# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 10:22 PM EST

| | | |
|---|---|---|
| PDB ID | : | 2FJ7 |
| Title | : | Crystal structure of Nucleosome Core Particle Containing a Poly (dA.dT) Sequence Element |
| Authors | : | Bao, Y.; White, C.L.; Luger, K. |
| Deposited on | : | 2005-12-31 |
| Resolution | : | 3.20 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 ⓘ 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 ⓘ) were used in the production of this report:

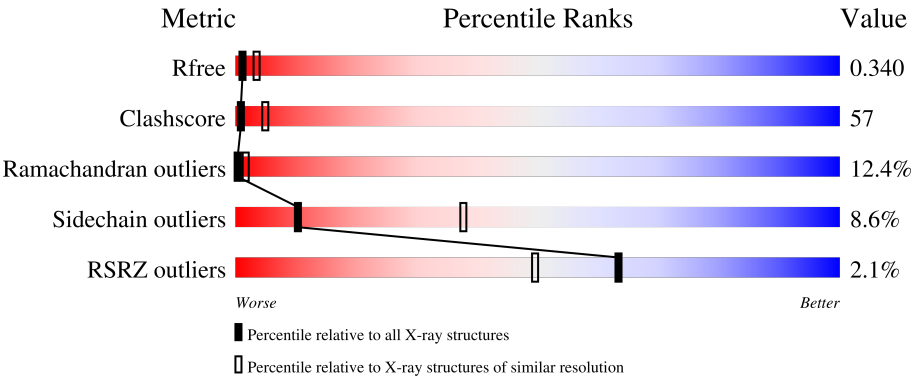
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 3.20 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 | 1133 (3.20-3.20) |
| Clashscore | 141614 | 1253 (3.20-3.20) |
| Ramachandran outliers | 138981 | 1234 (3.20-3.20) |
| Sidechain outliers | 138945 | 1233 (3.20-3.20) |
| RSRZ outliers | 127900 | 1095 (3.20-3.20) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | I | 147 | 5% 9% 91% |
| 2 | J | 147 | 3% 11% 85% |
| 3 | A | 135 | 2% 10% 47% 16% 27% |
| 3 | E | 135 | % 13% 47% 12% 27% |
| 4 | B | 102 | 21% 47% 10% 23% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 4 | F | 102 | 27% 48% 7% 18% |
| 5 | C | 129 | 24% 45% 13% 17% |
| 5 | G | 129 | % 25% 38% 17% 18% |
| 6 | D | 125 | 19% 45% 10% 26% |
| 6 | H | 125 | 3% 18% 48% 6% 26% |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12038 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 DNA chain called 147 bp DNA containing 16 bp poly dA element.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | I | 147 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3013 | 1443 | 555 | 869 | 146 | | | |

- Molecule 2 is a DNA chain called 147 bp DNA containing 16 bp poly dT element.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | J | 147 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 3008 | 1445 | 526 | 891 | 146 | | | |

- Molecule 3 is a protein called histone H3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 808 | 509 | 156 | 140 | 3 | | | |
| 3 | E | 98 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 808 | 509 | 156 | 140 | 3 | | | |

- Molecule 4 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | B | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 627 | 395 | 121 | 110 | 1 | | | |
| 4 | F | 84 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 673 | 424 | 133 | 115 | 1 | | | |

- Molecule 5 is a protein called histone H2A.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | C | 107 | Total | C | N | O | 0 | 0 | 0 |
| | | | 825 | 520 | 161 | 144 | | | |
| 5 | G | 106 | Total | C | N | O | 0 | 0 | 0 |
| | | | 818 | 516 | 160 | 142 | | | |

- Molecule 6 is a protein called Histone H2B.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | D | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 459 | 131 | 137 | 2 | | | |
| 6 | H | 93 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 729 | 459 | 131 | 137 | 2 | | | |

There are 2 discrepancies between the modelled and reference sequences:

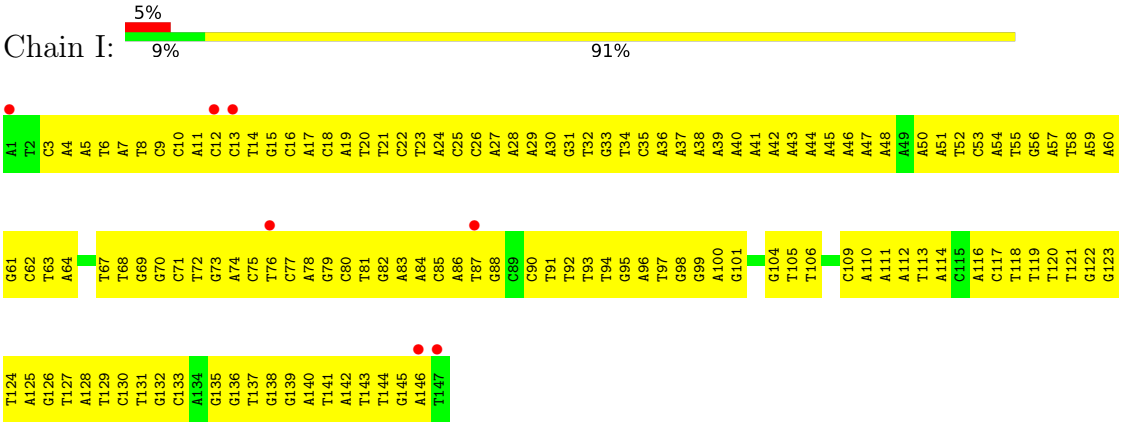
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 29 | THR | SER | conflict | UNP P02281 |
| H | 29 | THR | SER | conflict | UNP P02281 |

# 3 Residue-property plots (i)

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

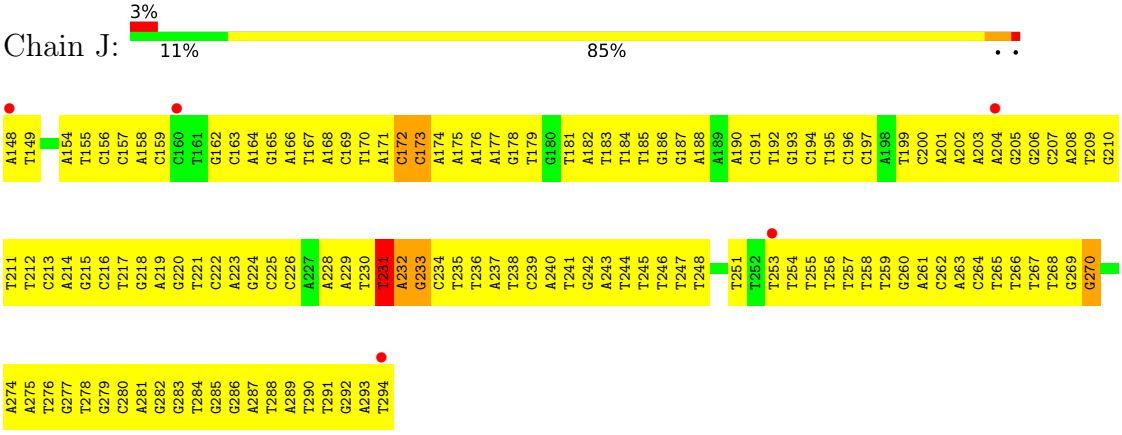
• Molecule 1: 147 bp DNA containing 16 bp poly dA element

Chain I:



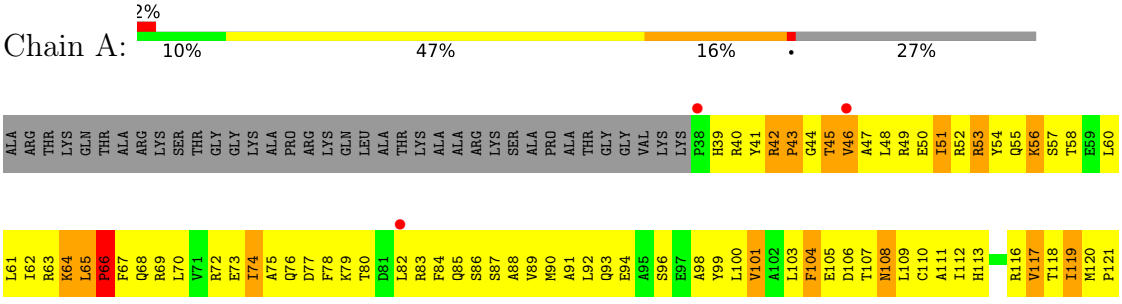

• Molecule 2: 147 bp DNA containing 16 bp poly dT element

Chain J:

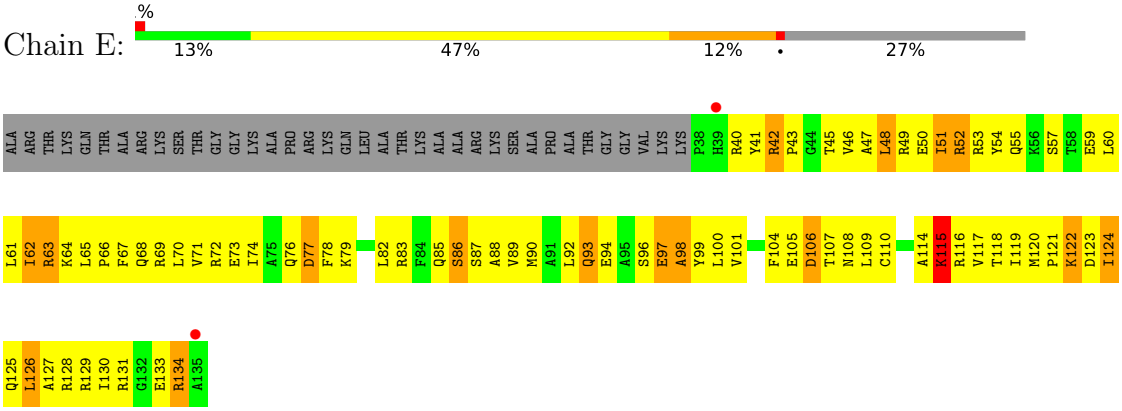



• Molecule 3: histone H3

Chain A:

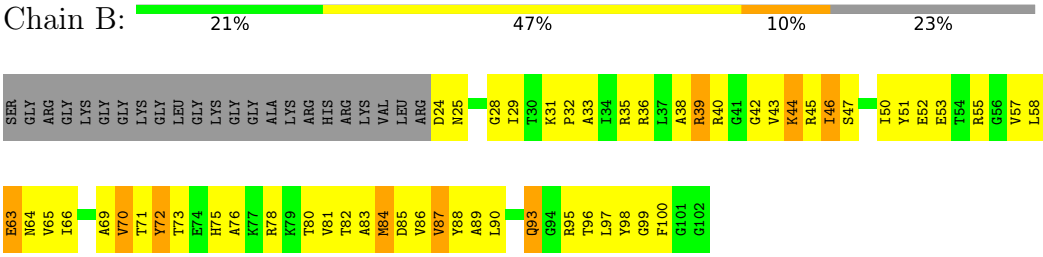


• Molecule 3: histone H3

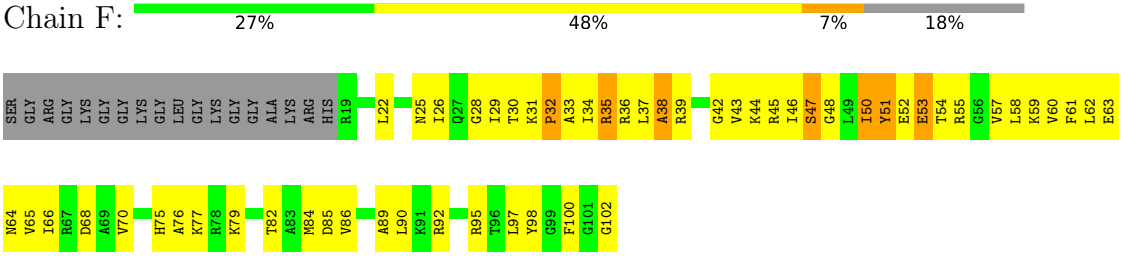




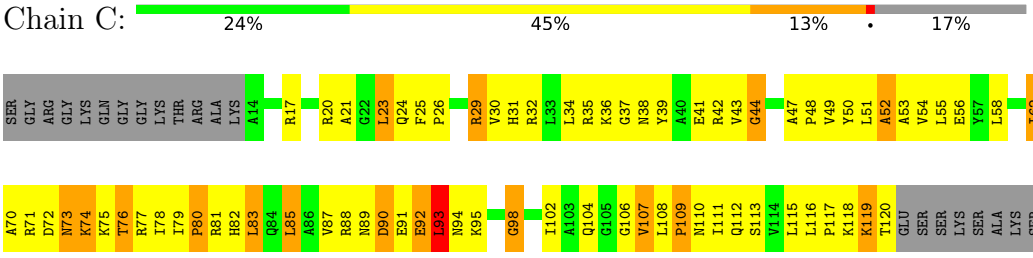

• Molecule 4: Histone H4



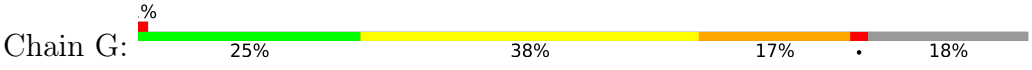

• Molecule 4: Histone H4

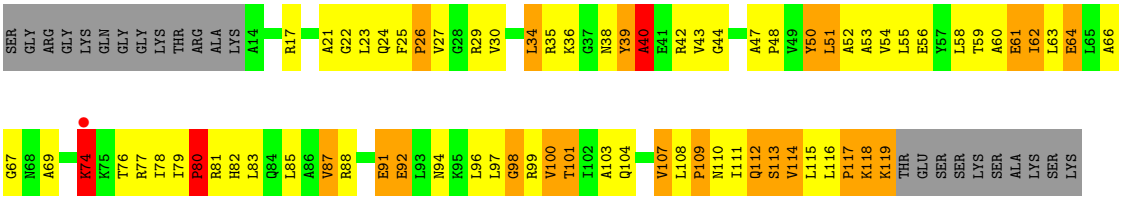



• Molecule 5: histone H2A

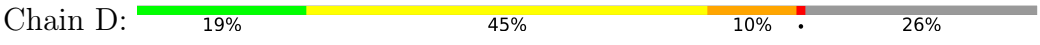


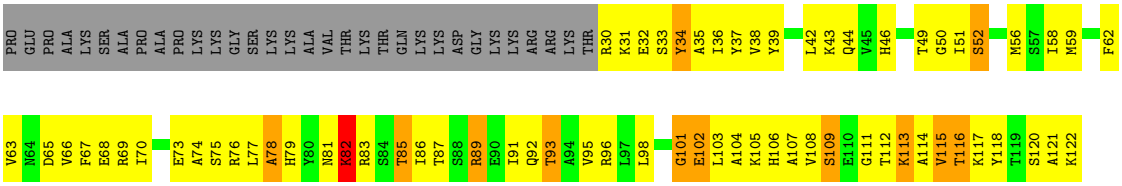

• Molecule 5: histone H2A



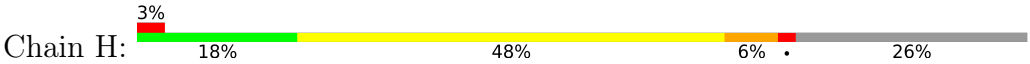


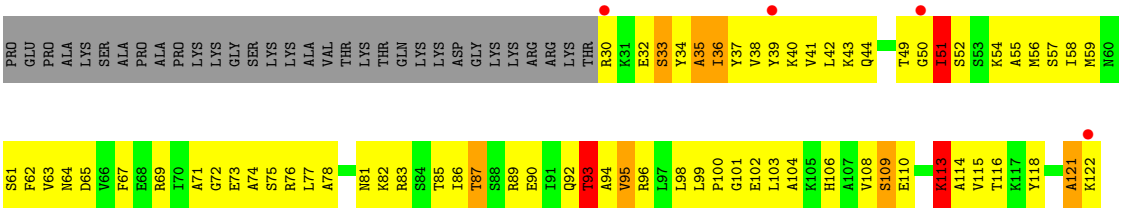

• Molecule 6: Histone H2B




• Molecule 6: Histone H2B



# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 104.92Å 109.60Å 177.97Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 3.20<br>37.89 – 2.69 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.2 (50.00-3.20)<br>78.9 (37.89-2.69) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 4.38 (at 2.69Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.280 , 0.350<br>0.278 , 0.340 | Depositor<br>DCC |
| $R_{free}$ test set | 2252 reflections (4.37%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 71.7 | Xtriage |
| Anisotropy | 0.698 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.26 , 81.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.27$ | Xtriage |
| Estimated twinning fraction | 0.035 for k,h,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.92 | EDS |
| Total number of atoms | 12038 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 126.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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 | I | 0.35 | 0/3384 | 0.73 | 0/5220 |
| 2 | J | 0.40 | 0/3370 | 0.93 | 10/5201 (0.2%) |
| 3 | A | 0.44 | 0/820 | 0.81 | 1/1099 (0.1%) |
| 3 | E | 0.57 | 0/820 | 0.84 | 1/1099 (0.1%) |
| 4 | B | 0.49 | 0/634 | 0.76 | 0/848 |
| 4 | F | 0.58 | 0/680 | 0.87 | 0/908 |
| 5 | C | 0.53 | 0/835 | 0.83 | 2/1127 (0.2%) |
| 5 | G | 0.39 | 0/828 | 1.02 | 5/1117 (0.4%) |
| 6 | D | 0.56 | 0/740 | 0.78 | 0/994 |
| 6 | H | 0.44 | 0/740 | 0.66 | 0/994 |
| All | All | 0.44 | 0/12851 | 0.83 | 19/18607 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 2 | J | 0 | 2 |
| 5 | G | 0 | 2 |
| All | All | 0 | 4 |

There are no bond length outliers.

All (19) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 5 | G | 40 | ALA | O-C-N | -20.12 | 90.50 | 122.70 |
| 2 | J | 173 | DC | O5'-P-OP2 | -19.42 | 87.39 | 110.70 |
| 2 | J | 172 | DC | OP2-P-O3' | -17.76 | 66.12 | 105.20 |
| 2 | J | 172 | DC | OP1-P-O3' | -17.68 | 66.30 | 105.20 |
| 2 | J | 173 | DC | O5'-P-OP1 | -15.76 | 91.51 | 105.70 |
| 3 | A | 66 | PRO | CA-N-CD | -10.34 | 97.03 | 111.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | J | 233 | DG | O5'-P-OP1 | -7.99 | 98.51 | 105.70 |
| 5 | G | 74 | LYS | CA-C-N | -7.92 | 99.78 | 117.20 |
| 2 | J | 231 | DT | C3'-C2'-C1' | -7.37 | 93.66 | 102.50 |
| 2 | J | 232 | DA | C5'-C4'-C3' | 7.21 | 127.09 | 114.10 |
| 3 | E | 77 | ASP | CB-CG-OD1 | 7.20 | 124.78 | 118.30 |
| 2 | J | 232 | DA | O5'-P-OP1 | 7.13 | 119.26 | 110.70 |
| 5 | G | 74 | LYS | C-N-CA | 6.84 | 138.80 | 121.70 |
| 5 | G | 74 | LYS | O-C-N | 6.26 | 132.72 | 122.70 |
| 5 | C | 83 | LEU | CB-CG-CD1 | -5.99 | 100.83 | 111.00 |
| 2 | J | 173 | DC | OP1-P-OP2 | 5.72 | 128.19 | 119.60 |
| 5 | C | 93 | LEU | CA-CB-CG | 5.50 | 127.94 | 115.30 |
| 5 | G | 40 | ALA | C-N-CA | 5.23 | 134.78 | 121.70 |
| 2 | J | 270 | DG | OP1-P-O3' | 5.02 | 116.25 | 105.20 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 5 | G | 40 | ALA | Mainchain,Peptide |
| 2 | J | 231 | DT | Sidechain |
| 2 | J | 270 | DG | Sidechain |

## 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 | I | 3013 | 0 | 1661 | 243 | 0 |
| 2 | J | 3008 | 0 | 1672 | 248 | 0 |
| 3 | A | 808 | 0 | 846 | 179 | 0 |
| 3 | E | 808 | 0 | 846 | 139 | 0 |
| 4 | B | 627 | 0 | 663 | 109 | 0 |
| 4 | F | 673 | 0 | 722 | 113 | 0 |
| 5 | C | 825 | 0 | 884 | 134 | 0 |
| 5 | G | 818 | 0 | 877 | 132 | 0 |
| 6 | D | 729 | 0 | 753 | 119 | 0 |
| 6 | H | 729 | 0 | 753 | 96 | 0 |
| All | All | 12038 | 0 | 9677 | 1230 | 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 57.

