:C:148:PRO:HB2 | 1:C:149:GLU:OE1 | 2.20 | 0.40 |
| 1:C:161:LEU:HD23 | 1:C:161:LEU:HA | 1.92 | 0.40 |
| 2:F:529:LEU:HD21 | 3:H:106:GLY:HA2 | 2.04 | 0.40 |
| 3:M:29:PHE:CE1 | 3:M:72:ARG:HD2 | 2.56 | 0.40 |
| 1:C:95:LYS:HB3 | 2:D:573:LEU:HB3 | 2.04 | 0.40 |
| 3:M:101:ARG:CZ | 6:I:3:BMA:C6 | 2.99 | 0.40 |
| 3:Q:36:TRP:CZ2 | 3:Q:79:LEU:HG | 2.56 | 0.40 |
| 1:A:194:PHE:CE1 | 2:B:519:THR:HG21 | 2.57 | 0.40 |
| 2:D:537:PRO:HD2 | 2:F:574:ARG:NH2 | 2.37 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:52:VAL:HB | 1:E:55:ASP:OD2 | 2.21 | 0.40 |
| 3:H:6:GLN:HE22 | 3:H:95:TYR:HA | 1.87 | 0.40 |
| 4:L:154:GLN:HB3 | 4:L:157:ASN:HD21 | 1.86 | 0.40 |
| 3:Q:71:SER:O | 3:Q:79:LEU:HD12 | 2.22 | 0.40 |
| 2:B:531:TRP:CE3 | 2:D:570:GLN:HG3 | 2.56 | 0.40 |
| 1:C:183:PHE:O | 1:C:184:LEU:HD12 | 2.21 | 0.40 |
| 1:E:149:GLU:HA | 1:E:149:GLU:OE1 | 2.22 | 0.40 |
| 3:M:128:PRO:HB3 | 3:M:154:TYR:HB3 | 2.03 | 0.40 |
| 4:N:185:TYR:CZ | 4:N:210:ARG:HG3 | 2.57 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:D:527:ILE:CB | 4:R:93:SER:O[2_565] | 1.99 | 0.21 |

## 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 | 160/162 (99%) | 156 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | C | 156/162 (96%) | 152 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | E | 153/162 (94%) | 147 (96%) | 6 (4%) | 0 | 100 | 100 |
| 2 | B | 102/111 (92%) | 96 (94%) | 6 (6%) | 0 | 100 | 100 |
| 2 | D | 102/111 (92%) | 98 (96%) | 4 (4%) | 0 | 100 | 100 |
| 2 | F | 101/111 (91%) | 97 (96%) | 4 (4%) | 0 | 100 | 100 |
| 3 | H | 209/233 (90%) | 204 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | M | 213/233 (91%) | 206 (97%) | 7 (3%) | 0 | 100 | 100 |
| 3 | Q | 220/233 (94%) | 214 (97%) | 6 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 4 | L | 206/213 (97%) | 198 (96%) | 8 (4%) | 0 | 100 | 100 |
| 4 | N | 210/213 (99%) | 201 (96%) | 9 (4%) | 0 | 100 | 100 |
| 4 | R | 209/213 (98%) | 205 (98%) | 4 (2%) | 0 | 100 | 100 |
| All | All | 2041/2157 (95%) | 1974 (97%) | 67 (3%) | 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 | 135/135 (100%) | 135 (100%) | 0 | 100 | 100 |
| 1 | C | 130/135 (96%) | 130 (100%) | 0 | 100 | 100 |
| 1 | E | 128/135 (95%) | 128 (100%) | 0 | 100 | 100 |
| 2 | B | 84/91 (92%) | 83 (99%) | 1 (1%) | 71 | 84 |
| 2 | D | 84/91 (92%) | 83 (99%) | 1 (1%) | 71 | 84 |
| 2 | F | 84/91 (92%) | 83 (99%) | 1 (1%) | 71 | 84 |
| 3 | H | 176/194 (91%) | 176 (100%) | 0 | 100 | 100 |
| 3 | M | 180/194 (93%) | 180 (100%) | 0 | 100 | 100 |
| 3 | Q | 183/194 (94%) | 183 (100%) | 0 | 100 | 100 |
| 4 | L | 184/187 (98%) | 184 (100%) | 0 | 100 | 100 |
| 4 | N | 186/187 (100%) | 186 (100%) | 0 | 100 | 100 |
| 4 | R | 185/187 (99%) | 185 (100%) | 0 | 100 | 100 |
| All | All | 1739/1821 (96%) | 1736 (100%) | 3 (0%) | 93 | 96 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 601 | CYS |
| 2 | D | 601 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | F | 601 | CYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 521 | GLN |
| 1 | C | 62 | GLN |
| 1 | C | 107 | ASN |
| 2 | D | 521 | GLN |
| 1 | E | 62 | GLN |
| 3 | H | 6 | GLN |
| 4 | L | 37 | GLN |
| 3 | Q | 77 | ASN |

