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

Feb 1, 2016 – 01:43 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 3UKF |
| Title | : | CRYSTAL STRUCTURE OF UDP-galactopyranose mutase from Aspergillus fumigatus in complex with UDPgalp (reduced) |
| Authors | : | Van Straaten, K.E.; Sanders, D.A.R. |
| Deposited on | : | 2011-11-09 |
| Resolution | : | 2.50 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

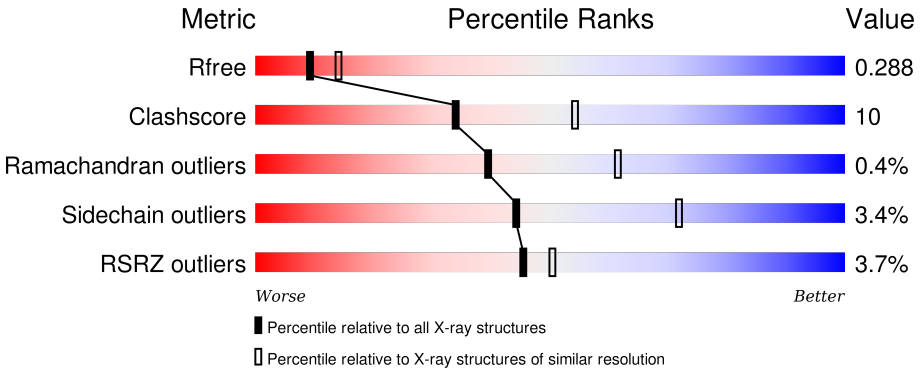
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 91344 | 3553 (2.50-2.50) |
| Clashscore | 102246 | 4242 (2.50-2.50) |
| Ramachandran outliers | 100387 | 4156 (2.50-2.50) |
| Sidechain outliers | 100360 | 4158 (2.50-2.50) |
| RSRZ outliers | 91569 | 3562 (2.50-2.50) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 509 | 78% 20% |
| 1 | B | 509 | 79% 20% |
| 1 | C | 509 | 78% 20% |
| 1 | D | 509 | 79% 20% |
| 1 | E | 509 | 8% 78% 21% |

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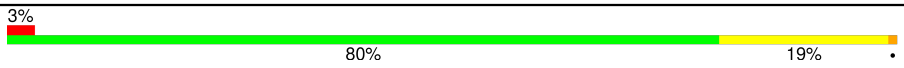
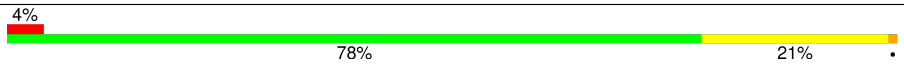
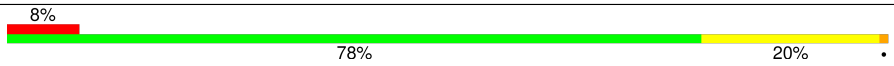
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 509 |   |
| 1 | G | 509 |   |
| 1 | H | 509 |   |

## 2 Entry composition (i)

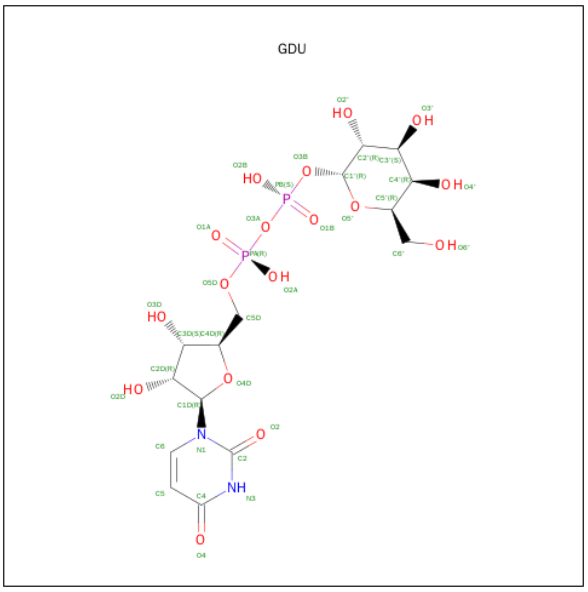
There are 5 unique types of molecules in this entry. The entry contains 33444 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-galactopyranose mutase.

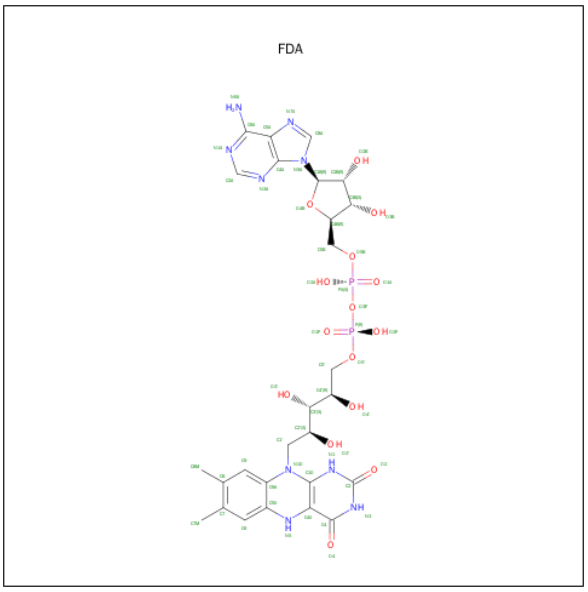
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | B | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | C | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | D | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | E | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | F | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | G | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |
| 1 | H | 509 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 3996 | 2534 | 686 | 755 | 7 | 14 | | | |

- Molecule 2 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |
| 2 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 36 | 15 | 2 | 17 | 2 | | |

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 3 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | G | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | E | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | H | 1 | Total | Cl | 0 | 0 |
| | | | 1 | 1 | | |
| 4 | B | 2 | Total | Cl | 0 | 0 |
| | | | 2 | 2 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 2 | Total Cl<br>2 2 | 0 | 0 |
| 4 | F | 1 | Total Cl<br>1 1 | 0 | 0 |

- Molecule 5 is water.