All (1230) 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) |
|---|---|---|---|
| 4:B:45:ARG:O | 4:B:46:ILE:HG13 | 1.25 | 1.28 |
| 2:J:281:DA:H2" | 2:J:282:DG:H5' | 1.25 | 1.15 |
| 3:E:61:LEU:HD12 | 4:F:37:LEU:HD23 | 1.28 | 1.15 |
| 3:A:117:VAL:HB | 4:B:44:LYS:HG2 | 1.23 | 1.14 |
| 5:G:26:PRO:HB2 | 5:G:29:ARG:HD2 | 1.32 | 1.12 |
| 3:A:76:GLN:HE22 | 3:A:80:THR:HA | 1.16 | 1.10 |
| 4:B:45:ARG:O | 4:B:46:ILE:CG1 | 2.00 | 1.10 |
| 3:A:69:ARG:HD2 | 4:B:25:ASN:OD1 | 1.51 | 1.09 |
| 5:C:39:TYR:HB3 | 6:D:75:SER:HB2 | 1.35 | 1.08 |
| 4:B:46:ILE:CG2 | 4:B:47:SER:H | 1.65 | 1.07 |
| 1:I:91:DT:H4' | 3:A:63:ARG:HD3 | 1.33 | 1.06 |
| 4:B:44:LYS:HD3 | 5:G:115:LEU:HD22 | 1.37 | 1.05 |
| 4:F:75:HIS:HB2 | 6:H:93:THR:HG21 | 1.35 | 1.04 |
| 1:I:81:DT:H4' | 4:B:45:ARG:HE | 1.16 | 1.03 |
| 3:A:76:GLN:NE2 | 3:A:80:THR:HA | 1.74 | 1.02 |
| 2:J:232:DA:H4' | 2:J:233:DG:OP1 | 1.56 | 1.01 |
| 1:I:12:DC:H1' | 1:I:13:DC:H5' | 1.43 | 1.00 |
| 2:J:247:DT:H4' | 2:J:248:DT:OP1 | 1.62 | 0.99 |
| 5:C:102:ILE:HG23 | 6:D:58:ILE:HD13 | 1.41 | 0.99 |
| 1:I:59:DA:H4' | 1:I:60:DA:OP1 | 1.60 | 0.99 |
| 5:G:107:VAL:HG12 | 5:G:108:LEU:H | 1.26 | 0.99 |
| 3:A:68:GLN:HG3 | 3:A:89:VAL:HG11 | 1.44 | 0.98 |
| 4:F:29:ILE:O | 4:F:34:ILE:HD11 | 1.63 | 0.98 |
| 2:J:187:DG:H4' | 2:J:188:DA:OP1 | 1.60 | 0.98 |
| 2:J:199:DT:H2" | 2:J:200:DC:H5" | 1.44 | 0.98 |
| 2:J:275:DA:H2" | 2:J:276:DT:OP2 | 1.65 | 0.97 |
| 3:E:119:ILE:HD13 | 4:F:43:VAL:HG11 | 1.46 | 0.97 |
| 5:G:119:LYS:HE3 | 5:G:119:LYS:HA | 1.46 | 0.97 |
| 1:I:81:DT:H4' | 4:B:45:ARG:NE | 1.79 | 0.96 |
| 2:J:255:DT:H4' | 2:J:256:DT:OP1 | 1.65 | 0.96 |
| 6:D:91:ILE:O | 6:D:95:VAL:HG23 | 1.63 | 0.96 |
| 1:I:75:DC:H2" | 1:I:76:DT:H5' | 1.45 | 0.95 |
| 2:J:239:DC:H2" | 2:J:240:DA:C8 | 2.00 | 0.95 |
| 2:J:283:DG:H4' | 2:J:284:DT:OP1 | 1.63 | 0.95 |
| 3:A:119:ILE:HG13 | 3:A:119:ILE:O | 1.66 | 0.94 |
| 4:B:46:ILE:CG2 | 4:B:47:SER:N | 2.26 | 0.94 |
| 6:D:34:TYR:O | 6:D:38:VAL:HG23 | 1.67 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:84:DA:H2" | 1:I:85:DC:OP2 | 1.66 | 0.94 |
| 1:I:5:DA:C4' | 3:A:39:HIS:HB2 | 1.97 | 0.93 |
| 1:I:87:DT:H1' | 1:I:88:DG:H5' | 1.50 | 0.93 |
| 2:J:291:DT:H4' | 2:J:292:DG:OP1 | 1.65 | 0.93 |
| 2:J:246:DT:H4' | 2:J:247:DT:OP1 | 1.69 | 0.93 |
| 5:G:26:PRO:CB | 5:G:29:ARG:HD2 | 1.99 | 0.92 |
| 2:J:173:DC:H2" | 2:J:174:DA:C8 | 2.04 | 0.92 |
| 4:B:46:ILE:HG22 | 4:B:47:SER:N | 1.81 | 0.92 |
| 4:B:47:SER:HB3 | 4:B:50:ILE:HG12 | 1.52 | 0.92 |
| 4:B:35:ARG:O | 4:B:39:ARG:HG2 | 1.67 | 0.92 |
| 1:I:5:DA:H4' | 3:A:39:HIS:HB2 | 1.48 | 0.92 |
| 5:C:58:LEU:O | 5:C:62:ILE:HG22 | 1.71 | 0.90 |
| 4:B:62:LEU:HD22 | 4:B:66:ILE:HD11 | 1.51 | 0.90 |
| 5:G:26:PRO:HD3 | 6:H:37:TYR:CG | 2.06 | 0.90 |
| 1:I:126:DG:H1' | 1:I:127:DT:O5' | 1.75 | 0.87 |
| 1:I:127:DT:P | 1:I:127:DT:H3' | 2.14 | 0.87 |
| 4:B:46:ILE:HG23 | 4:B:47:SER:H | 1.39 | 0.86 |
| 1:I:12:DC:H1' | 1:I:13:DC:C5' | 2.04 | 0.86 |
| 2:J:274:DA:H1' | 2:J:275:DA:O5' | 1.74 | 0.86 |
| 4:F:26:ILE:O | 4:F:55:ARG:HD3 | 1.77 | 0.84 |
| 5:G:77:ARG:HG2 | 5:G:78:ILE:H | 1.41 | 0.84 |
| 5:G:78:ILE:HA | 5:G:82:HIS:ND1 | 1.91 | 0.84 |
| 2:J:199:DT:C2' | 2:J:200:DC:H5" | 2.08 | 0.84 |
| 4:B:82:THR:HG23 | 4:B:85:ASP:OD2 | 1.78 | 0.83 |
| 2:J:225:DC:H1' | 2:J:226:DC:H5' | 1.59 | 0.82 |
| 4:B:52:GLU:OE1 | 4:B:55:ARG:HD2 | 1.79 | 0.82 |
| 5:G:51:LEU:HD21 | 6:H:67:PHE:CE1 | 2.15 | 0.82 |
| 4:B:46:ILE:HG22 | 4:B:47:SER:H | 1.42 | 0.82 |
| 6:D:82:LYS:HD2 | 6:D:82:LYS:N | 1.94 | 0.82 |
| 3:E:51:ILE:HG22 | 3:E:52:ARG:N | 1.94 | 0.82 |
| 2:J:282:DG:H4' | 2:J:283:DG:OP1 | 1.77 | 0.82 |
| 3:E:119:ILE:HD11 | 4:F:46:ILE:HG23 | 1.62 | 0.82 |
| 2:J:235:DT:H2" | 2:J:236:DT:H71 | 1.59 | 0.81 |
| 2:J:205:DG:H1' | 2:J:206:DG:C8 | 2.16 | 0.81 |
| 3:E:60:LEU:HD11 | 3:E:94:GLU:OE2 | 1.81 | 0.81 |
| 5:G:26:PRO:HB2 | 5:G:29:ARG:CD | 2.10 | 0.81 |
| 2:J:204:DA:H1' | 2:J:205:DG:O5' | 1.82 | 0.80 |
| 3:A:61:LEU:HD13 | 4:B:36:ARG:HB3 | 1.61 | 0.80 |
| 3:A:44:GLY:O | 3:A:48:LEU:HD13 | 1.80 | 0.80 |
| 3:E:61:LEU:HD12 | 4:F:37:LEU:HA | 1.64 | 0.80 |
| 5:C:23:LEU:HD12 | 5:C:23:LEU:N | 1.97 | 0.80 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:266:DT:H4' | 2:J:267:DT:OP1 | 1.83 | 0.79 |
| 4:B:66:ILE:O | 4:B:70:VAL:HG23 | 1.82 | 0.79 |
| 3:A:130:ILE:HG22 | 3:E:130:ILE:CG2 | 2.12 | 0.79 |
| 4:F:59:LYS:O | 4:F:63:GLU:HG3 | 1.82 | 0.79 |
| 5:G:17:ARG:HG2 | 6:H:118:TYR:OH | 1.83 | 0.79 |
| 2:J:246:DT:H2" | 2:J:247:DT:H71 | 1.63 | 0.79 |
| 4:F:30:THR:O | 4:F:34:ILE:HG13 | 1.83 | 0.78 |
| 5:C:107:VAL:HG23 | 5:C:108:LEU:N | 1.98 | 0.78 |
| 2:J:172:DC:C4' | 2:J:173:DC:OP2 | 2.30 | 0.78 |
| 2:J:242:DG:H2" | 2:J:243:DA:OP2 | 1.82 | 0.78 |
| 3:E:70:LEU:HD13 | 4:F:26:ILE:HA | 1.66 | 0.78 |
| 2:J:167:DT:H2" | 2:J:168:DA:H5" | 1.64 | 0.78 |
| 2:J:268:DT:H2" | 2:J:269:DG:C8 | 2.19 | 0.78 |
| 4:F:39:ARG:O | 4:F:42:GLY:N | 2.17 | 0.78 |
| 6:H:36:ILE:HD13 | 6:H:36:ILE:H | 1.48 | 0.77 |
| 1:I:12:DC:C6 | 1:I:12:DC:OP1 | 2.37 | 0.77 |
| 4:B:51:TYR:HB3 | 4:B:55:ARG:HH12 | 1.49 | 0.77 |
| 4:B:75:HIS:CD2 | 6:D:77:LEU:HD13 | 2.20 | 0.77 |
| 2:J:280:DC:H2" | 2:J:281:DA:OP2 | 1.84 | 0.77 |
| 3:E:50:GLU:HG2 | 4:F:39:ARG:HG3 | 1.66 | 0.77 |
| 2:J:247:DT:H2" | 2:J:248:DT:H72 | 1.66 | 0.77 |
| 1:I:95:DG:H2" | 1:I:96:DA:OP2 | 1.83 | 0.77 |
| 3:E:104:PHE:O | 3:E:107:THR:HB | 1.84 | 0.77 |
| 2:J:199:DT:H2" | 2:J:200:DC:C5' | 2.15 | 0.77 |
| 1:I:121:DT:H2" | 1:I:122:DG:C8 | 2.20 | 0.76 |
| 1:I:127:DT:H2" | 1:I:128:DA:OP2 | 1.84 | 0.76 |
| 2:J:183:DT:H2" | 2:J:184:DT:OP2 | 1.83 | 0.76 |
| 5:C:67:GLY:HA3 | 6:D:46:HIS:CD2 | 2.20 | 0.76 |
| 6:H:113:LYS:NZ | 6:H:113:LYS:HB3 | 1.98 | 0.76 |
| 5:C:35:ARG:O | 5:C:38:ASN:N | 2.18 | 0.76 |
| 1:I:83:DA:H5" | 3:A:43:PRO:HA | 1.66 | 0.76 |
| 3:E:87:SER:O | 3:E:89:VAL:N | 2.18 | 0.76 |
| 1:I:15:DG:H1' | 1:I:16:DC:H5' | 1.66 | 0.76 |
| 5:G:50:TYR:OH | 6:H:92:GLN:HG3 | 1.85 | 0.76 |
| 2:J:285:DG:H1' | 2:J:286:DG:H5' | 1.66 | 0.76 |
| 1:I:39:DA:H5" | 5:G:42:ARG:NE | 2.01 | 0.76 |
| 2:J:255:DT:H2" | 2:J:256:DT:H72 | 1.68 | 0.76 |
| 3:A:51:ILE:HG21 | 5:G:111:ILE:HD11 | 1.67 | 0.76 |
| 1:I:119:DT:H2" | 1:I:120:DT:H71 | 1.66 | 0.75 |
| 1:I:95:DG:H1' | 1:I:96:DA:C5' | 2.16 | 0.75 |
| 2:J:170:DT:H2" | 2:J:171:DA:OP2 | 1.86 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:32:PRO:HA | 4:B:35:ARG:HD3 | 1.67 | 0.75 |
| 5:C:83:LEU:O | 5:C:87:VAL:HG23 | 1.86 | 0.75 |
| 5:G:87:VAL:HG11 | 5:G:97:LEU:HD12 | 1.67 | 0.75 |
| 2:J:281:DA:C2' | 2:J:282:DG:H5' | 2.11 | 0.75 |
| 1:I:121:DT:H2" | 1:I:122:DG:N7 | 2.02 | 0.74 |
| 6:D:43:LYS:HE2 | 6:D:43:LYS:HA | 1.67 | 0.74 |
| 5:C:50:TYR:O | 5:C:53:ALA:HB3 | 1.87 | 0.74 |
| 1:I:129:DT:H1' | 1:I:130:DC:H5' | 1.69 | 0.74 |
| 5:G:67:GLY:HA2 | 5:G:78:ILE:HD11 | 1.69 | 0.74 |
| 1:I:137:DT:H2" | 1:I:138:DG:OP2 | 1.86 | 0.74 |
| 2:J:207:DC:H2" | 2:J:208:DA:OP2 | 1.86 | 0.74 |
| 1:I:123:DG:H4' | 6:D:30:ARG:HB2 | 1.69 | 0.73 |
| 1:I:17:DA:H1' | 1:I:18:DC:O4' | 1.86 | 0.73 |
| 5:G:80:PRO:HG3 | 6:H:54:LYS:O | 1.87 | 0.73 |
| 3:E:97:GLU:O | 3:E:99:TYR:N | 2.20 | 0.73 |
| 2:J:185:DT:H2" | 2:J:186:DG:N7 | 2.03 | 0.73 |
| 2:J:222:DC:H4' | 2:J:223:DA:OP1 | 1.89 | 0.73 |
| 3:E:69:ARG:HB3 | 4:F:25:ASN:OD1 | 1.88 | 0.73 |
| 1:I:105:DT:H2" | 1:I:106:DT:H71 | 1.71 | 0.73 |
| 3:A:130:ILE:HG22 | 3:E:130:ILE:HG22 | 1.69 | 0.73 |
| 5:G:111:ILE:O | 5:G:113:SER:N | 2.21 | 0.73 |
| 1:I:119:DT:H4' | 1:I:120:DT:OP1 | 1.86 | 0.72 |
| 1:I:82:DG:H1' | 1:I:83:DA:H5' | 1.70 | 0.72 |
| 1:I:95:DG:H1' | 1:I:96:DA:O5' | 1.89 | 0.72 |
| 1:I:116:DA:H1' | 1:I:117:DC:H5' | 1.72 | 0.72 |
| 2:J:154:DA:H4' | 3:E:49:ARG:HH21 | 1.54 | 0.72 |
| 2:J:172:DC:H4' | 2:J:173:DC:OP2 | 1.88 | 0.72 |
| 3:A:51:ILE:HG22 | 3:A:52:ARG:N | 2.04 | 0.72 |
| 5:C:78:ILE:N | 6:D:50:GLY:O | 2.18 | 0.72 |
| 3:E:61:LEU:O | 3:E:62:ILE:C | 2.28 | 0.72 |
| 4:F:45:ARG:HH11 | 4:F:45:ARG:HG2 | 1.54 | 0.72 |
| 1:I:69:DG:H5' | 3:E:43:PRO:HB2 | 1.72 | 0.72 |
| 5:C:113:SER:O | 5:C:116:LEU:HB2 | 1.90 | 0.71 |
| 2:J:194:DC:H2" | 2:J:195:DT:OP2 | 1.91 | 0.71 |
| 2:J:207:DC:H4' | 3:A:63:ARG:HH21 | 1.55 | 0.71 |
| 2:J:239:DC:P | 3:E:63:ARG:HE | 2.13 | 0.71 |
| 2:J:192:DT:H1' | 2:J:193:DG:C8 | 2.24 | 0.71 |
| 3:A:98:ALA:O | 3:A:101:VAL:HB | 1.90 | 0.71 |
| 5:C:30:VAL:HG21 | 5:C:52:ALA:HB2 | 1.71 | 0.71 |
| 5:G:25:PHE:HZ | 5:G:59:THR:HG21 | 1.56 | 0.71 |
| 1:I:75:DC:H2" | 1:I:76:DT:C5' | 2.18 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:50:GLU:O | 3:E:53:ARG:HB3 | 1.91 | 0.71 |
| 3:E:51:ILE:HA | 4:F:39:ARG:HB3 | 1.71 | 0.70 |
| 5:G:108:LEU:O | 5:G:110:ASN:N | 2.24 | 0.70 |
| 6:H:81:ASN:HB3 | 6:H:83:ARG:NE | 2.07 | 0.70 |
| 2:J:167:DT:H2" | 2:J:168:DA:C5' | 2.21 | 0.70 |
| 2:J:213:DC:H2" | 2:J:214:DA:OP2 | 1.91 | 0.70 |
| 3:A:92:LEU:HD21 | 4:B:86:VAL:CG2 | 2.21 | 0.70 |
| 3:A:129:ARG:HG3 | 3:A:130:ILE:N | 2.05 | 0.70 |
| 3:E:61:LEU:CD1 | 4:F:37:LEU:HD23 | 2.16 | 0.70 |
| 2:J:208:DA:H1' | 2:J:209:DT:H5' | 1.73 | 0.70 |
| 5:G:107:VAL:HG12 | 5:G:108:LEU:N | 2.05 | 0.70 |
| 5:C:119:LYS:HE3 | 5:C:119:LYS:HA | 1.74 | 0.70 |
| 5:G:54:VAL:HG21 | 6:H:95:VAL:HG21 | 1.74 | 0.70 |
| 1:I:95:DG:H1' | 1:I:96:DA:H5' | 1.72 | 0.69 |
| 2:J:256:DT:H2" | 2:J:257:DT:OP2 | 1.91 | 0.69 |
| 3:A:116:ARG:HH11 | 3:A:116:ARG:HB3 | 1.56 | 0.69 |
| 4:B:62:LEU:O | 4:B:63:GLU:C | 2.30 | 0.69 |
| 1:I:7:DA:H5' | 3:A:41:TYR:OH | 1.92 | 0.69 |
| 1:I:86:DA:H4' | 1:I:87:DT:OP2 | 1.93 | 0.69 |
| 2:J:171:DA:H2" | 2:J:172:DC:O5' | 1.91 | 0.69 |
| 5:G:42:ARG:O | 6:H:85:THR:HG23 | 1.92 | 0.69 |
| 2:J:158:DA:H1' | 2:J:159:DC:H5' | 1.72 | 0.69 |
| 2:J:262:DC:H2" | 2:J:263:DA:C8 | 2.28 | 0.69 |
| 1:I:86:DA:H61 | 2:J:209:DT:H3 | 1.40 | 0.69 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CD2 | 2.28 | 0.69 |
| 4:F:31:LYS:HG2 | 4:F:51:TYR:CD2 | 2.27 | 0.69 |
| 2:J:231:DT:OP2 | 3:E:41:TYR:HB2 | 1.91 | 0.69 |
| 4:B:51:TYR:O | 4:B:55:ARG:HG3 | 1.92 | 0.69 |
| 6:D:31:LYS:HZ3 | 6:D:32:GLU:HG3 | 1.58 | 0.69 |
| 5:G:25:PHE:O | 5:G:27:VAL:HG23 | 1.91 | 0.69 |
| 6:H:51:ILE:HD11 | 6:H:56:MET:N | 2.08 | 0.69 |
| 4:F:75:HIS:CD2 | 6:H:77:LEU:HD22 | 2.28 | 0.69 |
| 5:G:51:LEU:HD21 | 6:H:67:PHE:CD1 | 2.28 | 0.69 |
| 4:B:31:LYS:HE2 | 4:B:32:PRO:HD3 | 1.75 | 0.68 |
| 3:A:129:ARG:HE | 3:A:130:ILE:HD12 | 1.58 | 0.68 |
| 6:H:104:ALA:O | 6:H:108:VAL:HG23 | 1.93 | 0.68 |
| 3:E:61:LEU:O | 3:E:62:ILE:O | 2.11 | 0.68 |
| 2:J:288:DT:H1' | 2:J:289:DA:O5' | 1.92 | 0.68 |
| 5:C:71:ARG:NH1 | 5:C:71:ARG:HB3 | 2.08 | 0.68 |
| 4:F:47:SER:O | 4:F:51:TYR:HE1 | 1.76 | 0.68 |
| 1:I:67:DT:H2" | 1:I:68:DT:C7 | 2.23 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:157:DC:H1' | 2:J:158:DA:H5' | 1.75 | 0.68 |
| 2:J:253:DT:H2" | 2:J:254:DT:H72 | 1.76 | 0.68 |
| 4:B:96:THR:HG22 | 4:B:97:LEU:N | 2.09 | 0.68 |
| 4:B:45:ARG:O | 4:B:46:ILE:CB | 2.40 | 0.68 |
| 4:B:75:HIS:HB2 | 6:D:93:THR:HG21 | 1.76 | 0.68 |
| 3:A:104:PHE:O | 3:A:107:THR:HB | 1.94 | 0.68 |
| 6:D:102:GLU:O | 6:D:106:HIS:HD2 | 1.77 | 0.68 |
| 4:F:31:LYS:HA | 4:F:34:ILE:HD12 | 1.73 | 0.68 |
| 2:J:239:DC:H2" | 2:J:240:DA:N7 | 2.08 | 0.67 |
| 1:I:132:DG:H2" | 1:I:133:DC:C6 | 2.29 | 0.67 |
| 3:A:49:ARG:NH1 | 3:A:49:ARG:HB2 | 2.10 | 0.67 |
| 1:I:131:DT:H2" | 1:I:132:DG:OP2 | 1.95 | 0.67 |
| 5:C:51:LEU:O | 5:C:53:ALA:N | 2.28 | 0.67 |
| 4:B:39:ARG:HA | 4:B:39:ARG:HH11 | 1.59 | 0.67 |
| 5:C:38:ASN:ND2 | 5:G:38:ASN:HD22 | 1.93 | 0.67 |
| 1:I:69:DG:H2" | 1:I:70:DG:N7 | 2.09 | 0.67 |
| 4:B:97:LEU:HD13 | 5:G:101:THR:HG22 | 1.75 | 0.67 |
| 4:F:62:LEU:O | 4:F:66:ILE:HG12 | 1.95 | 0.67 |
| 2:J:238:DT:H4' | 3:E:63:ARG:HD3 | 1.76 | 0.67 |
| 3:E:45:THR:HG22 | 3:E:45:THR:O | 1.95 | 0.67 |
| 4:B:76:ALA:O | 4:B:78:ARG:HG3 | 1.94 | 0.67 |
| 1:I:113:DT:H5" | 5:C:42:ARG:HG2 | 1.76 | 0.66 |
| 1:I:101:DG:H4' | 3:A:83:ARG:HH11 | 1.61 | 0.66 |
| 3:A:74:ILE:HG21 | 4:B:66:ILE:HD12 | 1.78 | 0.66 |
| 5:C:26:PRO:O | 5:C:30:VAL:HG23 | 1.96 | 0.66 |
| 6:H:81:ASN:O | 6:H:82:LYS:HB2 | 1.96 | 0.66 |
| 3:A:116:ARG:O | 3:A:117:VAL:HG13 | 1.96 | 0.66 |
| 2:J:210:DG:H2" | 2:J:211:DT:OP2 | 1.95 | 0.66 |
| 3:A:53:ARG:O | 3:A:56:LYS:HB3 | 1.96 | 0.66 |
| 1:I:23:DT:H2" | 1:I:24:DA:OP2 | 1.95 | 0.65 |
| 1:I:120:DT:H1' | 1:I:121:DT:H5' | 1.76 | 0.65 |
| 2:J:167:DT:C2' | 2:J:168:DA:H5" | 2.26 | 0.65 |
| 4:B:24:ASP:O | 4:B:25:ASN:HB2 | 1.95 | 0.65 |
| 6:D:31:LYS:NZ | 6:D:32:GLU:HG3 | 2.12 | 0.65 |
| 2:J:206:DG:H2" | 2:J:207:DC:C5 | 2.31 | 0.65 |
| 3:A:83:ARG:HB2 | 4:B:80:THR:HG23 | 1.79 | 0.65 |
| 4:F:97:LEU:HD12 | 4:F:98:TYR:N | 2.12 | 0.65 |
| 1:I:68:DT:H1' | 3:E:43:PRO:HG2 | 1.77 | 0.65 |
| 5:G:63:LEU:O | 5:G:67:GLY:N | 2.30 | 0.65 |
| 5:C:50:TYR:HD2 | 6:D:91:ILE:HG22 | 1.61 | 0.65 |
| 6:H:81:ASN:HB2 | 6:H:83:ARG:HG2 | 1.79 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:10:DC:H1' | 1:I:11:DA:O5' | 1.97 | 0.65 |
| 1:I:55:DT:H2" | 1:I:56:DG:C8 | 2.31 | 0.65 |
| 4:B:69:ALA:O | 4:B:72:TYR:N | 2.29 | 0.65 |
| 5:C:43:VAL:O | 5:C:44:GLY:O | 2.15 | 0.65 |
| 1:I:5:DA:O4' | 3:A:39:HIS:HB2 | 1.96 | 0.64 |
| 1:I:78:DA:H2" | 1:I:79:DG:N7 | 2.11 | 0.64 |
| 5:G:119:LYS:HA | 5:G:119:LYS:CE | 2.22 | 0.64 |
| 1:I:105:DT:C2' | 1:I:106:DT:H71 | 2.28 | 0.64 |
| 3:A:124:ILE:O | 3:A:125:GLN:C | 2.36 | 0.64 |
| 1:I:90:DC:H2" | 1:I:91:DT:H71 | 1.79 | 0.64 |
| 1:I:123:DG:H2" | 1:I:124:DT:H71 | 1.79 | 0.64 |
| 1:I:132:DG:H2" | 1:I:133:DC:C5 | 2.32 | 0.64 |
| 2:J:230:DT:H3' | 3:E:46:VAL:HG21 | 1.78 | 0.64 |
| 5:C:42:ARG:HB2 | 6:D:85:THR:HG23 | 1.80 | 0.64 |
| 2:J:175:DA:H1' | 2:J:176:DA:H5' | 1.79 | 0.64 |
| 4:B:39:ARG:O | 4:B:42:GLY:N | 2.28 | 0.64 |
| 3:A:46:VAL:HG22 | 3:A:49:ARG:HH12 | 1.63 | 0.64 |
| 1:I:119:DT:H2" | 1:I:120:DT:C7 | 2.27 | 0.64 |
| 2:J:264:DC:C6 | 2:J:265:DT:H72 | 2.32 | 0.64 |
| 3:A:117:VAL:O | 4:B:44:LYS:HB3 | 1.98 | 0.64 |
| 5:C:72:ASP:C | 5:C:74:LYS:H | 2.01 | 0.64 |
| 6:H:92:GLN:C | 6:H:94:ALA:H | 2.00 | 0.64 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CG | 2.32 | 0.64 |
| 2:J:206:DG:H2" | 2:J:207:DC:C6 | 2.32 | 0.63 |
| 3:E:70:LEU:O | 3:E:74:ILE:HG13 | 1.99 | 0.63 |
| 2:J:215:DG:H4' | 3:A:42:ARG:NH2 | 2.14 | 0.63 |
| 4:B:96:THR:HG22 | 4:B:97:LEU:H | 1.62 | 0.63 |
| 3:E:92:LEU:HD11 | 4:F:66:ILE:HD12 | 1.81 | 0.63 |
| 1:I:21:DT:H1' | 1:I:22:DC:H5' | 1.79 | 0.63 |
| 3:E:119:ILE:CD1 | 4:F:43:VAL:HG11 | 2.24 | 0.63 |
| 5:G:38:ASN:C | 5:G:40:ALA:H | 2.01 | 0.63 |
| 3:A:76:GLN:C | 3:A:78:PHE:H | 2.02 | 0.63 |
| 1:I:61:DG:H2' | 4:F:32:PRO:HG2 | 1.80 | 0.63 |
| 2:J:220:DG:H2" | 2:J:221:DT:O5' | 1.98 | 0.63 |
| 1:I:69:DG:H5' | 3:E:43:PRO:CG | 2.29 | 0.62 |
| 1:I:135:DG:H2" | 1:I:136:DG:OP2 | 1.97 | 0.62 |
| 3:A:116:ARG:HH12 | 3:A:118:THR:HB | 1.64 | 0.62 |
| 5:G:83:LEU:HD13 | 6:H:58:ILE:HG22 | 1.80 | 0.62 |
| 2:J:230:DT:H4' | 2:J:231:DT:OP1 | 1.99 | 0.62 |
| 2:J:265:DT:H2" | 2:J:266:DT:O5' | 1.99 | 0.62 |
| 2:J:288:DT:H1' | 2:J:289:DA:C5' | 2.28 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:36:ARG:O | 4:B:39:ARG:HB2 | 1.99 | 0.62 |
| 1:I:61:DG:H1' | 1:I:62:DC:H5' | 1.81 | 0.62 |
| 3:A:116:ARG:NH2 | 3:A:118:THR:O | 2.30 | 0.62 |
| 5:C:102:ILE:CG2 | 6:D:58:ILE:HD13 | 2.23 | 0.62 |
| 3:E:114:ALA:O | 3:E:116:ARG:N | 2.33 | 0.62 |
| 4:F:29:ILE:HG22 | 4:F:34:ILE:HG12 | 1.80 | 0.62 |
| 4:F:97:LEU:HD12 | 4:F:98:TYR:H | 1.65 | 0.62 |
| 5:C:67:GLY:O | 5:C:70:ALA:N | 2.33 | 0.62 |
| 1:I:40:DA:H2" | 1:I:41:DA:OP2 | 1.99 | 0.62 |
| 5:C:90:ASP:OD2 | 5:C:93:LEU:HB2 | 2.00 | 0.62 |
| 4:F:36:ARG:HH11 | 4:F:36:ARG:HG3 | 1.64 | 0.62 |
| 3:A:45:THR:C | 3:A:47:ALA:H | 2.03 | 0.62 |
| 5:C:23:LEU:C | 5:C:24:GLN:HG2 | 2.20 | 0.62 |
| 5:G:64:GLU:O | 5:G:67:GLY:N | 2.33 | 0.62 |
| 5:G:103:ALA:O | 5:G:104:GLN:HB2 | 2.00 | 0.62 |
| 6:H:113:LYS:HB3 | 6:H:113:LYS:HZ3 | 1.64 | 0.62 |
| 6:D:81:ASN:O | 6:D:83:ARG:HG2 | 2.00 | 0.62 |
| 6:H:36:ILE:HD13 | 6:H:36:ILE:N | 2.13 | 0.62 |
| 4:F:84:MET:CE | 4:F:102:GLY:HA2 | 2.30 | 0.61 |
| 3:A:54:TYR:HA | 3:A:57:SER:OG | 1.99 | 0.61 |
| 2:J:258:DT:H1' | 2:J:259:DT:H5' | 1.81 | 0.61 |
| 1:I:7:DA:C3' | 3:A:49:ARG:HH21 | 2.13 | 0.61 |
| 1:I:59:DA:C4' | 1:I:60:DA:OP1 | 2.43 | 0.61 |
| 3:A:42:ARG:HG2 | 3:A:42:ARG:HH11 | 1.66 | 0.61 |