### 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)

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | NAG | G | 1 | 5 | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.45 | 0 |
| 5 | NAG | G | 2 | 5 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.51 | 0 |
| 5 | BMA | G | 3 | 5 | 11,11,12 | 0.64 | 0 | 15,15,17 | 0.93 | 1 (6%) |
| 5 | MAN | G | 4 | 5 | 11,11,12 | 0.74 | 0 | 15,15,17 | 1.21 | 2 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 5 | NAG | G | 5 | 5 | 14,14,15 | 0.31 | 0 | 17,19,21 | 1.01 | 1 (5%) |
| 5 | MAN | G | 6 | 5 | 11,11,12 | 0.96 | 1 (9%) | 15,15,17 | 1.13 | 2 (13%) |
| 6 | NAG | I | 1 | 6 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.44 | 0 |
| 6 | NAG | I | 2 | 6 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.51 | 0 |
| 6 | BMA | I | 3 | 6 | 11,11,12 | 0.64 | 0 | 15,15,17 | 0.93 | 1 (6%) |
| 6 | MAN | I | 4 | 6 | 11,11,12 | 0.73 | 0 | 15,15,17 | 1.21 | 2 (13%) |
| 6 | MAN | I | 5 | 6 | 11,11,12 | 0.96 | 1 (9%) | 15,15,17 | 1.13 | 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 |
|---|---|---|---|---|---|---|---|
| 5 | NAG | G | 1 | 5 | - | 0/6/23/26 | 0/1/1/1 |
| 5 | NAG | G | 2 | 5 | - | 1/6/23/26 | 0/1/1/1 |
| 5 | BMA | G | 3 | 5 | - | 2/2/19/22 | 0/1/1/1 |
| 5 | MAN | G | 4 | 5 | - | 1/2/19/22 | 0/1/1/1 |
| 5 | NAG | G | 5 | 5 | - | 3/6/23/26 | 0/1/1/1 |
| 5 | MAN | G | 6 | 5 | - | 0/2/19/22 | 0/1/1/1 |
| 6 | NAG | I | 1 | 6 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | I | 2 | 6 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | BMA | I | 3 | 6 | - | 2/2/19/22 | 0/1/1/1 |
| 6 | MAN | I | 4 | 6 | - | 1/2/19/22 | 0/1/1/1 |
| 6 | MAN | I | 5 | 6 | - | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 5 | G | 6 | MAN | C1-C2 | 2.75 | 1.58 | 1.52 |
| 6 | I | 5 | MAN | C1-C2 | 2.70 | 1.58 | 1.52 |

All (11) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | G | 5 | NAG | C2-N2-C7 | 3.43 | 127.79 | 122.90 |
| 5 | G | 4 | MAN | C1-O5-C5 | 3.23 | 116.57 | 112.19 |
| 6 | I | 4 | MAN | C1-O5-C5 | 3.22 | 116.56 | 112.19 |
| 5 | G | 3 | BMA | C1-O5-C5 | 2.52 | 115.60 | 112.19 |
| 5 | G | 4 | MAN | O2-C2-C3 | -2.49 | 105.14 | 110.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | I | 3 | BMA | C1-O5-C5 | 2.49 | 115.56 | 112.19 |
| 6 | I | 4 | MAN | O2-C2-C3 | -2.48 | 105.16 | 110.14 |
| 6 | I | 5 | MAN | O2-C2-C3 | -2.33 | 105.47 | 110.14 |
| 5 | G | 6 | MAN | O2-C2-C3 | -2.32 | 105.50 | 110.14 |
| 5 | G | 6 | MAN | C1-O5-C5 | 2.27 | 115.26 | 112.19 |
| 6 | I | 5 | MAN | C1-O5-C5 | 2.26 | 115.26 | 112.19 |

There are no chirality outliers.