| 4:B:33:ALA:HA | 4:B:36:ARG:NH1 | 2.14 | 0.61 |
| 5:C:29:ARG:HG3 | 5:C:32:ARG:HH21 | 1.64 | 0.61 |
| 1:I:76:DT:H2" | 1:I:77:DC:OP2 | 2.01 | 0.61 |
| 1:I:113:DT:C5' | 5:C:42:ARG:HG2 | 2.31 | 0.61 |
| 6:D:101:GLY:O | 6:D:103:LEU:N | 2.34 | 0.61 |
| 2:J:237:DA:H2" | 2:J:238:DT:OP2 | 2.01 | 0.61 |
| 3:E:61:LEU:CD1 | 4:F:37:LEU:HA | 2.29 | 0.61 |
| 1:I:84:DA:H5' | 3:A:40:ARG:NH1 | 2.15 | 0.60 |
| 3:E:121:PRO:O | 3:E:125:GLN:HG3 | 2.01 | 0.60 |
| 1:I:5:DA:H61 | 2:J:290:DT:H3 | 1.49 | 0.60 |
| 1:I:50:DA:H2" | 1:I:51:DA:C8 | 2.36 | 0.60 |
| 1:I:117:DC:H2" | 1:I:118:DT:OP2 | 2.01 | 0.60 |
| 3:A:107:THR:O | 3:A:110:CYS:HB2 | 2.00 | 0.60 |
| 5:C:25:PHE:CE1 | 5:C:56:GLU:HA | 2.35 | 0.60 |
| 6:D:35:ALA:HA | 6:D:56:MET:SD | 2.40 | 0.60 |
| 1:I:6:DT:H2" | 1:I:7:DA:OP2 | 2.01 | 0.60 |
| 3:A:130:ILE:HG22 | 3:E:130:ILE:HG21 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:267:DT:H2" | 2:J:268:DT:OP2 | 2.01 | 0.60 |
| 5:C:38:ASN:HD21 | 5:G:38:ASN:HD22 | 1.50 | 0.60 |
| 6:D:69:ARG:HB3 | 6:D:98:LEU:HD21 | 1.84 | 0.60 |
| 1:I:69:DG:H5' | 3:E:43:PRO:CB | 2.32 | 0.60 |
| 2:J:169:DC:H1' | 2:J:170:DT:O5' | 2.01 | 0.60 |
| 2:J:284:DT:H2" | 2:J:285:DG:OP2 | 2.01 | 0.60 |
| 3:E:108:ASN:O | 3:E:110:CYS:N | 2.35 | 0.60 |
| 4:F:54:THR:O | 4:F:57:VAL:HG12 | 2.01 | 0.60 |
| 3:A:116:ARG:CZ | 3:A:120:MET:HE3 | 2.32 | 0.60 |
| 1:I:22:DC:H2" | 1:I:23:DT:OP2 | 2.01 | 0.60 |
| 2:J:291:DT:H1' | 2:J:292:DG:C8 | 2.36 | 0.60 |
| 5:G:83:LEU:HD13 | 6:H:58:ILE:CG2 | 2.32 | 0.60 |
| 6:H:113:LYS:O | 6:H:114:ALA:C | 2.40 | 0.60 |
| 2:J:201:DA:H2" | 2:J:202:DA:OP2 | 2.02 | 0.59 |
| 3:E:105:GLU:C | 3:E:107:THR:H | 2.05 | 0.59 |
| 6:D:102:GLU:O | 6:D:106:HIS:CD2 | 2.55 | 0.59 |
| 3:E:96:SER:HA | 4:F:61:PHE:CE2 | 2.38 | 0.59 |
| 5:G:58:LEU:O | 5:G:62:ILE:HG12 | 2.02 | 0.59 |
| 2:J:247:DT:H2" | 2:J:248:DT:C7 | 2.30 | 0.59 |
| 5:C:79:ILE:HG22 | 6:D:52:SER:HB3 | 1.83 | 0.59 |
| 6:D:116:THR:HG22 | 6:D:117:LYS:N | 2.16 | 0.59 |
| 1:I:26:DC:H4' | 1:I:27:DA:OP1 | 2.03 | 0.59 |
| 2:J:177:DA:H1' | 2:J:178:DG:C8 | 2.38 | 0.59 |
| 3:E:51:ILE:O | 3:E:53:ARG:N | 2.35 | 0.59 |
| 4:B:51:TYR:HB3 | 4:B:55:ARG:NH1 | 2.17 | 0.59 |
| 2:J:216:DC:H2" | 2:J:217:DT:C6 | 2.38 | 0.59 |
| 3:E:105:GLU:O | 3:E:107:THR:N | 2.35 | 0.59 |
| 5:G:24:GLN:OE1 | 6:H:40:LYS:HB3 | 2.03 | 0.59 |
| 1:I:47:DA:H1' | 1:I:48:DA:H5' | 1.85 | 0.59 |
| 1:I:53:DC:H2" | 1:I:54:DA:OP2 | 2.02 | 0.59 |
| 2:J:292:DG:OP2 | 3:A:42:ARG:HB2 | 2.03 | 0.59 |
| 5:C:90:ASP:OD2 | 5:C:93:LEU:N | 2.35 | 0.59 |
| 5:G:26:PRO:HD3 | 6:H:37:TYR:CD1 | 2.38 | 0.59 |
| 1:I:27:DA:H2" | 1:I:28:DA:OP2 | 2.03 | 0.59 |
| 1:I:33:DG:H1' | 1:I:34:DT:H5' | 1.84 | 0.59 |
| 2:J:163:DC:H2" | 2:J:164:DA:N7 | 2.18 | 0.59 |
| 3:A:58:THR:C | 4:B:40:ARG:HH22 | 2.05 | 0.59 |
| 5:C:24:GLN:NE2 | 6:D:44:GLN:NE2 | 2.51 | 0.59 |
| 3:E:60:LEU:HA | 3:E:97:GLU:OE2 | 2.03 | 0.59 |
| 3:E:67:PHE:CD2 | 3:E:93:GLN:HG3 | 2.38 | 0.59 |
| 2:J:231:DT:H5' | 3:E:40:ARG:HG2 | 1.84 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:241:DT:H1' | 2:J:242:DG:H5' | 1.85 | 0.58 |
| 5:G:77:ARG:HG2 | 5:G:78:ILE:N | 2.15 | 0.58 |
| 5:G:96:LEU:HD12 | 5:G:96:LEU:O | 2.03 | 0.58 |
| 1:I:11:DA:H1' | 1:I:12:DC:OP1 | 2.03 | 0.58 |
| 1:I:16:DC:H2" | 1:I:17:DA:OP2 | 2.01 | 0.58 |
| 2:J:208:DA:H5' | 3:A:63:ARG:NH2 | 2.19 | 0.58 |
| 3:A:87:SER:HB2 | 4:B:83:ALA:HB2 | 1.85 | 0.58 |
| 3:A:101:VAL:O | 3:A:104:PHE:HB2 | 2.03 | 0.58 |
| 5:G:51:LEU:HD21 | 6:H:67:PHE:HE1 | 1.63 | 0.58 |
| 3:A:84:PHE:HB3 | 3:A:89:VAL:HG23 | 1.84 | 0.58 |
| 5:G:25:PHE:CE1 | 5:G:56:GLU:HA | 2.38 | 0.58 |
| 1:I:36:DA:H2" | 1:I:37:DA:OP2 | 2.02 | 0.58 |
| 6:D:36:ILE:HG13 | 6:D:37:TYR:N | 2.17 | 0.58 |
| 4:F:37:LEU:O | 4:F:39:ARG:N | 2.37 | 0.58 |
| 5:G:78:ILE:HA | 5:G:82:HIS:CE1 | 2.39 | 0.58 |
| 6:H:54:LYS:O | 6:H:58:ILE:HD13 | 2.03 | 0.58 |
| 1:I:132:DG:H4' | 5:C:77:ARG:NH2 | 2.19 | 0.58 |
| 5:C:47:ALA:HB1 | 6:D:91:ILE:HD12 | 1.84 | 0.58 |
| 3:E:123:ASP:O | 3:E:126:LEU:N | 2.36 | 0.58 |
| 4:F:31:LYS:HB3 | 4:F:32:PRO:HD3 | 1.85 | 0.58 |
| 1:I:30:DA:H2" | 1:I:31:DG:OP2 | 2.03 | 0.58 |
| 2:J:277:DG:H2" | 2:J:278:DT:OP2 | 2.03 | 0.58 |
| 4:B:33:ALA:HB1 | 4:B:36:ARG:NH2 | 2.18 | 0.58 |
| 4:F:45:ARG:HG2 | 4:F:45:ARG:NH1 | 2.16 | 0.58 |
| 2:J:260:DG:H3' | 5:G:35:ARG:HH12 | 1.68 | 0.58 |
| 5:G:26:PRO:HD3 | 6:H:37:TYR:CD2 | 2.39 | 0.58 |
| 5:G:26:PRO:HB3 | 6:H:37:TYR:CZ | 2.39 | 0.58 |
| 3:A:103:LEU:CD2 | 3:A:128:ARG:HD2 | 2.33 | 0.58 |
| 4:F:50:ILE:HG22 | 4:F:51:TYR:N | 2.18 | 0.58 |
| 5:G:43:VAL:HG12 | 5:G:44:GLY:O | 2.04 | 0.58 |
| 2:J:155:DT:H1' | 2:J:156:DC:H5' | 1.85 | 0.57 |
| 5:C:35:ARG:O | 5:C:37:GLY:N | 2.37 | 0.57 |
| 1:I:5:DA:H4' | 3:A:39:HIS:CB | 2.27 | 0.57 |
| 1:I:84:DA:C2' | 1:I:85:DC:OP2 | 2.47 | 0.57 |
| 2:J:217:DT:H2" | 2:J:218:DG:N7 | 2.19 | 0.57 |
| 3:A:73:GLU:OE1 | 4:B:25:ASN:HB3 | 2.05 | 0.57 |
| 3:A:85:GLN:HG3 | 4:B:82:THR:HA | 1.85 | 0.57 |
| 3:A:116:ARG:HB3 | 3:A:116:ARG:NH1 | 2.18 | 0.57 |
| 5:C:92:GLU:HA | 5:C:92:GLU:OE2 | 2.03 | 0.57 |
| 5:C:23:LEU:HD23 | 5:C:53:ALA:HA | 1.86 | 0.57 |
| 3:E:118:THR:OG1 | 4:F:45:ARG:HG2 | 2.05 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:47:SER:OG | 4:F:48:GLY:N | 2.37 | 0.57 |
| 1:I:58:DT:O2 | 1:I:59:DA:N1 | 2.37 | 0.57 |
| 1:I:58:DT:O2 | 1:I:59:DA:C2 | 2.58 | 0.57 |
| 1:I:83:DA:H2" | 1:I:84:DA:OP2 | 2.03 | 0.57 |
| 2:J:215:DG:H4' | 3:A:42:ARG:CZ | 2.35 | 0.57 |
| 3:A:49:ARG:O | 3:A:53:ARG:HB2 | 2.05 | 0.57 |
| 3:A:67:PHE:O | 3:A:70:LEU:HB3 | 2.05 | 0.57 |
| 3:A:92:LEU:HD21 | 4:B:86:VAL:HG22 | 1.85 | 0.57 |
| 3:A:92:LEU:HD23 | 4:B:86:VAL:HG11 | 1.86 | 0.57 |
| 3:E:119:ILE:O | 4:F:47:SER:HB3 | 2.04 | 0.57 |
| 3:A:61:LEU:N | 3:A:61:LEU:HD23 | 2.19 | 0.57 |
| 3:A:123:ASP:O | 3:A:124:ILE:C | 2.42 | 0.57 |
| 5:C:30:VAL:O | 5:C:34:LEU:HD12 | 2.04 | 0.57 |
| 6:H:36:ILE:H | 6:H:36:ILE:CD1 | 2.17 | 0.57 |
| 5:C:26:PRO:HG3 | 5:C:29:ARG:HD2 | 1.85 | 0.57 |
| 5:C:50:TYR:HE1 | 6:D:112:THR:N | 2.02 | 0.57 |
| 3:E:60:LEU:HG | 3:E:97:GLU:OE2 | 2.05 | 0.57 |
| 5:C:31:HIS:O | 5:C:34:LEU:HB2 | 2.05 | 0.57 |
| 3:E:87:SER:O | 3:E:90:MET:N | 2.35 | 0.57 |
| 5:G:112:GLN:O | 5:G:114:VAL:N | 2.38 | 0.57 |
| 2:J:148:DA:H2" | 2:J:149:DT:H72 | 1.86 | 0.56 |
| 6:D:69:ARG:HB3 | 6:D:98:LEU:CD2 | 2.35 | 0.56 |
| 1:I:141:DT:H2" | 1:I:142:DA:C8 | 2.40 | 0.56 |
| 2:J:247:DT:C2' | 2:J:248:DT:H72 | 2.34 | 0.56 |
| 3:E:99:TYR:HE1 | 3:E:131:ARG:HH12 | 1.52 | 0.56 |
| 3:E:108:ASN:OD1 | 4:F:43:VAL:HG22 | 2.05 | 0.56 |
| 4:B:44:LYS:CD | 5:G:115:LEU:HD22 | 2.24 | 0.56 |
| 1:I:121:DT:O4 | 2:J:173:DC:N4 | 2.38 | 0.56 |
| 4:F:57:VAL:CG1 | 4:F:58:LEU:N | 2.67 | 0.56 |
| 5:C:23:LEU:CD2 | 5:C:53:ALA:HA | 2.35 | 0.56 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CE2 | 2.40 | 0.56 |
| 6:D:51:ILE:HD13 | 6:D:56:MET:CE | 2.36 | 0.56 |
| 3:E:108:ASN:C | 3:E:110:CYS:H | 2.09 | 0.56 |
| 4:F:75:HIS:CB | 6:H:93:THR:HG21 | 2.24 | 0.56 |
| 1:I:137:DT:C2 | 1:I:138:DG:N7 | 2.74 | 0.56 |
| 3:E:119:ILE:HD13 | 4:F:43:VAL:CG1 | 2.30 | 0.56 |
| 3:E:120:MET:O | 3:E:123:ASP:HB2 | 2.04 | 0.56 |
| 5:G:47:ALA:N | 5:G:48:PRO:HD2 | 2.20 | 0.56 |
| 3:A:120:MET:C | 4:B:50:ILE:HD11 | 2.26 | 0.56 |
| 1:I:25:DC:H2" | 1:I:26:DC:OP2 | 2.05 | 0.56 |
| 1:I:31:DG:H2" | 1:I:32:DT:OP2 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:90:DC:H2" | 1:I:91:DT:C7 | 2.35 | 0.56 |
| 6:D:39:TYR:O | 6:D:42:LEU:HB3 | 2.05 | 0.56 |
| 3:E:120:MET:HG2 | 4:F:47:SER:HB2 | 1.88 | 0.56 |
| 2:J:288:DT:H1' | 2:J:289:DA:H5' | 1.88 | 0.55 |
| 3:A:130:ILE:CG2 | 3:E:130:ILE:CG2 | 2.84 | 0.55 |
| 4:B:47:SER:HB3 | 4:B:50:ILE:CG1 | 2.33 | 0.55 |
| 5:C:51:LEU:C | 5:C:53:ALA:N | 2.59 | 0.55 |
| 1:I:23:DT:OP1 | 1:I:23:DT:H3' | 2.06 | 0.55 |
| 2:J:203:DA:C6 | 2:J:204:DA:N6 | 2.74 | 0.55 |
| 5:C:39:TYR:O | 6:D:75:SER:OG | 2.21 | 0.55 |
| 2:J:164:DA:H2" | 2:J:165:DG:C8 | 2.41 | 0.55 |
| 2:J:205:DG:H1' | 2:J:206:DG:N7 | 2.20 | 0.55 |
| 5:G:52:ALA:O | 5:G:55:LEU:HB2 | 2.06 | 0.55 |
| 5:G:96:LEU:HG | 5:G:97:LEU:HD23 | 1.88 | 0.55 |
| 2:J:154:DA:H4' | 3:E:49:ARG:NH2 | 2.21 | 0.55 |
| 2:J:204:DA:C1' | 2:J:205:DG:O5' | 2.54 | 0.55 |
| 3:A:49:ARG:HB2 | 3:A:49:ARG:HH11 | 1.72 | 0.55 |
| 4:F:82:THR:O | 4:F:85:ASP:HB2 | 2.07 | 0.55 |
| 5:G:50:TYR:HD2 | 5:G:50:TYR:O | 1.89 | 0.55 |
| 6:H:106:HIS:O | 6:H:109:SER:HB3 | 2.07 | 0.55 |
| 1:I:57:DA:H2" | 1:I:58:DT:OP2 | 2.06 | 0.55 |
| 1:I:109:DC:C5 | 1:I:110:DA:C6 | 2.94 | 0.55 |
| 2:J:229:DA:H2" | 2:J:230:DT:O5' | 2.04 | 0.55 |
| 2:J:275:DA:H3' | 2:J:275:DA:OP1 | 2.06 | 0.55 |
| 6:H:51:ILE:HD13 | 6:H:52:SER:O | 2.06 | 0.55 |
| 5:C:50:TYR:HD2 | 6:D:91:ILE:CG2 | 2.20 | 0.55 |
| 1:I:84:DA:H5" | 3:A:40:ARG:HG2 | 1.88 | 0.55 |
| 2:J:215:DG:H1' | 2:J:216:DC:H5' | 1.87 | 0.55 |
| 4:B:38:ALA:O | 4:B:43:VAL:HG23 | 2.07 | 0.55 |
| 1:I:4:DA:H2" | 1:I:5:DA:OP2 | 2.06 | 0.55 |
| 2:J:229:DA:H2' | 2:J:230:DT:H71 | 1.87 | 0.55 |
| 3:A:42:ARG:CZ | 3:A:42:ARG:HA | 2.37 | 0.55 |
| 3:A:45:THR:HG22 | 3:A:49:ARG:NH1 | 2.22 | 0.55 |
| 3:A:75:ALA:O | 3:A:78:PHE:N | 2.37 | 0.55 |
| 3:A:76:GLN:HA | 3:A:79:LYS:O | 2.06 | 0.55 |
| 5:C:67:GLY:HA3 | 6:D:46:HIS:HD2 | 1.69 | 0.55 |
| 6:D:39:TYR:HA | 6:D:42:LEU:HB3 | 1.89 | 0.55 |
| 2:J:230:DT:P | 3:E:46:VAL:HB | 2.47 | 0.55 |
| 1:I:126:DG:H2" | 1:I:127:DT:OP2 | 2.07 | 0.55 |
| 2:J:241:DT:H2" | 2:J:242:DG:H5' | 1.89 | 0.55 |
| 2:J:255:DT:H2" | 2:J:256:DT:C7 | 2.36 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:60:LEU:C | 3:A:61:LEU:HD23 | 2.27 | 0.55 |
| 4:B:97:LEU:CD1 | 5:G:101:THR:HG22 | 2.36 | 0.55 |
| 5:C:107:VAL:CG2 | 5:C:108:LEU:N | 2.70 | 0.55 |
| 2:J:260:DG:H2" | 2:J:261:DA:C8 | 2.41 | 0.54 |
| 3:E:108:ASN:ND2 | 4:F:42:GLY:O | 2.40 | 0.54 |
| 6:H:71:ALA:O | 6:H:75:SER:N | 2.37 | 0.54 |
| 1:I:41:DA:H2" | 1:I:42:DA:OP2 | 2.05 | 0.54 |
| 3:A:74:ILE:HG22 | 3:A:75:ALA:N | 2.22 | 0.54 |
| 5:C:50:TYR:CD2 | 6:D:91:ILE:HG22 | 2.42 | 0.54 |
| 6:D:34:TYR:CE2 | 6:D:63:VAL:HG11 | 2.42 | 0.54 |
| 5:G:22:GLY:O | 5:G:23:LEU:HD23 | 2.07 | 0.54 |
| 1:I:69:DG:H2" | 1:I:70:DG:C8 | 2.43 | 0.54 |
| 2:J:275:DA:C2' | 2:J:276:DT:OP2 | 2.50 | 0.54 |
| 3:E:108:ASN:C | 3:E:110:CYS:N | 2.60 | 0.54 |
| 4:F:33:ALA:HA | 4:F:36:ARG:NH1 | 2.22 | 0.54 |
| 4:F:86:VAL:O | 4:F:89:ALA:HB3 | 2.06 | 0.54 |
| 2:J:285:DG:H2" | 2:J:286:DG:O5' | 2.07 | 0.54 |
| 5:C:76:THR:O | 6:D:50:GLY:N | 2.39 | 0.54 |
| 4:F:31:LYS:HG2 | 4:F:51:TYR:CE2 | 2.42 | 0.54 |
| 3:A:45:THR:O | 3:A:48:LEU:N | 2.40 | 0.54 |
| 5:C:94:ASN:O | 5:C:98:GLY:N | 2.40 | 0.54 |
| 3:E:108:ASN:HD21 | 4:F:43:VAL:HA | 1.71 | 0.54 |
| 1:I:20:DT:H2" | 1:I:21:DT:OP2 | 2.08 | 0.54 |
| 4:B:38:ALA:HB1 | 4:B:43:VAL:HG21 | 1.89 | 0.54 |
| 1:I:41:DA:H1' | 1:I:42:DA:H5' | 1.90 | 0.54 |
| 1:I:86:DA:N6 | 2:J:209:DT:H3 | 2.05 | 0.54 |
| 1:I:26:DC:H2" | 1:I:27:DA:N7 | 2.22 | 0.54 |
| 1:I:91:DT:H4' | 3:A:63:ARG:CD | 2.23 | 0.54 |
| 1:I:95:DG:C1' | 1:I:96:DA:H5' | 2.37 | 0.54 |
| 2:J:253:DT:C2' | 2:J:254:DT:H72 | 2.38 | 0.54 |
| 3:A:116:ARG:NH1 | 3:A:118:THR:HB | 2.21 | 0.54 |
| 5:C:35:ARG:C | 5:C:37:GLY:H | 2.10 | 0.54 |
| 6:D:101:GLY:O | 6:D:102:GLU:C | 2.46 | 0.54 |
| 3:E:65:LEU:HB3 | 3:E:66:PRO:HD3 | 1.90 | 0.54 |
| 3:E:104:PHE:CD1 | 4:F:38:ALA:HA | 2.43 | 0.54 |
| 3:E:117:VAL:O | 4:F:45:ARG:HB3 | 2.07 | 0.54 |
| 3:A:76:GLN:C | 3:A:78:PHE:N | 2.62 | 0.54 |
| 4:B:29:ILE:N | 4:B:29:ILE:HD12 | 2.23 | 0.54 |
| 5:C:80:PRO:HB3 | 6:D:58:ILE:CD1 | 2.38 | 0.54 |
| 5:C:110:ASN:O | 3:E:55:GLN:OE1 | 2.26 | 0.54 |
| 4:F:35:ARG:HG2 | 4:F:36:ARG:N | 2.23 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:75:HIS:HA | 6:H:89:ARG:HH12 | 1.73 | 0.54 |
| 5:G:97:LEU:O | 5:G:99:ARG:N | 2.41 | 0.54 |
| 1:I:71:DC:OP1 | 3:E:116:ARG:HB3 | 2.08 | 0.54 |
| 2:J:275:DA:H3' | 2:J:275:DA:P | 2.48 | 0.53 |
| 5:C:72:ASP:O | 5:C:74:LYS:N | 2.38 | 0.53 |
| 4:F:76:ALA:O | 4:F:77:LYS:HB2 | 2.08 | 0.53 |
| 1:I:12:DC:H2" | 1:I:13:DC:OP2 | 2.08 | 0.53 |
| 4:B:33:ALA:O | 4:B:36:ARG:HB2 | 2.09 | 0.53 |
| 5:C:23:LEU:HD12 | 5:C:23:LEU:H | 1.71 | 0.53 |
| 6:D:118:TYR:C | 6:D:120:SER:H | 2.11 | 0.53 |
| 3:E:124:ILE:O | 3:E:128:ARG:HG3 | 2.08 | 0.53 |
| 5:G:30:VAL:O | 5:G:34:LEU:HB2 | 2.08 | 0.53 |
| 6:D:34:TYR:CD1 | 6:D:34:TYR:N | 2.77 | 0.53 |
| 5:G:116:LEU:HB3 | 5:G:117:PRO:HD2 | 1.89 | 0.53 |
| 2:J:178:DG:H2' | 2:J:179:DT:H72 | 1.91 | 0.53 |
| 2:J:268:DT:H2" | 2:J:269:DG:N7 | 2.24 | 0.53 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CD1 | 2.43 | 0.53 |
| 1:I:81:DT:H2" | 1:I:82:DG:OP2 | 2.08 | 0.53 |
| 1:I:82:DG:H5" | 4:B:45:ARG:HG3 | 1.90 | 0.53 |
| 1:I:9:DC:H2" | 1:I:10:DC:OP2 | 2.07 | 0.53 |
| 1:I:121:DT:H2" | 1:I:122:DG:C5 | 2.43 | 0.53 |
| 5:C:35:ARG:C | 5:C:37:GLY:N | 2.62 | 0.53 |
| 4:F:28:GLY:O | 4:F:30:THR:HG23 | 2.08 | 0.53 |
| 6:H:71:ALA:O | 6:H:74:ALA:HB3 | 2.08 | 0.53 |
| 1:I:23:DT:H1' | 1:I:24:DA:O4' | 2.08 | 0.53 |
| 2:J:232:DA:H2" | 2:J:233:DG:C8 | 2.44 | 0.53 |
| 5:C:24:GLN:HE22 | 6:D:44:GLN:NE2 | 2.06 | 0.53 |
| 5:C:116:LEU:HD23 | 5:C:117:PRO:HD2 | 1.90 | 0.53 |
| 5:G:23:LEU:HD12 | 5:G:27:VAL:HG21 | 1.91 | 0.53 |
| 3:E:76:GLN:OE1 | 4:F:22:LEU:HD12 | 2.09 | 0.53 |
| 5:C:17:ARG:CD | 6:D:118:TYR:OH | 2.56 | 0.53 |
| 6:D:51:ILE:HD13 | 6:D:56:MET:HE3 | 1.91 | 0.53 |
| 5:G:39:TYR:O | 5:G:40:ALA:HB2 | 2.08 | 0.53 |
| 6:H:95:VAL:HG12 | 6:H:96:ARG:N | 2.23 | 0.53 |
| 6:H:99:LEU:O | 6:H:104:ALA:HB2 | 2.09 | 0.53 |
| 1:I:15:DG:H1' | 1:I:16:DC:C5' | 2.38 | 0.53 |
| 1:I:81:DT:C4' | 4:B:45:ARG:HE | 2.05 | 0.53 |
| 1:I:101:DG:H5" | 3:A:83:ARG:HD2 | 1.90 | 0.53 |
| 2:J:289:DA:C2' | 2:J:290:DT:H72 | 2.39 | 0.53 |
| 3:A:45:THR:HG22 | 3:A:49:ARG:HH11 | 1.74 | 0.53 |
| 3:A:60:LEU:HD13 | 3:A:93:GLN:HG2 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:B:98:TYR:CZ | 5:G:100:VAL:HG21 | 2.44 | 0.53 |
| 1:I:141:DT:H2" | 1:I:142:DA:H8 | 1.72 | 0.52 |
| 2:J:279:DG:H4' | 2:J:280:DC:OP1 | 2.09 | 0.52 |
| 4:F:65:VAL:O | 4:F:66:ILE:C | 2.46 | 0.52 |
| 3:A:60:LEU:HD21 | 3:A:94:GLU:OE1 | 2.10 | 0.52 |
| 3:A:129:ARG:HE | 3:A:130:ILE:CD1 | 2.21 | 0.52 |
| 5:C:116:LEU:CD2 | 5:C:117:PRO:HD2 | 2.40 | 0.52 |
| 3:E:118:THR:HA | 4:F:45:ARG:HB3 | 1.91 | 0.52 |
| 6:H:75:SER:O | 6:H:78:ALA:HB3 | 2.10 | 0.52 |
| 3:A:60:LEU:HD21 | 3:A:94:GLU:CD | 2.30 | 0.52 |
| 5:C:79:ILE:O | 5:C:81:ARG:N | 2.42 | 0.52 |
| 3:E:51:ILE:O | 3:E:52:ARG:C | 2.48 | 0.52 |
| 1:I:51:DA:OP1 | 3:E:72:ARG:NH1 | 2.42 | 0.52 |
| 3:A:120:MET:HB3 | 3:A:122:LYS:HG2 | 1.91 | 0.52 |
| 1:I:45:DA:H2" | 1:I:46:DA:OP2 | 2.09 | 0.52 |
| 2:J:207:DC:C4' | 3:A:63:ARG:HH21 | 2.22 | 0.52 |
| 6:H:51:ILE:HD11 | 6:H:56:MET:CA | 2.39 | 0.52 |
| 1:I:28:DA:H2" | 1:I:29:DA:OP2 | 2.09 | 0.52 |
| 1:I:113:DT:P | 5:C:35:ARG:HH22 | 2.33 | 0.52 |
| 2:J:239:DC:OP1 | 3:E:63:ARG:NE | 2.37 | 0.52 |
| 3:A:54:TYR:O | 3:A:57:SER:N | 2.41 | 0.52 |
| 3:A:92:LEU:HD21 | 4:B:86:VAL:HG21 | 1.91 | 0.52 |
| 3:E:120:MET:CA | 4:F:50:ILE:HD11 | 2.40 | 0.52 |
| 6:H:36:ILE:HG12 | 6:H:37:TYR:CD1 | 2.45 | 0.52 |
| 1:I:12:DC:H1' | 1:I:13:DC:O5' | 2.09 | 0.52 |
| 5:C:39:TYR:CB | 6:D:75:SER:HB2 | 2.23 | 0.52 |
| 5:C:50:TYR:CE1 | 6:D:112:THR:N | 2.78 | 0.52 |
| 6:D:115:VAL:O | 6:D:116:THR:C | 2.48 | 0.52 |
| 6:H:92:GLN:C | 6:H:94:ALA:N | 2.61 | 0.52 |
| 1:I:3:DC:H2" | 1:I:4:DA:OP2 | 2.09 | 0.52 |
| 1:I:145:DG:H2" | 1:I:146:DA:OP2 | 2.10 | 0.52 |
| 5:C:50:TYR:HE2 | 6:D:92:GLN:HA | 1.75 | 0.52 |
| 5:C:107:VAL:HG23 | 5:C:108:LEU:H | 1.74 | 0.52 |
| 5:C:112:GLN:HB2 | 5:C:115:LEU:CD1 | 2.40 | 0.52 |
| 3:E:105:GLU:C | 3:E:107:THR:N | 2.62 | 0.52 |
| 3:E:119:ILE:CD1 | 4:F:46:ILE:HG23 | 2.36 | 0.52 |
| 6:H:81:ASN:HB3 | 6:H:83:ARG:HE | 1.72 | 0.52 |
| 3:E:66:PRO:HB3 | 4:F:28:GLY:HA3 | 1.91 | 0.52 |
| 3:E:97:GLU:O | 3:E:98:ALA:C | 2.48 | 0.52 |
| 1:I:87:DT:H2" | 1:I:88:DG:O5' | 2.09 | 0.51 |
| 3:A:117:VAL:HB | 4:B:44:LYS:CG | 2.16 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:D:36:ILE:HD11 | 6:D:37:TYR:CZ | 2.45 | 0.51 |
| 2:J:169:DC:H2" | 2:J:170:DT:O5' | 2.09 | 0.51 |
| 2:J:232:DA:H1' | 2:J:233:DG:C8 | 2.46 | 0.51 |
| 3:A:108:ASN:HD21 | 3:A:112:ILE:HD11 | 1.76 | 0.51 |
| 5:C:102:ILE:HG23 | 6:D:58:ILE:CD1 | 2.27 | 0.51 |
| 3:E:119:ILE:HG12 | 4:F:46:ILE:HA | 1.92 | 0.51 |