All (11) torsion outliers are listed below:

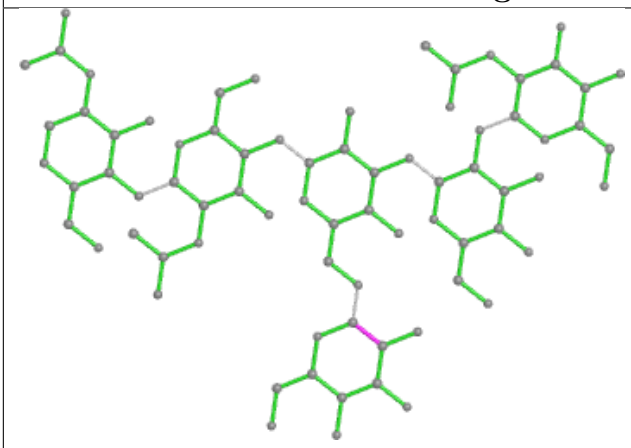
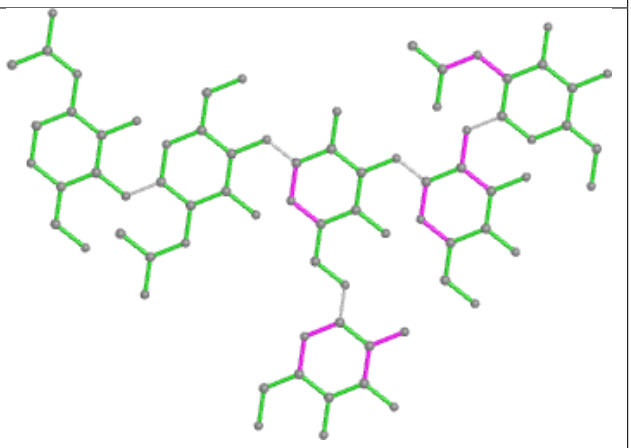
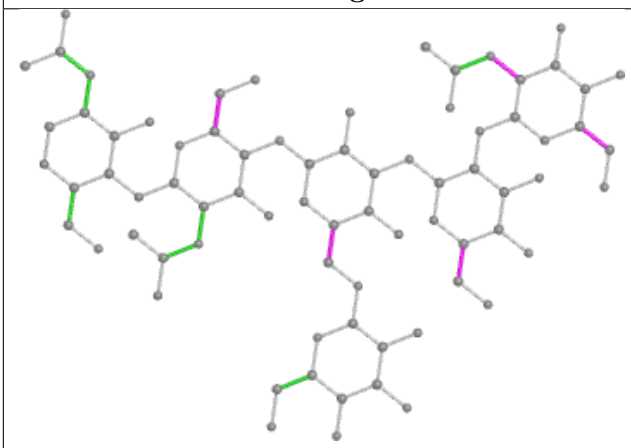
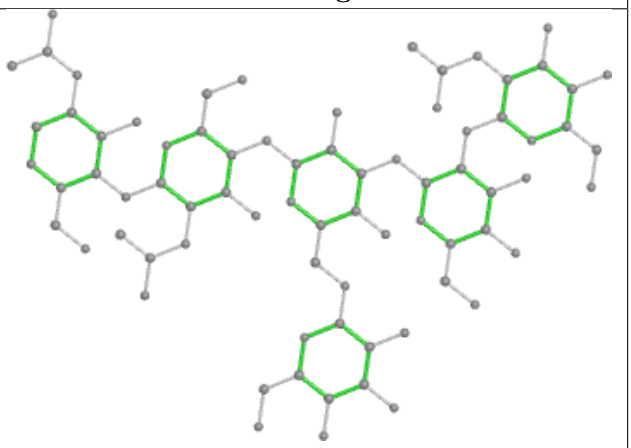
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | G | 5 | NAG | C3-C2-N2-C7 |
| 5 | G | 3 | BMA | C4-C5-C6-O6 |
| 6 | I | 3 | BMA | C4-C5-C6-O6 |
| 5 | G | 3 | BMA | O5-C5-C6-O6 |
| 6 | I | 3 | BMA | O5-C5-C6-O6 |
| 5 | G | 5 | NAG | O5-C5-C6-O6 |
| 5 | G | 2 | NAG | O5-C5-C6-O6 |
| 5 | G | 4 | MAN | O5-C5-C6-O6 |
| 6 | I | 2 | NAG | O5-C5-C6-O6 |
| 6 | I | 4 | MAN | O5-C5-C6-O6 |
| 5 | G | 5 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