| 2:J:255:DT:C2' | 2:J:256:DT:H72 | 2.38 | 0.51 |
| 5:C:77:ARG:HA | 6:D:50:GLY:O | 2.11 | 0.51 |
| 3:E:51:ILE:HG22 | 3:E:52:ARG:H | 1.75 | 0.51 |
| 1:I:84:DA:OP1 | 3:A:40:ARG:HA | 2.11 | 0.51 |
| 2:J:215:DG:H2" | 2:J:216:DC:OP2 | 2.10 | 0.51 |
| 2:J:291:DT:C4' | 2:J:292:DG:OP1 | 2.50 | 0.51 |
| 3:A:119:ILE:O | 3:A:119:ILE:CG1 | 2.49 | 0.51 |
| 5:C:31:HIS:CD2 | 5:C:48:PRO:HG3 | 2.45 | 0.51 |
| 3:E:41:TYR:O | 3:E:42:ARG:O | 2.28 | 0.51 |
| 6:H:36:ILE:HG12 | 6:H:37:TYR:N | 2.25 | 0.51 |
| 2:J:255:DT:H1' | 2:J:256:DT:C6 | 2.46 | 0.51 |
| 3:A:92:LEU:O | 3:A:96:SER:N | 2.40 | 0.51 |
| 4:B:78:ARG:NH1 | 4:B:82:THR:HG21 | 2.25 | 0.51 |
| 3:E:107:THR:O | 3:E:110:CYS:HB2 | 2.10 | 0.51 |
| 1:I:82:DG:C5' | 4:B:45:ARG:HG3 | 2.40 | 0.51 |
| 3:A:76:GLN:HE22 | 3:A:80:THR:CA | 2.06 | 0.51 |
| 3:A:85:GLN:O | 3:A:86:SER:C | 2.48 | 0.51 |
| 5:C:111:ILE:HG22 | 5:C:112:GLN:O | 2.10 | 0.51 |
| 3:E:64:LYS:HE2 | 3:E:90:MET:HE1 | 1.92 | 0.51 |
| 1:I:24:DA:H2" | 1:I:25:DC:OP2 | 2.09 | 0.51 |
| 3:A:42:ARG:NH2 | 3:A:43:PRO:HD3 | 2.25 | 0.51 |
| 5:C:108:LEU:HD23 | 5:C:109:PRO:HD2 | 1.93 | 0.51 |
| 3:A:86:SER:O | 3:A:90:MET:HG2 | 2.11 | 0.51 |
| 5:C:39:TYR:O | 6:D:75:SER:CB | 2.59 | 0.51 |
| 3:E:51:ILE:CG2 | 3:E:52:ARG:N | 2.66 | 0.51 |
| 1:I:84:DA:OP1 | 3:A:40:ARG:CA | 2.58 | 0.51 |
| 1:I:91:DT:C4' | 3:A:63:ARG:HD3 | 2.21 | 0.51 |
| 2:J:283:DG:H2" | 2:J:284:DT:H71 | 1.93 | 0.51 |
| 4:F:66:ILE:HD13 | 4:F:66:ILE:N | 2.25 | 0.51 |
| 6:H:73:GLU:OE1 | 6:H:73:GLU:HA | 2.11 | 0.51 |
| 1:I:69:DG:H5' | 3:E:43:PRO:HG2 | 1.92 | 0.50 |
| 2:J:196:DC:H2" | 2:J:197:DC:C5 | 2.46 | 0.50 |
| 6:D:111:GLY:O | 6:D:112:THR:C | 2.48 | 0.50 |
| 6:H:94:ALA:O | 6:H:98:LEU:HD13 | 2.12 | 0.50 |
| 2:J:229:DA:C5 | 2:J:230:DT:C4 | 2.98 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:235:DT:H2" | 2:J:236:DT:C7 | 2.35 | 0.50 |
| 3:A:129:ARG:HG3 | 3:A:130:ILE:HD13 | 1.93 | 0.50 |
| 3:E:126:LEU:O | 3:E:129:ARG:N | 2.44 | 0.50 |
| 6:H:59:MET:O | 6:H:63:VAL:HG23 | 2.11 | 0.50 |
| 3:A:85:GLN:O | 3:A:88:ALA:N | 2.44 | 0.50 |
| 5:C:104:GLN:N | 3:E:94:GLU:OE1 | 2.37 | 0.50 |
| 5:G:17:ARG:HG2 | 6:H:118:TYR:CZ | 2.46 | 0.50 |
| 3:E:120:MET:HA | 4:F:50:ILE:HD11 | 1.93 | 0.50 |
| 4:F:46:ILE:CG2 | 4:F:50:ILE:HG21 | 2.42 | 0.50 |
| 2:J:274:DA:H1' | 2:J:275:DA:C5' | 2.41 | 0.50 |
| 2:J:285:DG:H1' | 2:J:286:DG:C5' | 2.40 | 0.50 |
| 3:A:126:LEU:O | 3:A:129:ARG:N | 2.37 | 0.50 |
| 3:E:85:GLN:HG3 | 4:F:82:THR:HA | 1.93 | 0.50 |
| 5:G:51:LEU:CD2 | 6:H:67:PHE:HE1 | 2.25 | 0.50 |
| 5:G:60:ALA:O | 5:G:62:ILE:N | 2.45 | 0.50 |
| 1:I:5:DA:N6 | 2:J:290:DT:H3 | 2.10 | 0.50 |
| 1:I:17:DA:H2" | 1:I:18:DC:OP2 | 2.11 | 0.50 |
| 1:I:83:DA:C5' | 3:A:43:PRO:HA | 2.38 | 0.50 |
| 2:J:155:DT:H2" | 2:J:156:DC:O5' | 2.11 | 0.50 |
| 2:J:242:DG:OP2 | 2:J:242:DG:H3' | 2.11 | 0.50 |
| 4:B:99:GLY:HA2 | 6:H:58:ILE:HD12 | 1.93 | 0.50 |
| 1:I:23:DT:H3' | 1:I:23:DT:P | 2.50 | 0.50 |
| 2:J:181:DT:H2" | 2:J:182:DA:OP2 | 2.12 | 0.50 |
| 3:E:70:LEU:HD13 | 4:F:26:ILE:CA | 2.41 | 0.50 |
| 4:F:39:ARG:NH1 | 4:F:44:LYS:HA | 2.27 | 0.50 |
| 4:F:66:ILE:HG22 | 4:F:70:VAL:HG23 | 1.93 | 0.50 |
| 5:G:26:PRO:O | 5:G:29:ARG:HG2 | 2.11 | 0.50 |
| 5:G:38:ASN:O | 5:G:40:ALA:N | 2.43 | 0.50 |
| 1:I:54:DA:H2" | 1:I:55:DT:O5' | 2.11 | 0.50 |
| 1:I:127:DT:H3' | 1:I:127:DT:OP2 | 2.10 | 0.50 |
| 2:J:185:DT:O3' | 2:J:186:DG:C8 | 2.65 | 0.50 |
| 3:A:130:ILE:CG2 | 3:E:130:ILE:HG21 | 2.41 | 0.50 |
| 4:B:58:LEU:HD12 | 4:B:58:LEU:O | 2.11 | 0.50 |
| 5:C:30:VAL:HG13 | 5:C:51:LEU:HD23 | 1.92 | 0.50 |
| 6:D:67:PHE:CD2 | 6:D:67:PHE:C | 2.85 | 0.50 |
| 1:I:7:DA:H2" | 1:I:8:DT:OP2 | 2.12 | 0.49 |
| 3:A:103:LEU:HD21 | 3:A:128:ARG:HD2 | 1.92 | 0.49 |
| 4:F:66:ILE:HD13 | 4:F:66:ILE:H | 1.77 | 0.49 |
| 1:I:39:DA:H4' | 5:G:42:ARG:HE | 1.77 | 0.49 |
| 2:J:259:DT:H4' | 5:G:42:ARG:NH2 | 2.27 | 0.49 |
| 2:J:261:DA:P | 5:G:35:ARG:HH12 | 2.35 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:274:DA:C1' | 2:J:275:DA:O5' | 2.53 | 0.49 |
| 3:A:100:LEU:HD11 | 4:B:58:LEU:HB2 | 1.94 | 0.49 |
| 3:E:61:LEU:HD12 | 4:F:37:LEU:CA | 2.39 | 0.49 |
| 5:G:91:GLU:O | 5:G:92:GLU:C | 2.50 | 0.49 |
| 5:G:117:PRO:O | 5:G:118:LYS:C | 2.50 | 0.49 |
| 1:I:99:DG:H1' | 1:I:100:DA:C8 | 2.47 | 0.49 |
| 3:A:85:GLN:C | 3:A:87:SER:N | 2.65 | 0.49 |
| 5:C:73:ASN:O | 5:C:75:LYS:HD3 | 2.12 | 0.49 |
| 4:F:86:VAL:O | 4:F:89:ALA:N | 2.45 | 0.49 |
| 1:I:11:DA:H1' | 1:I:12:DC:P | 2.52 | 0.49 |
| 3:A:85:GLN:O | 3:A:87:SER:N | 2.46 | 0.49 |
| 4:B:86:VAL:O | 4:B:87:VAL:C | 2.50 | 0.49 |
| 5:G:78:ILE:HG23 | 5:G:82:HIS:HB2 | 1.93 | 0.49 |
| 6:D:104:ALA:O | 6:D:107:ALA:N | 2.45 | 0.49 |
| 5:G:25:PHE:O | 5:G:27:VAL:N | 2.40 | 0.49 |
| 2:J:269:DG:H5" | 6:H:37:TYR:OH | 2.13 | 0.49 |
| 3:E:123:ASP:O | 3:E:124:ILE:C | 2.51 | 0.49 |
| 3:A:122:LYS:HG3 | 3:A:123:ASP:N | 2.27 | 0.49 |
| 6:D:96:ARG:HH21 | 6:D:108:VAL:HG11 | 1.78 | 0.49 |
| 5:G:116:LEU:HB3 | 5:G:117:PRO:CD | 2.43 | 0.49 |
| 6:H:87:THR:HG23 | 6:H:90:GLU:OE1 | 2.13 | 0.49 |
| 2:J:168:DA:C2 | 2:J:169:DC:C4 | 3.00 | 0.49 |
| 5:G:80:PRO:HD3 | 6:H:55:ALA:HB2 | 1.95 | 0.49 |
| 5:G:81:ARG:HE | 5:G:85:LEU:HD11 | 1.76 | 0.49 |
| 1:I:110:DA:H2" | 1:I:111:DA:OP2 | 2.13 | 0.48 |
| 2:J:174:DA:C2 | 2:J:175:DA:C2 | 3.01 | 0.48 |
| 2:J:192:DT:O3' | 2:J:193:DG:H8 | 1.96 | 0.48 |
| 2:J:283:DG:H1' | 2:J:284:DT:C6 | 2.48 | 0.48 |
| 4:B:60:VAL:O | 4:B:64:ASN:ND2 | 2.45 | 0.48 |
| 5:C:79:ILE:HG12 | 5:C:82:HIS:CE1 | 2.47 | 0.48 |
| 3:A:64:LYS:NZ | 3:A:64:LYS:HB3 | 2.27 | 0.48 |
| 4:F:38:ALA:O | 4:F:43:VAL:HB | 2.13 | 0.48 |
| 3:A:67:PHE:O | 3:A:70:LEU:N | 2.46 | 0.48 |
| 5:C:47:ALA:HB3 | 5:C:48:PRO:CD | 2.43 | 0.48 |
| 4:F:26:ILE:O | 4:F:26:ILE:HG13 | 2.13 | 0.48 |
| 1:I:92:DT:O4 | 2:J:202:DA:N6 | 2.45 | 0.48 |
| 2:J:236:DT:H2" | 2:J:237:DA:C8 | 2.48 | 0.48 |
| 3:A:85:GLN:HB3 | 3:A:87:SER:OG | 2.12 | 0.48 |
| 3:A:103:LEU:HD22 | 3:A:128:ARG:HD2 | 1.95 | 0.48 |
| 5:C:23:LEU:O | 5:C:24:GLN:HG2 | 2.14 | 0.48 |
| 5:C:78:ILE:HA | 5:C:82:HIS:ND1 | 2.27 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:132:DG:H4' | 5:C:77:ARG:HH21 | 1.77 | 0.48 |
| 4:B:62:LEU:O | 4:B:65:VAL:N | 2.46 | 0.48 |
| 5:C:17:ARG:HD2 | 6:D:118:TYR:OH | 2.13 | 0.48 |
| 4:F:100:PHE:CD1 | 4:F:100:PHE:N | 2.81 | 0.48 |
| 1:I:142:DA:H2" | 1:I:143:DT:OP2 | 2.13 | 0.48 |
| 4:B:84:MET:O | 4:B:85:ASP:C | 2.52 | 0.48 |
| 6:D:82:LYS:HD2 | 6:D:82:LYS:H | 1.74 | 0.48 |
| 4:F:47:SER:HB3 | 4:F:50:ILE:HG12 | 1.95 | 0.48 |
| 5:G:42:ARG:HH11 | 5:G:42:ARG:HG2 | 1.79 | 0.48 |
| 5:G:81:ARG:HG3 | 5:G:81:ARG:O | 2.14 | 0.48 |
| 2:J:190:DA:C4 | 2:J:191:DC:C5 | 3.02 | 0.48 |
| 4:B:52:GLU:O | 4:B:55:ARG:N | 2.47 | 0.48 |
| 5:C:23:LEU:N | 5:C:23:LEU:CD1 | 2.67 | 0.48 |
| 6:D:115:VAL:O | 6:D:118:TYR:N | 2.46 | 0.48 |
| 3:E:53:ARG:NH1 | 3:E:54:TYR:OH | 2.47 | 0.48 |
| 1:I:57:DA:C8 | 1:I:58:DT:H72 | 2.48 | 0.48 |
| 1:I:81:DT:H2" | 1:I:82:DG:C8 | 2.49 | 0.48 |
| 1:I:122:DG:N2 | 2:J:173:DC:N3 | 2.58 | 0.48 |
| 3:A:61:LEU:CD1 | 4:B:36:ARG:HB3 | 2.37 | 0.48 |
| 4:B:96:THR:CG2 | 4:B:97:LEU:N | 2.77 | 0.48 |
| 5:C:71:ARG:HB3 | 5:C:71:ARG:CZ | 2.44 | 0.48 |
| 3:E:93:GLN:O | 3:E:97:GLU:HG3 | 2.14 | 0.48 |
| 1:I:127:DT:C2' | 1:I:128:DA:OP2 | 2.58 | 0.48 |
| 5:G:118:LYS:HG3 | 5:G:118:LYS:O | 2.13 | 0.48 |
| 6:H:32:GLU:O | 6:H:33:SER:HB2 | 2.14 | 0.48 |
| 1:I:47:DA:H2" | 1:I:48:DA:OP2 | 2.14 | 0.48 |
| 2:J:162:DG:H2" | 2:J:163:DC:C5 | 2.49 | 0.48 |
| 2:J:225:DC:C1' | 2:J:226:DC:H5' | 2.39 | 0.48 |
| 2:J:258:DT:O2 | 2:J:259:DT:C2 | 2.67 | 0.48 |
| 3:A:50:GLU:O | 3:A:53:ARG:HB3 | 2.14 | 0.48 |
| 3:A:65:LEU:O | 3:A:66:PRO:C | 2.48 | 0.48 |
| 3:A:91:ALA:O | 3:A:94:GLU:N | 2.46 | 0.48 |
| 6:D:107:ALA:O | 6:D:108:VAL:C | 2.52 | 0.48 |
| 4:F:33:ALA:CA | 4:F:36:ARG:NH1 | 2.77 | 0.48 |
| 1:I:61:DG:H3' | 4:F:30:THR:HB | 1.95 | 0.47 |
| 2:J:169:DC:C2' | 2:J:170:DT:O5' | 2.62 | 0.47 |
| 2:J:231:DT:H4' | 2:J:232:DA:OP1 | 2.14 | 0.47 |
| 5:C:51:LEU:O | 5:C:54:VAL:N | 2.46 | 0.47 |
| 1:I:97:DT:H1' | 1:I:98:DG:H5' | 1.96 | 0.47 |
| 3:A:76:GLN:O | 3:A:78:PHE:N | 2.48 | 0.47 |
| 5:C:51:LEU:O | 5:C:52:ALA:C | 2.51 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:47:ALA:HB1 | 4:F:39:ARG:NH1 | 2.29 | 0.47 |
| 5:G:94:ASN:O | 5:G:98:GLY:N | 2.46 | 0.47 |
| 1:I:93:DT:O4 | 2:J:201:DA:N6 | 2.47 | 0.47 |
| 1:I:95:DG:OP2 | 1:I:95:DG:H3' | 2.15 | 0.47 |
| 3:A:116:ARG:NH1 | 3:A:116:ARG:CB | 2.77 | 0.47 |
| 6:D:66:VAL:O | 6:D:70:ILE:HG13 | 2.13 | 0.47 |
| 3:E:73:GLU:OE1 | 4:F:25:ASN:ND2 | 2.47 | 0.47 |
| 5:G:116:LEU:O | 5:G:117:PRO:O | 2.32 | 0.47 |
| 1:I:56:DG:H2" | 1:I:57:DA:O5' | 2.13 | 0.47 |
| 3:A:91:ALA:O | 3:A:92:LEU:C | 2.52 | 0.47 |
| 3:E:110:CYS:SG | 3:E:126:LEU:CD2 | 3.03 | 0.47 |
| 3:A:65:LEU:C | 3:A:67:PHE:N | 2.65 | 0.47 |
| 3:E:97:GLU:O | 3:E:100:LEU:N | 2.46 | 0.47 |
| 5:G:53:ALA:HB2 | 6:H:114:ALA:CB | 2.43 | 0.47 |
| 1:I:7:DA:N1 | 2:J:288:DT:O4 | 2.47 | 0.47 |
| 2:J:222:DC:H2" | 2:J:223:DA:C8 | 2.49 | 0.47 |
| 5:C:110:ASN:CG | 5:C:111:ILE:N | 2.68 | 0.47 |
| 6:D:62:PHE:O | 6:D:63:VAL:C | 2.51 | 0.47 |
| 6:H:109:SER:O | 6:H:110:GLU:C | 2.52 | 0.47 |
| 2:J:218:DG:H2" | 2:J:219:DA:C8 | 2.49 | 0.47 |
| 2:J:240:DA:H2" | 2:J:241:DT:OP2 | 2.14 | 0.47 |
| 2:J:241:DT:C2' | 2:J:242:DG:H5' | 2.45 | 0.47 |
| 2:J:292:DG:C2 | 2:J:293:DA:C6 | 3.02 | 0.47 |
| 2:J:292:DG:H5' | 3:A:39:HIS:CE1 | 2.49 | 0.47 |
| 4:B:52:GLU:O | 4:B:53:GLU:C | 2.53 | 0.47 |
| 4:B:75:HIS:CG | 6:D:77:LEU:HD13 | 2.49 | 0.47 |
| 6:D:67:PHE:HD2 | 6:D:68:GLU:N | 2.11 | 0.47 |
| 3:E:85:GLN:O | 3:E:86:SER:C | 2.52 | 0.47 |
| 5:G:29:ARG:NH2 | 6:H:32:GLU:OE1 | 2.46 | 0.47 |
| 6:H:43:LYS:HA | 6:H:43:LYS:HE2 | 1.96 | 0.47 |
| 6:H:92:GLN:O | 6:H:94:ALA:N | 2.47 | 0.47 |
| 6:H:115:VAL:O | 6:H:118:TYR:N | 2.48 | 0.47 |
| 5:C:17:ARG:HA | 5:C:20:ARG:HB2 | 1.97 | 0.47 |
| 3:E:126:LEU:O | 3:E:127:ALA:C | 2.53 | 0.47 |
| 4:F:47:SER:O | 4:F:51:TYR:CE1 | 2.62 | 0.47 |
| 5:G:17:ARG:HG2 | 6:H:118:TYR:CE1 | 2.50 | 0.47 |
| 6:H:72:GLY:O | 6:H:75:SER:N | 2.48 | 0.47 |
| 2:J:286:DG:C2 | 2:J:287:DA:C2 | 3.03 | 0.47 |
| 3:A:45:THR:O | 3:A:47:ALA:N | 2.39 | 0.47 |
| 3:A:61:LEU:O | 3:A:62:ILE:HD13 | 2.15 | 0.47 |
| 6:D:51:ILE:HD11 | 6:D:56:MET:HA | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:E:124:ILE:H | 3:E:124:ILE:HG12 | 1.59 | 0.47 |
| 1:I:69:DG:C5' | 3:E:43:PRO:HB2 | 2.43 | 0.47 |
| 5:C:17:ARG:HA | 5:C:20:ARG:CB | 2.45 | 0.47 |
| 5:C:26:PRO:HB2 | 5:C:29:ARG:HB2 | 1.97 | 0.47 |
| 6:D:103:LEU:O | 6:D:106:HIS:HB2 | 2.14 | 0.47 |
| 6:H:51:ILE:HD13 | 6:H:51:ILE:C | 2.36 | 0.47 |
| 1:I:14:DT:H4' | 1:I:15:DG:OP1 | 2.15 | 0.46 |
| 3:A:72:ARG:HH11 | 3:A:72:ARG:HG2 | 1.79 | 0.46 |
| 4:B:44:LYS:HB2 | 5:G:115:LEU:HD22 | 1.96 | 0.46 |
| 1:I:124:DT:H2" | 1:I:125:DA:O5' | 2.14 | 0.46 |
| 1:I:129:DT:H1' | 1:I:130:DC:C5' | 2.42 | 0.46 |
| 2:J:176:DA:C2 | 2:J:177:DA:N1 | 2.83 | 0.46 |
| 2:J:279:DG:H2" | 2:J:280:DC:C5 | 2.50 | 0.46 |
| 3:A:130:ILE:CG2 | 3:E:130:ILE:HG22 | 2.43 | 0.46 |
| 5:G:79:ILE:HB | 5:G:80:PRO:HD2 | 1.97 | 0.46 |
| 5:G:103:ALA:O | 5:G:104:GLN:CB | 2.62 | 0.46 |
| 1:I:80:DC:H2" | 1:I:81:DT:OP2 | 2.16 | 0.46 |
| 2:J:232:DA:H2" | 2:J:233:DG:H8 | 1.80 | 0.46 |
| 2:J:244:DT:C2' | 2:J:245:DT:H72 | 2.45 | 0.46 |
| 4:B:73:THR:OG1 | 4:B:81:VAL:HG22 | 2.15 | 0.46 |
| 2:J:224:DG:H2" | 2:J:225:DC:OP2 | 2.15 | 0.46 |
| 4:B:44:LYS:HG3 | 4:B:45:ARG:N | 2.29 | 0.46 |
| 1:I:27:DA:C2 | 2:J:269:DG:N2 | 2.83 | 0.46 |
| 1:I:56:DG:N2 | 2:J:240:DA:C2 | 2.83 | 0.46 |
| 3:E:61:LEU:HB2 | 4:F:37:LEU:HD21 | 1.97 | 0.46 |
| 4:F:84:MET:O | 4:F:85:ASP:C | 2.54 | 0.46 |
| 6:H:71:ALA:O | 6:H:74:ALA:N | 2.49 | 0.46 |
| 5:C:23:LEU:HD11 | 6:D:114:ALA:HB1 | 1.96 | 0.46 |
| 6:D:77:LEU:O | 6:D:78:ALA:C | 2.54 | 0.46 |
| 3:E:67:PHE:CE2 | 3:E:93:GLN:HG3 | 2.50 | 0.46 |
| 3:E:127:ALA:O | 3:E:131:ARG:HB2 | 2.15 | 0.46 |
| 5:G:113:SER:OG | 5:G:114:VAL:N | 2.46 | 0.46 |
| 1:I:79:DG:H1 | 2:J:216:DC:H42 | 1.64 | 0.46 |
| 2:J:244:DT:H2' | 2:J:245:DT:H72 | 1.96 | 0.46 |
| 3:A:58:THR:CA | 4:B:40:ARG:NH2 | 2.79 | 0.46 |
| 3:A:116:ARG:HH12 | 3:A:118:THR:CB | 2.29 | 0.46 |
| 4:B:57:VAL:O | 4:B:58:LEU:C | 2.52 | 0.46 |
| 5:C:20:ARG:HG3 | 6:D:121:ALA:HB3 | 1.98 | 0.46 |
| 6:D:77:LEU:HD23 | 6:D:77:LEU:HA | 1.81 | 0.46 |
| 1:I:74:DA:H2" | 1:I:75:DC:C5 | 2.51 | 0.46 |
| 3:A:128:ARG:O | 3:A:133:GLU:HB2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:C:43:VAL:HA | 6:D:86:ILE:HG22 | 1.97 | 0.46 |
| 3:E:68:GLN:O | 3:E:71:VAL:HB | 2.16 | 0.46 |
| 1:I:136:DG:O6 | 2:J:159:DC:N4 | 2.46 | 0.46 |
| 3:A:44:GLY:O | 3:A:47:ALA:HB3 | 2.16 | 0.46 |
| 3:E:73:GLU:O | 3:E:76:GLN:HB3 | 2.15 | 0.46 |
| 3:E:114:ALA:O | 3:E:116:ARG:HG3 | 2.16 | 0.46 |
| 1:I:70:DG:H1 | 2:J:225:DC:H42 | 1.63 | 0.46 |
| 1:I:82:DG:N2 | 2:J:214:DA:C2 | 2.84 | 0.46 |
| 2:J:148:DA:H2" | 2:J:149:DT:C7 | 2.46 | 0.46 |
| 2:J:204:DA:H1' | 2:J:205:DG:C5' | 2.46 | 0.46 |
| 3:A:103:LEU:O | 3:A:107:THR:N | 2.49 | 0.46 |
| 3:A:122:LYS:HA | 3:A:125:GLN:OE1 | 2.16 | 0.46 |
| 5:C:72:ASP:C | 5:C:74:LYS:N | 2.69 | 0.46 |
| 3:E:65:LEU:HD12 | 3:E:65:LEU:HA | 1.82 | 0.46 |
| 4:F:33:ALA:O | 4:F:34:ILE:C | 2.52 | 0.46 |
| 6:H:58:ILE:HG22 | 6:H:58:ILE:O | 2.16 | 0.46 |
| 1:I:15:DG:H2" | 1:I:16:DC:O5' | 2.15 | 0.45 |
| 1:I:34:DT:H2" | 1:I:35:DC:OP2 | 2.15 | 0.45 |
| 1:I:143:DT:H2' | 1:I:144:DT:H72 | 1.98 | 0.45 |
| 2:J:245:DT:C4 | 2:J:246:DT:O4 | 2.70 | 0.45 |
| 1:I:59:DA:C5 | 1:I:60:DA:C6 | 3.05 | 0.45 |
| 1:I:112:DA:H4' | 5:C:42:ARG:NH2 | 2.30 | 0.45 |
| 2:J:244:DT:H2" | 2:J:245:DT:C6 | 2.51 | 0.45 |
| 2:J:260:DG:H2" | 2:J:261:DA:H8 | 1.80 | 0.45 |
| 6:D:43:LYS:NZ | 6:D:49:THR:O | 2.34 | 0.45 |
| 4:F:31:LYS:HE3 | 4:F:35:ARG:HH12 | 1.80 | 0.45 |
| 5:G:38:ASN:C | 5:G:40:ALA:N | 2.69 | 0.45 |
| 1:I:17:DA:H2" | 1:I:18:DC:C6 | 2.50 | 0.45 |
| 1:I:42:DA:C6 | 1:I:43:DA:C6 | 3.05 | 0.45 |
| 1:I:94:DT:H2" | 1:I:95:DG:H5' | 1.99 | 0.45 |
| 2:J:148:DA:H2" | 2:J:149:DT:OP2 | 2.17 | 0.45 |
| 5:G:74:LYS:HD2 | 5:G:74:LYS:HA | 1.56 | 0.45 |
| 1:I:116:DA:H2" | 1:I:117:DC:O5' | 2.17 | 0.45 |
| 2:J:288:DT:C1' | 2:J:289:DA:O5' | 2.64 | 0.45 |
| 3:A:56:LYS:HG3 | 3:A:56:LYS:O | 2.15 | 0.45 |
| 3:A:110:CYS:SG | 3:A:127:ALA:HB2 | 2.56 | 0.45 |
| 4:B:61:PHE:HE1 | 4:B:95:ARG:HD3 | 1.81 | 0.45 |
| 6:D:34:TYR:H | 6:D:34:TYR:HD1 | 1.63 | 0.45 |
| 3:E:68:GLN:CD | 3:E:72:ARG:HH21 | 2.19 | 0.45 |
| 1:I:5:DA:C4' | 3:A:39:HIS:CB | 2.82 | 0.45 |
| 1:I:32:DT:H2" | 1:I:33:DG:C8 | 2.52 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:138:DG:H2” | 1:I:139:DG:O4’ | 2.17 | 0.45 |
| 2:J:288:DT:H2” | 2:J:289:DA:O5’ | 2.15 | 0.45 |
| 3:A:99:TYR:CD2 | 4:B:61:PHE:CD1 | 3.05 | 0.45 |
| 4:B:69:ALA:O | 4:B:71:THR:N | 2.49 | 0.45 |
| 5:C:47:ALA:HB1 | 6:D:91:ILE:CD1 | 2.47 | 0.45 |
| 5:C:49:VAL:HG11 | 6:D:115:VAL:HA | 1.98 | 0.45 |
| 1:I:113:DT:C6 | 1:I:114:DA:N7 | 2.85 | 0.45 |
| 2:J:231:DT:H5” | 3:E:40:ARG:HA | 1.98 | 0.45 |
| 3:A:55:GLN:OE1 | 5:G:109:PRO:HA | 2.16 | 0.45 |
| 3:A:57:SER:C | 4:B:40:ARG:HH21 | 2.20 | 0.45 |
| 5:C:92:GLU:O | 5:C:95:LYS:N | 2.49 | 0.45 |
| 6:D:73:GLU:OE2 | 6:D:76:ARG:NH1 | 2.49 | 0.45 |
| 5:G:63:LEU:HA | 5:G:66:ALA:HB3 | 1.97 | 0.45 |
| 2:J:219:DA:C4 | 2:J:220:DG:N7 | 2.84 | 0.45 |
| 2:J:262:DC:C4 | 2:J:263:DA:N6 | 2.84 | 0.45 |
| 4:F:31:LYS:CA | 4:F:34:ILE:HD12 | 2.46 | 0.45 |
| 4:F:35:ARG:CG | 4:F:36:ARG:N | 2.78 | 0.45 |
| 1:I:10:DC:H2” | 1:I:11:DA:O5’ | 2.16 | 0.45 |
| 1:I:11:DA:C1’ | 1:I:12:DC:P | 3.04 | 0.45 |
| 1:I:52:DT:H1’ | 1:I:53:DC:H5’ | 1.98 | 0.45 |
| 1:I:136:DG:O6 | 2:J:159:DC:N3 | 2.50 | 0.45 |
| 6:H:76:ARG:O | 6:H:77:LEU:C | 2.55 | 0.45 |
| 1:I:123:DG:OP1 | 5:C:29:ARG:NH2 | 2.38 | 0.45 |
| 3:A:64:LYS:NZ | 3:A:64:LYS:CB | 2.80 | 0.45 |
| 4:B:96:THR:CG2 | 4:B:97:LEU:H | 2.29 | 0.45 |
| 5:C:42:ARG:CB | 6:D:85:THR:HG23 | 2.47 | 0.45 |
| 5:C:50:TYR:CE2 | 6:D:92:GLN:HB2 | 2.51 | 0.45 |
| 5:C:51:LEU:C | 5:C:53:ALA:H | 2.19 | 0.45 |
| 5:C:92:GLU:O | 5:C:94:ASN:N | 2.50 | 0.45 |
| 1:I:67:DT:H2” | 1:I:68:DT:H73 | 1.96 | 0.45 |
| 2:J:158:DA:H1’ | 2:J:159:DC:C5’ | 2.43 | 0.45 |
| 2:J:173:DC:P | 2:J:173:DC:C6 | 3.10 | 0.45 |
| 3:A:60:LEU:HD13 | 3:A:93:GLN:CG | 2.46 | 0.45 |
| 3:A:120:MET:SD | 3:A:122:LYS:HE2 | 2.57 | 0.45 |