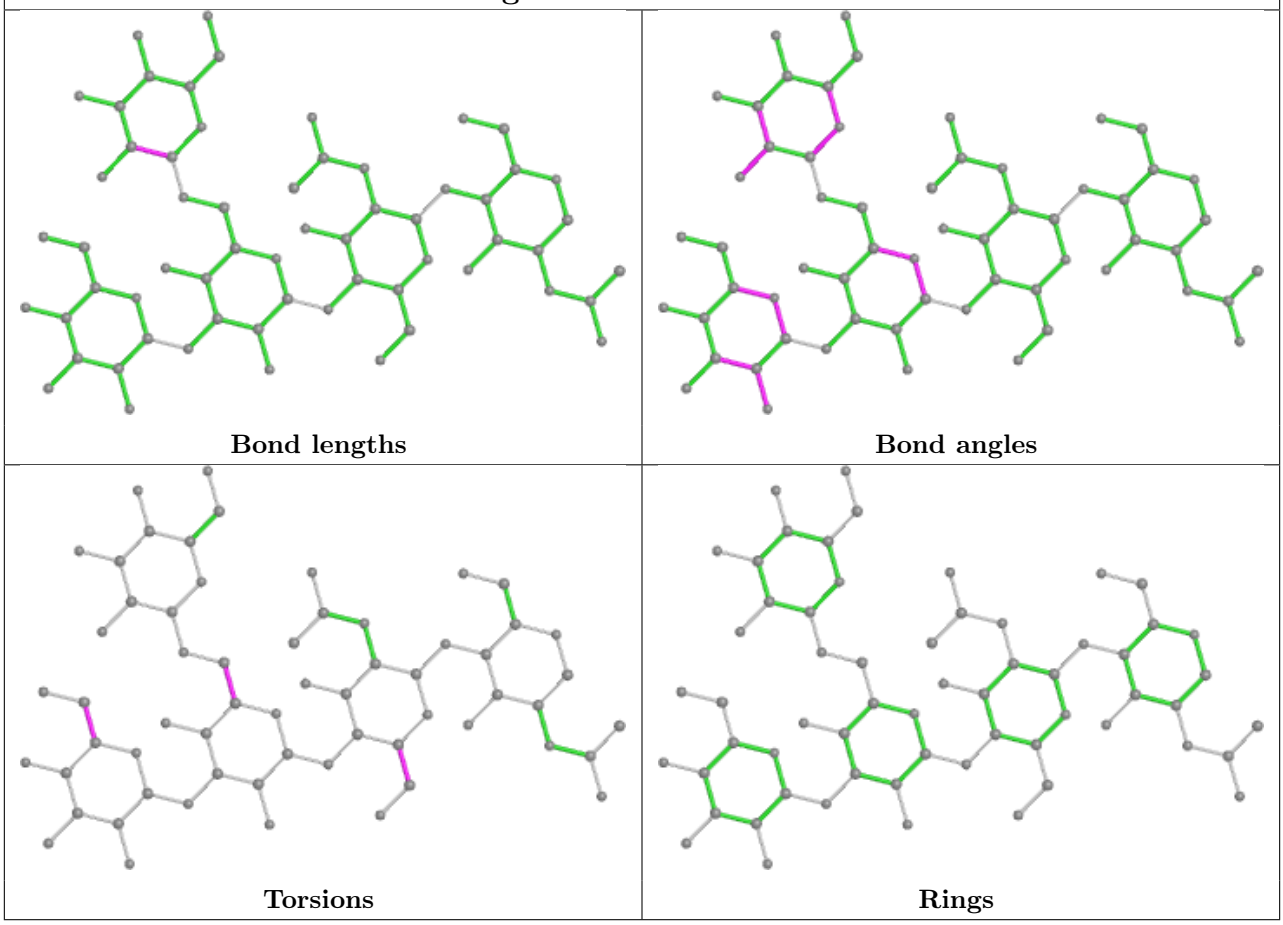
9 monomers are involved in 22 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | I | 5 | MAN | 1 | 0 |
| 5 | G | 3 | BMA | 1 | 0 |
| 5 | G | 6 | MAN | 1 | 0 |
| 6 | I | 3 | BMA | 7 | 0 |
| 5 | G | 5 | NAG | 1 | 0 |
| 5 | G | 1 | NAG | 8 | 0 |
| 5 | G | 2 | NAG | 1 | 0 |
| 6 | I | 1 | NAG | 3 | 0 |
| 6 | I | 2 | NAG | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

| Oligosaccharide Chain G | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

**Oligosaccharide Chain I**




## 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 7 | NAG | B | 701 | - | 14,14,15 | 0.38 | 0 | 17,19,21 | 0.48 | 0 |
| 7 | NAG | A | 201 | 1 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.45 | 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 |
|---|---|---|---|---|---|---|---|
| 7 | NAG | B | 701 | - | - | 2/6/23/26 | 0/1/1/1 |
| 7 | NAG | A | 201 | 1 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 7 | B | 701 | NAG | O5-C5-C6-O6 |
| 7 | B | 701 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