| 4:F:50:ILE:O | 4:F:52:GLU:N | 2.49 | 0.45 |
| 5:G:87:VAL:CG1 | 5:G:97:LEU:HD12 | 2.42 | 0.45 |
| 5:C:120:THR:O | 5:C:120:THR:HG23 | 2.17 | 0.44 |
| 3:E:45:THR:O | 3:E:45:THR:CG2 | 2.65 | 0.44 |
| 3:E:60:LEU:N | 3:E:60:LEU:CD1 | 2.79 | 0.44 |
| 5:G:60:ALA:O | 5:G:61:GLU:C | 2.56 | 0.44 |
| 5:G:76:THR:O | 6:H:49:THR:HG23 | 2.17 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:41:DA:H1' | 1:I:42:DA:C5' | 2.47 | 0.44 |
| 1:I:82:DG:N1 | 1:I:83:DA:C2 | 2.86 | 0.44 |
| 2:J:241:DT:C4 | 2:J:242:DG:N7 | 2.85 | 0.44 |
| 2:J:253:DT:H2" | 2:J:254:DT:C7 | 2.46 | 0.44 |
| 6:D:109:SER:C | 6:D:111:GLY:N | 2.70 | 0.44 |
| 3:E:104:PHE:O | 3:E:105:GLU:C | 2.55 | 0.44 |
| 4:F:39:ARG:HH12 | 4:F:44:LYS:HA | 1.81 | 0.44 |
| 5:G:25:PHE:CD1 | 5:G:56:GLU:HA | 2.51 | 0.44 |
| 6:H:42:LEU:HD21 | 6:H:50:GLY:O | 2.17 | 0.44 |
| 1:I:97:DT:H2" | 1:I:98:DG:OP2 | 2.16 | 0.44 |
| 2:J:229:DA:H5" | 4:F:45:ARG:HD2 | 1.99 | 0.44 |
| 3:E:42:ARG:HG2 | 3:E:43:PRO:HD2 | 2.00 | 0.44 |
| 4:F:31:LYS:CE | 4:F:35:ARG:HH12 | 2.30 | 0.44 |
| 1:I:5:DA:H2" | 1:I:6:DT:OP2 | 2.16 | 0.44 |
| 1:I:10:DC:C2' | 1:I:11:DA:O5' | 2.65 | 0.44 |
| 2:J:183:DT:C2' | 2:J:184:DT:OP2 | 2.61 | 0.44 |
| 6:D:87:THR:C | 6:D:89:ARG:N | 2.69 | 0.44 |
| 1:I:83:DA:H5" | 3:A:43:PRO:CA | 2.41 | 0.44 |
| 1:I:118:DT:C4 | 1:I:119:DT:C4 | 3.06 | 0.44 |
| 2:J:217:DT:H2" | 2:J:218:DG:C8 | 2.53 | 0.44 |
| 2:J:288:DT:C2' | 2:J:289:DA:O5' | 2.65 | 0.44 |
| 3:A:72:ARG:O | 3:A:73:GLU:C | 2.56 | 0.44 |
| 3:A:103:LEU:HD11 | 3:A:128:ARG:HG3 | 1.99 | 0.44 |
| 6:D:76:ARG:HE | 6:D:76:ARG:HB2 | 1.63 | 0.44 |
| 4:F:26:ILE:O | 4:F:55:ARG:CD | 2.59 | 0.44 |
| 5:G:113:SER:O | 5:G:115:LEU:N | 2.50 | 0.44 |
| 6:H:34:TYR:O | 6:H:38:VAL:HG23 | 2.17 | 0.44 |
| 1:I:12:DC:C1' | 1:I:13:DC:H5' | 2.30 | 0.44 |
| 5:C:51:LEU:HD13 | 6:D:91:ILE:CD1 | 2.48 | 0.44 |
| 4:F:60:VAL:O | 4:F:64:ASN:OD1 | 2.36 | 0.44 |
| 5:G:39:TYR:O | 5:G:40:ALA:CB | 2.65 | 0.44 |
| 6:H:89:ARG:O | 6:H:90:GLU:C | 2.56 | 0.44 |
| 2:J:238:DT:H2" | 2:J:239:DC:H6 | 1.82 | 0.44 |
| 5:C:17:ARG:HD3 | 6:D:118:TYR:OH | 2.17 | 0.44 |
| 5:C:20:ARG:HG3 | 6:D:121:ALA:CB | 2.47 | 0.44 |
| 1:I:93:DT:H1' | 1:I:94:DT:C6 | 2.53 | 0.44 |
| 2:J:184:DT:H2" | 2:J:185:DT:C6 | 2.53 | 0.44 |
| 2:J:276:DT:H1' | 2:J:277:DG:H5' | 2.00 | 0.44 |
| 3:A:88:ALA:HB2 | 4:B:82:THR:O | 2.17 | 0.44 |
| 4:B:33:ALA:O | 4:B:36:ARG:N | 2.41 | 0.44 |
| 6:D:74:ALA:O | 6:D:75:SER:C | 2.56 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:F:84:MET:HE1 | 4:F:102:GLY:HA2 | 1.98 | 0.44 |
| 5:G:92:GLU:HB3 | 6:H:103:LEU:HB2 | 1.99 | 0.44 |
| 1:I:32:DT:C2 | 1:I:33:DG:C5 | 3.06 | 0.44 |
| 1:I:104:DG:H1' | 1:I:105:DT:H5' | 1.99 | 0.44 |
| 2:J:176:DA:OP1 | 5:C:32:ARG:NH1 | 2.51 | 0.44 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CZ | 2.53 | 0.44 |
| 6:D:38:VAL:HG11 | 6:D:59:MET:HG2 | 2.00 | 0.44 |
| 6:H:102:GLU:C | 6:H:104:ALA:H | 2.20 | 0.44 |
| 1:I:63:DT:N3 | 1:I:64:DA:N6 | 2.66 | 0.43 |
| 2:J:192:DT:H1' | 2:J:193:DG:N7 | 2.33 | 0.43 |
| 2:J:231:DT:C5' | 3:E:40:ARG:HG2 | 2.46 | 0.43 |
| 4:B:36:ARG:HG3 | 4:B:36:ARG:HH11 | 1.82 | 0.43 |
| 4:F:33:ALA:C | 4:F:35:ARG:N | 2.69 | 0.43 |
| 5:G:25:PHE:HE1 | 6:H:41:VAL:HG21 | 1.83 | 0.43 |
| 5:G:88:ARG:HA | 5:G:88:ARG:HD3 | 1.90 | 0.43 |
| 5:G:116:LEU:HD23 | 5:G:116:LEU:HA | 1.87 | 0.43 |
| 5:G:119:LYS:HE3 | 5:G:119:LYS:CA | 2.31 | 0.43 |
| 3:A:90:MET:O | 3:A:94:GLU:HG2 | 2.19 | 0.43 |
| 5:C:76:THR:O | 5:C:76:THR:OG1 | 2.35 | 0.43 |
| 1:I:72:DT:H2" | 1:I:73:DG:C8 | 2.53 | 0.43 |
| 3:A:42:ARG:HG2 | 3:A:42:ARG:NH1 | 2.31 | 0.43 |
| 4:B:38:ALA:O | 4:B:43:VAL:CG2 | 2.66 | 0.43 |
| 4:B:98:TYR:CE2 | 6:H:62:PHE:HA | 2.53 | 0.43 |
| 6:D:79:HIS:HE1 | 5:G:36:LYS:O | 2.01 | 0.43 |
| 6:D:87:THR:C | 6:D:89:ARG:H | 2.22 | 0.43 |
| 3:E:115:LYS:HE3 | 3:E:115:LYS:N | 2.33 | 0.43 |
| 5:G:60:ALA:C | 5:G:62:ILE:N | 2.72 | 0.43 |
| 2:J:217:DT:H1' | 2:J:218:DG:C8 | 2.52 | 0.43 |
| 2:J:264:DC:N1 | 2:J:265:DT:H72 | 2.34 | 0.43 |
| 5:C:23:LEU:H | 5:C:23:LEU:CD1 | 2.31 | 0.43 |
| 5:C:63:LEU:HD12 | 6:D:42:LEU:HA | 2.00 | 0.43 |
| 3:E:60:LEU:CG | 3:E:97:GLU:OE2 | 2.66 | 0.43 |
| 3:E:72:ARG:O | 3:E:76:GLN:HB2 | 2.18 | 0.43 |
| 2:J:274:DA:C2' | 2:J:275:DA:O5' | 2.66 | 0.43 |
| 3:A:121:PRO:N | 4:B:50:ILE:HD11 | 2.33 | 0.43 |
| 5:C:51:LEU:HB2 | 6:D:91:ILE:HD13 | 2.00 | 0.43 |
| 1:I:79:DG:H1 | 2:J:216:DC:N4 | 2.17 | 0.43 |
| 1:I:126:DG:C1' | 1:I:127:DT:O5' | 2.57 | 0.43 |
| 2:J:230:DT:OP1 | 3:E:46:VAL:HB | 2.18 | 0.43 |
| 4:B:87:VAL:O | 4:B:89:ALA:N | 2.52 | 0.43 |
| 5:C:37:GLY:HA3 | 5:C:39:TYR:CE1 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:C:55:LEU:HD21 | 6:D:66:VAL:HG12 | 2.01 | 0.43 |
| 6:D:67:PHE:CD2 | 6:D:68:GLU:N | 2.87 | 0.43 |
| 6:D:78:ALA:O | 6:D:79:HIS:C | 2.57 | 0.43 |
| 6:D:109:SER:O | 6:D:111:GLY:N | 2.52 | 0.43 |
| 2:J:176:DA:C2 | 2:J:177:DA:C2 | 3.06 | 0.43 |
| 3:A:109:LEU:O | 3:A:113:HIS:N | 2.42 | 0.43 |
| 6:D:51:ILE:CD1 | 6:D:56:MET:HE2 | 2.49 | 0.43 |
| 3:E:104:PHE:O | 3:E:107:THR:N | 2.44 | 0.43 |
| 1:I:137:DT:C2' | 1:I:138:DG:OP2 | 2.62 | 0.43 |
| 5:C:34:LEU:HB3 | 5:C:43:VAL:HG21 | 2.00 | 0.43 |
| 5:C:107:VAL:HG11 | 3:E:101:VAL:HG11 | 1.99 | 0.43 |
| 6:D:46:HIS:HB3 | 6:D:49:THR:OG1 | 2.19 | 0.43 |
| 5:G:17:ARG:HA | 6:H:118:TYR:HE1 | 1.84 | 0.43 |
| 5:G:96:LEU:HD12 | 6:H:69:ARG:HH12 | 1.82 | 0.43 |
| 6:H:81:ASN:O | 6:H:82:LYS:CB | 2.66 | 0.43 |
| 6:H:121:ALA:O | 6:H:122:LYS:OXT | 2.37 | 0.43 |
| 1:I:41:DA:H1' | 1:I:42:DA:O4' | 2.18 | 0.42 |
| 1:I:86:DA:H1' | 1:I:87:DT:OP1 | 2.18 | 0.42 |
| 3:E:61:LEU:HB2 | 4:F:37:LEU:CD2 | 2.49 | 0.42 |
| 6:H:99:LEU:HA | 6:H:100:PRO:HD3 | 1.74 | 0.42 |
| 6:H:102:GLU:C | 6:H:104:ALA:N | 2.70 | 0.42 |
| 1:I:43:DA:H2" | 1:I:44:DA:C8 | 2.54 | 0.42 |
| 2:J:157:DC:H2" | 2:J:158:DA:O5' | 2.19 | 0.42 |
| 3:A:92:LEU:HD23 | 4:B:86:VAL:CG1 | 2.48 | 0.42 |
| 4:B:53:GLU:OE1 | 4:B:53:GLU:HA | 2.18 | 0.42 |
| 4:F:30:THR:HB | 4:F:32:PRO:HD2 | 2.01 | 0.42 |
| 5:G:36:LYS:C | 5:G:38:ASN:H | 2.21 | 0.42 |
| 1:I:32:DT:C4 | 1:I:33:DG:O6 | 2.72 | 0.42 |
| 1:I:38:DA:H1' | 1:I:39:DA:C8 | 2.55 | 0.42 |
| 1:I:41:DA:P | 1:I:41:DA:H3' | 2.59 | 0.42 |
| 1:I:92:DT:H2" | 1:I:93:DT:O5' | 2.19 | 0.42 |
| 2:J:246:DT:H1' | 2:J:247:DT:C6 | 2.54 | 0.42 |
| 2:J:274:DA:H2" | 2:J:275:DA:OP2 | 2.18 | 0.42 |
| 3:A:123:ASP:O | 3:A:126:LEU:N | 2.52 | 0.42 |
| 5:C:88:ARG:HD3 | 5:C:88:ARG:HA | 1.52 | 0.42 |
| 1:I:83:DA:C8 | 1:I:84:DA:N7 | 2.88 | 0.42 |
| 2:J:289:DA:H2' | 2:J:290:DT:H72 | 2.01 | 0.42 |
| 3:A:108:ASN:C | 3:A:108:ASN:HD22 | 2.22 | 0.42 |
| 4:B:93:GLN:HE21 | 4:B:93:GLN:HB3 | 1.46 | 0.42 |
| 6:D:122:LYS:HG2 | 6:D:122:LYS:OXT | 2.19 | 0.42 |
| 5:G:67:GLY:C | 5:G:69:ALA:N | 2.72 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:10:DC:H1' | 1:I:11:DA:C5' | 2.49 | 0.42 |
| 1:I:61:DG:H5" | 4:F:30:THR:HG21 | 2.01 | 0.42 |
| 1:I:83:DA:O3' | 3:A:41:TYR:HB2 | 2.20 | 0.42 |
| 2:J:230:DT:OP2 | 3:E:46:VAL:HB | 2.19 | 0.42 |
| 2:J:254:DT:H2" | 2:J:255:DT:OP2 | 2.20 | 0.42 |
| 2:J:290:DT:H2" | 2:J:291:DT:OP2 | 2.19 | 0.42 |
| 3:A:61:LEU:HB3 | 4:B:36:ARG:HB3 | 2.01 | 0.42 |
| 4:B:44:LYS:HD3 | 5:G:115:LEU:CD2 | 2.28 | 0.42 |
| 5:G:79:ILE:HG22 | 6:H:52:SER:HB2 | 2.02 | 0.42 |
| 1:I:40:DA:H1' | 1:I:41:DA:O5' | 2.18 | 0.42 |
| 3:A:46:VAL:HG22 | 3:A:49:ARG:NH1 | 2.31 | 0.42 |
| 3:A:116:ARG:NH1 | 3:A:118:THR:H | 2.17 | 0.42 |
| 4:F:65:VAL:O | 4:F:68:ASP:N | 2.50 | 0.42 |
| 5:G:23:LEU:HB2 | 5:G:27:VAL:HG21 | 2.02 | 0.42 |
| 6:H:57:SER:C | 6:H:59:MET:N | 2.73 | 0.42 |
| 1:I:74:DA:H2" | 1:I:75:DC:C6 | 2.55 | 0.42 |
| 1:I:128:DA:H2" | 1:I:129:DT:OP2 | 2.19 | 0.42 |
| 2:J:163:DC:H2" | 2:J:164:DA:C8 | 2.54 | 0.42 |
| 4:B:52:GLU:OE1 | 4:B:52:GLU:HA | 2.20 | 0.42 |
| 6:D:38:VAL:O | 6:D:42:LEU:N | 2.47 | 0.42 |
| 6:D:43:LYS:O | 6:D:44:GLN:C | 2.58 | 0.42 |
| 3:E:50:GLU:O | 3:E:51:ILE:C | 2.58 | 0.42 |
| 3:E:76:GLN:C | 3:E:78:PHE:H | 2.23 | 0.42 |
| 3:E:128:ARG:NH2 | 3:E:133:GLU:OE1 | 2.50 | 0.42 |
| 4:F:30:THR:CB | 4:F:32:PRO:HD2 | 2.50 | 0.42 |
| 4:F:33:ALA:HB2 | 4:F:36:ARG:HH12 | 1.84 | 0.42 |
| 1:I:32:DT:N3 | 1:I:33:DG:C6 | 2.88 | 0.42 |
| 2:J:238:DT:H2" | 2:J:239:DC:C6 | 2.54 | 0.42 |
| 3:A:45:THR:C | 3:A:47:ALA:N | 2.71 | 0.42 |
| 4:B:33:ALA:HB1 | 4:B:36:ARG:HH22 | 1.84 | 0.42 |
| 5:C:26:PRO:HD3 | 6:D:37:TYR:CE1 | 2.55 | 0.42 |
| 5:C:92:GLU:O | 5:C:93:LEU:C | 2.58 | 0.42 |
| 6:D:78:ALA:O | 6:D:81:ASN:N | 2.39 | 0.42 |
| 5:G:50:TYR:HH | 6:H:92:GLN:HG3 | 1.80 | 0.42 |
| 6:H:58:ILE:CG2 | 6:H:58:ILE:O | 2.68 | 0.42 |
| 1:I:67:DT:H2" | 1:I:68:DT:C5 | 2.54 | 0.42 |
| 2:J:229:DA:C5' | 4:F:45:ARG:HD2 | 2.49 | 0.42 |
| 6:D:65:ASP:HB3 | 4:F:98:TYR:OH | 2.20 | 0.42 |
| 6:D:112:THR:O | 6:D:113:LYS:C | 2.58 | 0.42 |
| 3:E:49:ARG:HG2 | 3:E:50:GLU:N | 2.33 | 0.42 |
| 5:G:52:ALA:O | 5:G:56:GLU:N | 2.45 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:G:101:THR:HG22 | 5:G:101:THR:O | 2.20 | 0.42 |
| 5:G:110:ASN:O | 5:G:111:ILE:HD13 | 2.19 | 0.42 |
| 6:H:63:VAL:O | 6:H:64:ASN:C | 2.57 | 0.42 |
| 1:I:12:DC:C5 | 1:I:13:DC:C5 | 3.07 | 0.42 |
| 2:J:177:DA:C4 | 2:J:178:DG:N7 | 2.88 | 0.42 |
| 2:J:182:DA:H2" | 2:J:183:DT:O5' | 2.20 | 0.42 |
| 2:J:266:DT:H2" | 2:J:267:DT:H71 | 2.02 | 0.42 |
| 2:J:293:DA:H2" | 2:J:294:DT:OP2 | 2.20 | 0.42 |
| 6:D:121:ALA:O | 6:D:122:LYS:HB3 | 2.20 | 0.42 |
| 5:G:42:ARG:C | 6:H:85:THR:HG23 | 2.39 | 0.42 |
| 6:H:39:TYR:O | 6:H:43:LYS:N | 2.35 | 0.42 |
| 1:I:39:DA:H2" | 1:I:40:DA:OP2 | 2.19 | 0.41 |
| 1:I:123:DG:H2" | 1:I:124:DT:OP2 | 2.20 | 0.41 |
| 2:J:171:DA:C2' | 2:J:172:DC:O5' | 2.65 | 0.41 |
| 2:J:174:DA:H2" | 2:J:175:DA:C8 | 2.55 | 0.41 |
| 3:A:70:LEU:HB2 | 4:B:25:ASN:O | 2.20 | 0.41 |
| 3:A:116:ARG:HH12 | 3:A:118:THR:H | 1.66 | 0.41 |
| 5:C:41:GLU:OE1 | 5:C:41:GLU:HA | 2.20 | 0.41 |
| 6:D:74:ALA:C | 6:D:86:ILE:HD11 | 2.39 | 0.41 |
| 5:G:21:ALA:HB2 | 6:H:118:TYR:HD1 | 1.85 | 0.41 |
| 5:G:96:LEU:HG | 5:G:97:LEU:CD2 | 2.48 | 0.41 |
| 6:H:85:THR:HG22 | 6:H:86:ILE:O | 2.19 | 0.41 |
| 1:I:7:DA:N1 | 2:J:288:DT:C4 | 2.88 | 0.41 |
| 1:I:7:DA:H3' | 3:A:49:ARG:HH21 | 1.82 | 0.41 |
| 2:J:238:DT:C6 | 2:J:239:DC:C5 | 3.08 | 0.41 |
| 2:J:268:DT:H2" | 2:J:269:DG:C5 | 2.55 | 0.41 |
| 3:A:55:GLN:HG2 | 5:G:107:VAL:HB | 2.01 | 0.41 |
| 3:A:106:ASP:O | 3:A:110:CYS:SG | 2.59 | 0.41 |
| 3:A:108:ASN:O | 3:A:111:ALA:N | 2.52 | 0.41 |
| 3:A:110:CYS:O | 3:A:113:HIS:HB3 | 2.20 | 0.41 |
| 4:B:45:ARG:HB3 | 4:B:46:ILE:H | 1.63 | 0.41 |
| 5:G:51:LEU:HD12 | 5:G:51:LEU:O | 2.20 | 0.41 |
| 1:I:18:DC:H2" | 1:I:19:DA:C8 | 2.55 | 0.41 |
| 2:J:203:DA:C4' | 2:J:204:DA:OP1 | 2.69 | 0.41 |
| 3:A:79:LYS:HB3 | 3:A:82:LEU:HD21 | 2.03 | 0.41 |
| 6:D:118:TYR:C | 6:D:120:SER:N | 2.74 | 0.41 |
| 3:E:64:LYS:HE2 | 3:E:90:MET:CE | 2.50 | 0.41 |
| 3:E:99:TYR:HE1 | 3:E:131:ARG:NH1 | 2.18 | 0.41 |
| 4:F:65:VAL:HG11 | 4:F:90:LEU:HD21 | 2.01 | 0.41 |
| 5:G:26:PRO:HB2 | 5:G:29:ARG:CG | 2.50 | 0.41 |
| 5:G:66:ALA:O | 5:G:69:ALA:HB3 | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:71:DC:H2" | 1:I:72:DT:O5' | 2.21 | 0.41 |
| 1:I:127:DT:H6 | 1:I:127:DT:H2' | 1.63 | 0.41 |
| 2:J:231:DT:OP1 | 3:E:40:ARG:HB3 | 2.20 | 0.41 |
| 3:A:45:THR:HG22 | 3:A:46:VAL:N | 2.36 | 0.41 |
| 3:A:104:PHE:O | 3:A:105:GLU:C | 2.58 | 0.41 |
| 3:A:126:LEU:O | 3:A:127:ALA:C | 2.58 | 0.41 |
| 5:C:17:ARG:O | 5:C:20:ARG:HB3 | 2.21 | 0.41 |
| 6:D:36:ILE:CG1 | 6:D:37:TYR:N | 2.83 | 0.41 |
| 4:F:36:ARG:HG3 | 4:F:36:ARG:NH1 | 2.34 | 0.41 |
| 4:F:54:THR:O | 4:F:55:ARG:C | 2.59 | 0.41 |
| 5:G:24:GLN:HB2 | 5:G:56:GLU:OE1 | 2.20 | 0.41 |
| 6:H:49:THR:HG22 | 6:H:50:GLY:N | 2.36 | 0.41 |
| 1:I:29:DA:H5' | 6:H:30:ARG:NH2 | 2.36 | 0.41 |
| 1:I:78:DA:C2 | 1:I:79:DG:C2 | 3.09 | 0.41 |
| 1:I:137:DT:C2 | 1:I:138:DG:C8 | 3.09 | 0.41 |
| 3:A:54:TYR:C | 3:A:56:LYS:N | 2.74 | 0.41 |
| 3:A:65:LEU:HB3 | 3:A:66:PRO:CD | 2.51 | 0.41 |
| 3:A:130:ILE:HD12 | 3:A:130:ILE:HA | 1.84 | 0.41 |
| 5:G:67:GLY:C | 5:G:69:ALA:H | 2.23 | 0.41 |
| 1:I:123:DG:H4' | 6:D:30:ARG:CB | 2.46 | 0.41 |
| 3:A:84:PHE:O | 3:A:85:GLN:C | 2.58 | 0.41 |
| 3:A:92:LEU:O | 3:A:93:GLN:C | 2.59 | 0.41 |
| 5:C:21:ALA:HB2 | 6:D:118:TYR:HD1 | 1.85 | 0.41 |
| 5:C:85:LEU:O | 5:C:89:ASN:HB2 | 2.21 | 0.41 |
| 6:D:34:TYR:CD2 | 6:D:63:VAL:HG11 | 2.56 | 0.41 |
| 3:E:87:SER:C | 3:E:89:VAL:N | 2.74 | 0.41 |
| 4:F:31:LYS:N | 4:F:32:PRO:CD | 2.84 | 0.41 |
| 1:I:101:DG:C4' | 3:A:83:ARG:HH11 | 2.32 | 0.41 |
| 2:J:232:DA:C4' | 2:J:233:DG:OP1 | 2.46 | 0.41 |
| 5:C:78:ILE:N | 5:C:78:ILE:HD12 | 2.35 | 0.41 |
| 5:G:78:ILE:HG23 | 5:G:82:HIS:CB | 2.51 | 0.41 |
| 5:G:81:ARG:HG3 | 5:G:85:LEU:CD1 | 2.50 | 0.41 |
| 1:I:10:DC:C1' | 1:I:11:DA:O5' | 2.67 | 0.41 |
| 1:I:77:DC:H42 | 2:J:218:DG:H1 | 1.67 | 0.41 |
| 1:I:83:DA:N6 | 2:J:211:DT:O4 | 2.54 | 0.41 |
| 2:J:175:DA:N1 | 2:J:176:DA:C2 | 2.89 | 0.41 |
| 2:J:233:DG:H2" | 2:J:234:DC:OP2 | 2.20 | 0.41 |
| 2:J:287:DA:H2" | 2:J:288:DT:OP2 | 2.20 | 0.41 |
| 2:J:292:DG:OP2 | 3:A:42:ARG:HG3 | 2.21 | 0.41 |
| 4:F:25:ASN:HD22 | 4:F:25:ASN:N | 2.18 | 0.41 |
| 5:G:25:PHE:CE1 | 6:H:41:VAL:HG21 | 2.55 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:H:51:ILE:O | 6:H:51:ILE:HG23 | 2.20 | 0.41 |
| 1:I:29:DA:H5' | 6:H:30:ARG:HH21 | 1.86 | 0.41 |
| 2:J:166:DA:H5" | 5:C:77:ARG:HD3 | 2.03 | 0.41 |
| 2:J:194:DC:C2 | 2:J:195:DT:C4 | 3.09 | 0.41 |
| 4:B:62:LEU:HD23 | 4:B:62:LEU:HA | 1.88 | 0.41 |
| 5:C:62:ILE:HD13 | 5:C:87:VAL:HG22 | 2.03 | 0.41 |
| 4:F:52:GLU:O | 4:F:54:THR:N | 2.54 | 0.41 |
| 4:F:90:LEU:HB3 | 4:F:95:ARG:O | 2.20 | 0.41 |
| 5:G:27:VAL:HG22 | 5:G:52:ALA:CB | 2.50 | 0.41 |
| 1:I:16:DC:H1' | 1:I:17:DA:C8 | 2.56 | 0.41 |
| 1:I:68:DT:C4 | 1:I:69:DG:C6 | 3.09 | 0.41 |
| 2:J:228:DA:OP1 | 4:F:47:SER:HA | 2.21 | 0.41 |
| 2:J:242:DG:H1' | 2:J:243:DA:H5' | 2.03 | 0.41 |
| 2:J:260:DG:OP1 | 5:G:43:VAL:N | 2.45 | 0.41 |
| 3:A:92:LEU:CD2 | 4:B:86:VAL:CG1 | 2.99 | 0.41 |
| 3:E:47:ALA:O | 3:E:48:LEU:C | 2.58 | 0.41 |
| 3:E:79:LYS:HB3 | 3:E:82:LEU:HD11 | 2.02 | 0.41 |
| 4:F:52:GLU:O | 4:F:53:GLU:C | 2.59 | 0.41 |
| 5:C:25:PHE:HA | 6:D:37:TYR:CD2 | 2.56 | 0.40 |
| 1:I:124:DT:H1' | 1:I:125:DA:H5' | 2.02 | 0.40 |
| 2:J:199:DT:C1' | 2:J:200:DC:H5" | 2.51 | 0.40 |
| 2:J:219:DA:P | 3:A:120:MET:HE2 | 2.62 | 0.40 |
| 4:B:90:LEU:HB3 | 4:B:95:ARG:O | 2.22 | 0.40 |
| 3:E:122:LYS:NZ | 3:E:122:LYS:HB2 | 2.35 | 0.40 |
| 1:I:40:DA:N6 | 1:I:41:DA:N6 | 2.68 | 0.40 |
| 2:J:211:DT:H2" | 2:J:212:DT:OP2 | 2.20 | 0.40 |
| 2:J:220:DG:C2 | 2:J:221:DT:C2 | 3.09 | 0.40 |
| 2:J:242:DG:H1' | 2:J:243:DA:C5' | 2.51 | 0.40 |
| 2:J:246:DT:C2' | 2:J:247:DT:H71 | 2.44 | 0.40 |
| 2:J:251:DT:H6 | 2:J:251:DT:H2' | 1.75 | 0.40 |
| 3:A:66:PRO:HB3 | 4:B:28:GLY:HA3 | 2.02 | 0.40 |
| 4:B:75:HIS:NE2 | 6:D:77:LEU:HD13 | 2.34 | 0.40 |
| 5:C:30:VAL:HG11 | 5:C:51:LEU:HB3 | 2.03 | 0.40 |
| 6:H:35:ALA:O | 6:H:38:VAL:HB | 2.20 | 0.40 |
| 1:I:140:DA:H2' | 1:I:141:DT:H72 | 2.03 | 0.40 |
| 2:J:248:DT:H5" | 3:E:83:ARG:HD2 | 2.03 | 0.40 |
| 4:B:98:TYR:OH | 6:H:65:ASP:OD2 | 2.38 | 0.40 |
| 3:E:57:SER:HB2 | 3:E:59:GLU:OE2 | 2.22 | 0.40 |
| 3:E:70:LEU:O | 3:E:70:LEU:HG | 2.20 | 0.40 |
| 5:G:51:LEU:HD12 | 5:G:51:LEU:C | 2.42 | 0.40 |
| 2:J:156:DC:C2 | 2:J:157:DC:N4 | 2.89 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:J:257:DT:C6 | 2:J:258:DT:H71 | 2.57 | 0.40 |
| 3:A:117:VAL:HG12 | 5:G:115:LEU:CD2 | 2.52 | 0.40 |
| 4:B:100:PHE:CD1 | 4:B:100:PHE:N | 2.89 | 0.40 |
| 6:D:104:ALA:O | 6:D:106:HIS:N | 2.54 | 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 | |
|---|---|---|---|---|---|---|---|
| 3 | A | 96/135 (71%) | 55 (57%) | 25 (26%) | 16 (17%) | 0 | 0 |
| 3 | E | 96/135 (71%) | 61 (64%) | 21 (22%) | 14 (15%) | 0 | 1 |
| 4 | B | 77/102 (76%) | 45 (58%) | 25 (32%) | 7 (9%) | 1 | 3 |
| 4 | F | 82/102 (80%) | 57 (70%) | 19 (23%) | 6 (7%) | 1 | 7 |
| 5 | C | 105/129 (81%) | 73 (70%) | 20 (19%) | 12 (11%) | 0 | 2 |
| 5 | G | 104/129 (81%) | 64 (62%) | 21 (20%) | 19 (18%) | 0 | 0 |
| 6 | D | 91/125 (73%) | 59 (65%) | 23 (25%) | 9 (10%) | 0 | 3 |
| 6 | H | 91/125 (73%) | 56 (62%) | 26 (29%) | 9 (10%) | 0 | 3 |
| All | All | 742/982 (76%) | 470 (63%) | 180 (24%) | 92 (12%) | 0 | 2 |