2 monomers are involved in 10 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 7 | B | 701 | NAG | 4 | 0 |
| 7 | A | 201 | NAG | 6 | 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

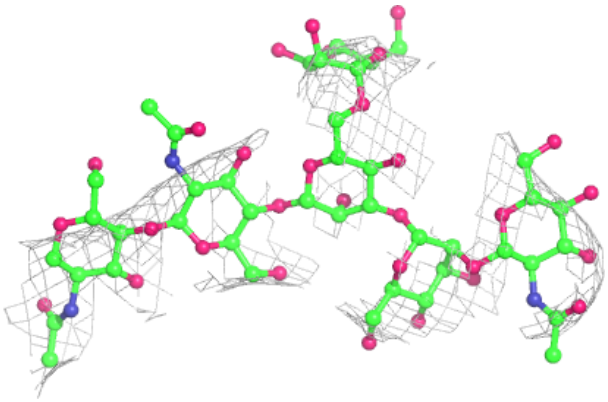
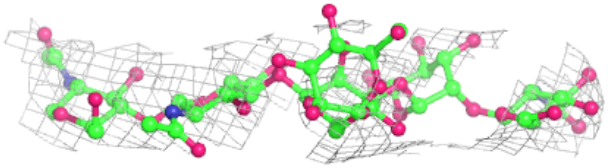
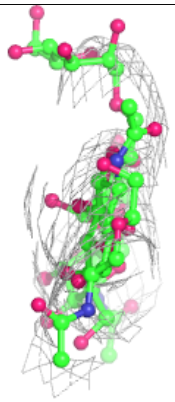
## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

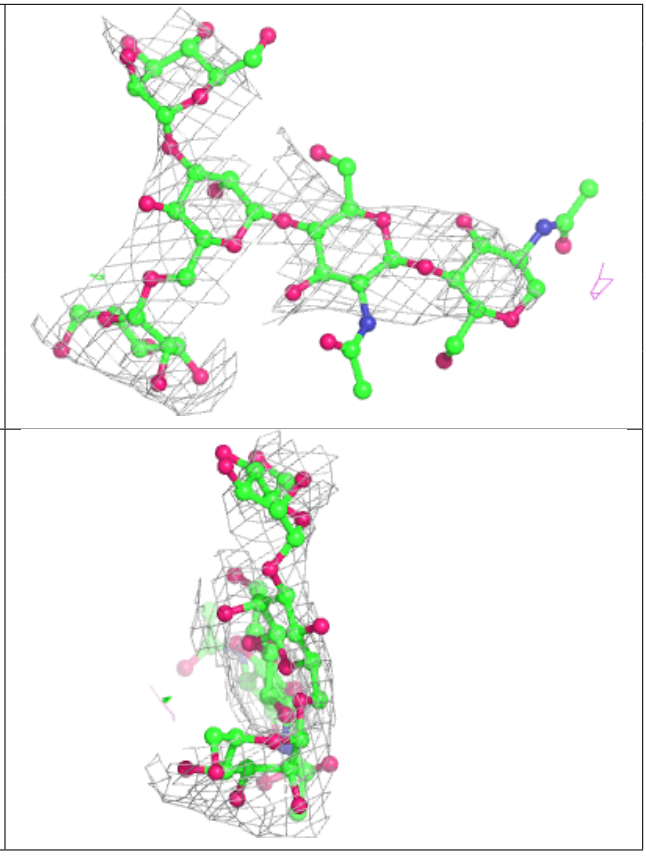
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

<table>
<tr><td>Electron density around Chain G:<br><br>2m$F_o$-D$F_c$ (at 0.7 rmsd) in gray<br>m$F_o$-D$F_c$ (at 3 rmsd) in purple (negative)<br>and green (positive)</td><td>  </td></tr>
<tr><td>  </td><td>  </td></tr>
</table>

**Electron density around Chain I:**

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



## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.