All (92) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 45 | THR |
| 3 | A | 65 | LEU |
| 3 | A | 117 | VAL |
| 3 | A | 124 | ILE |
| 3 | A | 126 | LEU |
| 4 | B | 46 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | C | 80 | PRO |
| 5 | C | 92 | GLU |
| 6 | D | 101 | GLY |
| 6 | D | 102 | GLU |
| 3 | E | 51 | ILE |
| 3 | E | 62 | ILE |
| 3 | E | 88 | ALA |
| 3 | E | 97 | GLU |
| 3 | E | 98 | ALA |
| 3 | E | 115 | LYS |
| 3 | E | 134 | ARG |
| 4 | F | 38 | ALA |
| 4 | F | 47 | SER |
| 5 | G | 40 | ALA |
| 5 | G | 64 | GLU |
| 5 | G | 98 | GLY |
| 5 | G | 112 | GLN |
| 5 | G | 113 | SER |
| 5 | G | 114 | VAL |
| 5 | G | 117 | PRO |
| 5 | G | 118 | LYS |
| 3 | A | 46 | VAL |
| 3 | A | 64 | LYS |
| 4 | B | 44 | LYS |
| 4 | B | 62 | LEU |
| 5 | C | 36 | LYS |
| 5 | C | 44 | GLY |
| 5 | C | 52 | ALA |
| 5 | C | 73 | ASN |
| 5 | C | 74 | LYS |
| 5 | C | 93 | LEU |
| 6 | D | 82 | LYS |
| 3 | E | 52 | ARG |
| 3 | E | 106 | ASP |
| 3 | E | 109 | LEU |
| 3 | E | 124 | ILE |
| 4 | F | 51 | TYR |
| 5 | G | 91 | GLU |
| 5 | G | 92 | GLU |
| 5 | G | 109 | PRO |
| 6 | H | 101 | GLY |
| 6 | H | 109 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 6 | H | 121 | ALA |
| 3 | A | 53 | ARG |
| 4 | B | 63 | GLU |
| 4 | B | 87 | VAL |
| 4 | B | 88 | TYR |
| 3 | E | 42 | ARG |
| 5 | G | 61 | GLU |
| 5 | G | 74 | LYS |
| 6 | H | 51 | ILE |
| 6 | H | 93 | THR |
| 3 | A | 74 | ILE |
| 3 | A | 77 | ASP |
| 5 | C | 23 | LEU |
| 6 | D | 113 | LYS |
| 6 | D | 115 | VAL |
| 4 | F | 53 | GLU |
| 5 | G | 26 | PRO |
| 5 | G | 39 | TYR |
| 5 | G | 87 | VAL |
| 3 | A | 125 | GLN |
| 5 | C | 98 | GLY |
| 5 | C | 109 | PRO |
| 6 | D | 52 | SER |
| 6 | D | 109 | SER |
| 3 | E | 77 | ASP |
| 3 | E | 86 | SER |
| 6 | H | 33 | SER |
| 6 | H | 44 | GLN |
| 6 | H | 113 | LYS |
| 3 | A | 51 | ILE |
| 3 | A | 123 | ASP |
| 6 | D | 78 | ALA |
| 6 | D | 105 | LYS |
| 4 | F | 50 | ILE |
| 6 | H | 35 | ALA |
| 3 | A | 43 | PRO |
| 3 | A | 119 | ILE |
| 4 | F | 32 | PRO |
| 5 | G | 62 | ILE |
| 3 | A | 101 | VAL |
| 4 | B | 70 | VAL |
| 5 | C | 106 | GLY |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | G | 80 | PRO |
| 5 | G | 107 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 3 | A | 85/110 (77%) | 78 (92%) | 7 (8%) | 11 41 |
| 3 | E | 85/110 (77%) | 77 (91%) | 8 (9%) | 8 33 |
| 4 | B | 64/78 (82%) | 60 (94%) | 4 (6%) | 18 52 |
| 4 | F | 69/78 (88%) | 66 (96%) | 3 (4%) | 29 64 |
| 5 | C | 85/101 (84%) | 76 (89%) | 9 (11%) | 6 27 |
| 5 | G | 84/101 (83%) | 76 (90%) | 8 (10%) | 8 32 |
| 6 | D | 79/105 (75%) | 72 (91%) | 7 (9%) | 9 35 |
| 6 | H | 79/105 (75%) | 71 (90%) | 8 (10%) | 7 29 |
| All | All | 630/788 (80%) | 576 (91%) | 54 (9%) | 10 38 |

All (54) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 42 | ARG |
| 3 | A | 56 | LYS |
| 3 | A | 66 | PRO |
| 3 | A | 104 | PHE |
| 3 | A | 108 | ASN |
| 3 | A | 129 | ARG |
| 3 | A | 130 | ILE |
| 4 | B | 39 | ARG |
| 4 | B | 72 | TYR |
| 4 | B | 84 | MET |
| 4 | B | 93 | GLN |
| 5 | C | 29 | ARG |
| 5 | C | 62 | ILE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | C | 76 | THR |
| 5 | C | 85 | LEU |
| 5 | C | 90 | ASP |
| 5 | C | 91 | GLU |
| 5 | C | 107 | VAL |
| 5 | C | 118 | LYS |
| 5 | C | 119 | LYS |
| 6 | D | 33 | SER |
| 6 | D | 34 | TYR |
| 6 | D | 82 | LYS |
| 6 | D | 85 | THR |
| 6 | D | 89 | ARG |
| 6 | D | 93 | THR |
| 6 | D | 116 | THR |
| 3 | E | 48 | LEU |
| 3 | E | 63 | ARG |
| 3 | E | 93 | GLN |
| 3 | E | 106 | ASP |
| 3 | E | 115 | LYS |
| 3 | E | 122 | LYS |
| 3 | E | 126 | LEU |
| 3 | E | 134 | ARG |
| 4 | F | 35 | ARG |
| 4 | F | 79 | LYS |
| 4 | F | 92 | ARG |
| 5 | G | 34 | LEU |
| 5 | G | 50 | TYR |
| 5 | G | 51 | LEU |
| 5 | G | 74 | LYS |
| 5 | G | 80 | PRO |
| 5 | G | 100 | VAL |
| 5 | G | 101 | THR |
| 5 | G | 119 | LYS |
| 6 | H | 36 | ILE |
| 6 | H | 51 | ILE |
| 6 | H | 61 | SER |
| 6 | H | 87 | THR |
| 6 | H | 93 | THR |
| 6 | H | 95 | VAL |
| 6 | H | 113 | LYS |
| 6 | H | 116 | THR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 76 | GLN |
| 3 | A | 108 | ASN |
| 4 | B | 93 | GLN |
| 5 | C | 31 | HIS |
| 5 | C | 38 | ASN |
| 5 | C | 89 | ASN |
| 5 | C | 104 | GLN |
| 6 | D | 44 | GLN |
| 6 | D | 79 | HIS |
| 6 | D | 106 | HIS |
| 3 | E | 125 | GLN |
| 5 | G | 38 | ASN |
| 6 | H | 64 | ASN |
| 6 | H | 81 | ASN |
| 6 | H | 92 | GLN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no monosaccharides in this entry.

### 5.6 Ligand geometry

There are no ligands in this entry.

### 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 | I | 147/147 (100%) | -0.06 | 7 (4%) 30 18 | 77, 171, 203, 203 | 0 |
| 2 | J | 147/147 (100%) | -0.11 | 5 (3%) 45 29 | 82, 169, 203, 203 | 0 |
| 3 | A | 98/135 (72%) | -0.12 | 3 (3%) 49 32 | 41, 96, 171, 181 | 0 |
| 3 | E | 98/135 (72%) | -0.22 | 2 (2%) 65 51 | 21, 69, 145, 196 | 0 |
| 4 | B | 79/102 (77%) | -0.19 | 0 100 100 | 34, 87, 158, 192 | 0 |
| 4 | F | 84/102 (82%) | -0.36 | 0 100 100 | 24, 55, 103, 131 | 0 |
| 5 | C | 107/129 (82%) | -0.35 | 0 100 100 | 17, 62, 145, 184 | 0 |
| 5 | G | 106/129 (82%) | -0.21 | 1 (0%) 84 75 | 40, 95, 163, 201 | 0 |
| 6 | D | 93/125 (74%) | -0.28 | 0 100 100 | 25, 62, 118, 170 | 0 |
| 6 | H | 93/125 (74%) | -0.16 | 4 (4%) 35 22 | 25, 85, 164, 203 | 0 |
| All | All | 1052/1276 (82%) | -0.19 | 22 (2%) 63 49 | 17, 94, 200, 203 | 0 |

All (22) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | E | 135 | ALA | 5.4 |
| 1 | I | 147 | DT | 4.9 |
| 3 | E | 39 | HIS | 4.4 |
| 6 | H | 39 | TYR | 3.9 |
| 2 | J | 148 | DA | 3.3 |
| 1 | I | 12 | DC | 3.3 |
| 1 | I | 76 | DT | 3.0 |
| 3 | A | 38 | PRO | 3.0 |
| 2 | J | 204 | DA | 2.7 |
| 2 | J | 160 | DC | 2.6 |
| 1 | I | 87 | DT | 2.6 |
| 1 | I | 13 | DC | 2.5 |
| 3 | A | 82 | LEU | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | J | 253 | DT | 2.4 |
| 2 | J | 294 | DT | 2.3 |
| 1 | I | 146 | DA | 2.3 |
| 6 | H | 50 | GLY | 2.3 |
| 6 | H | 30 | ARG | 2.2 |
| 1 | I | 1 | DA | 2.2 |
| 6 | H | 122 | LYS | 2.1 |
| 5 | G | 74 | LYS | 2.0 |
| 3 | A | 46 | VAL | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.