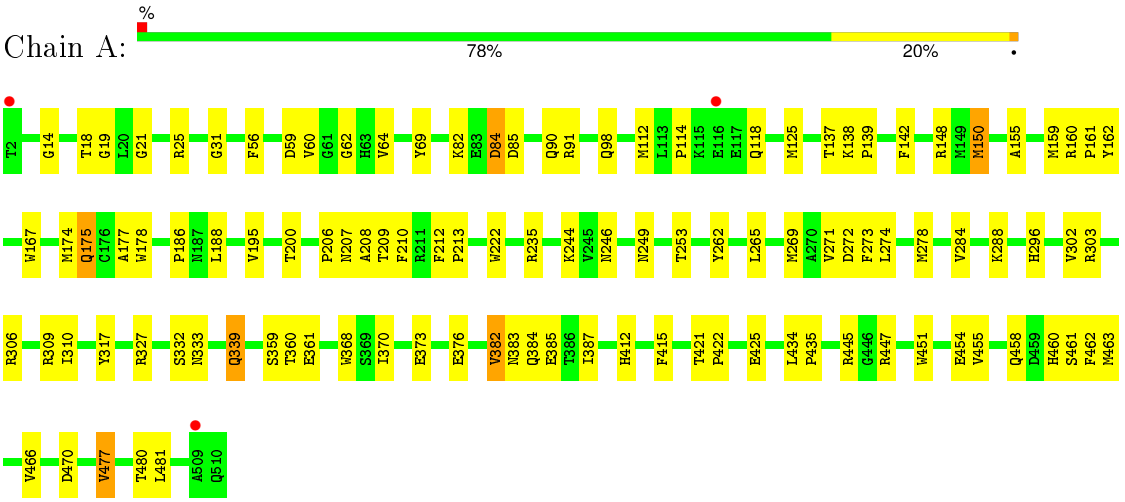
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 109 | Total O<br>109 109 | 0 | 0 |
| 5 | B | 122 | Total O<br>122 122 | 0 | 0 |
| 5 | C | 71 | Total O<br>71 71 | 0 | 0 |
| 5 | D | 104 | Total O<br>104 104 | 0 | 0 |
| 5 | E | 90 | Total O<br>90 90 | 0 | 0 |
| 5 | F | 78 | Total O<br>78 78 | 0 | 0 |
| 5 | G | 97 | Total O<br>97 97 | 0 | 0 |
| 5 | H | 85 | Total O<br>85 85 | 0 | 0 |

# 3 Residue-property plots (i)

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

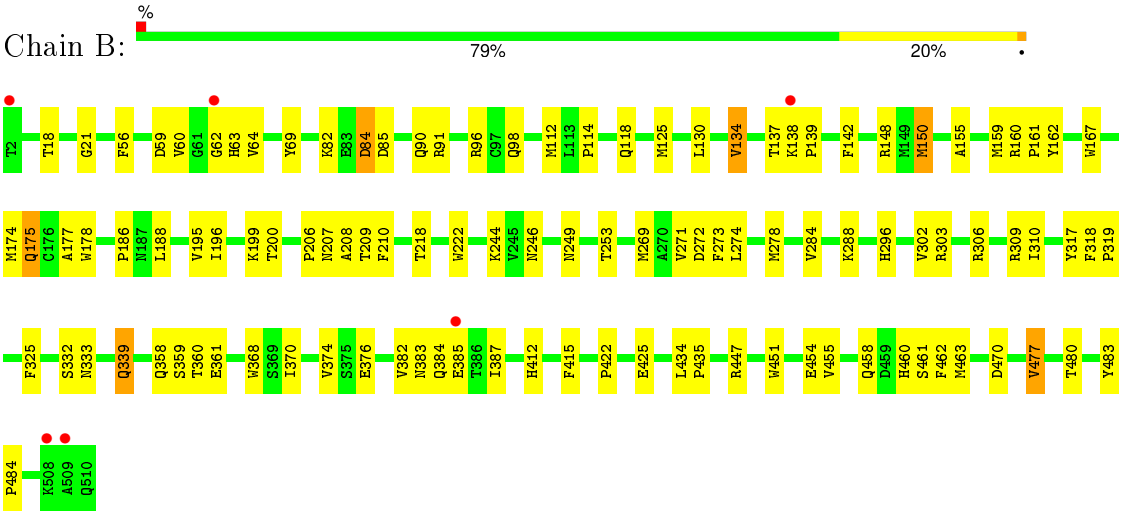
- Molecule 1: UDP-galactopyranose mutase

Chain A:



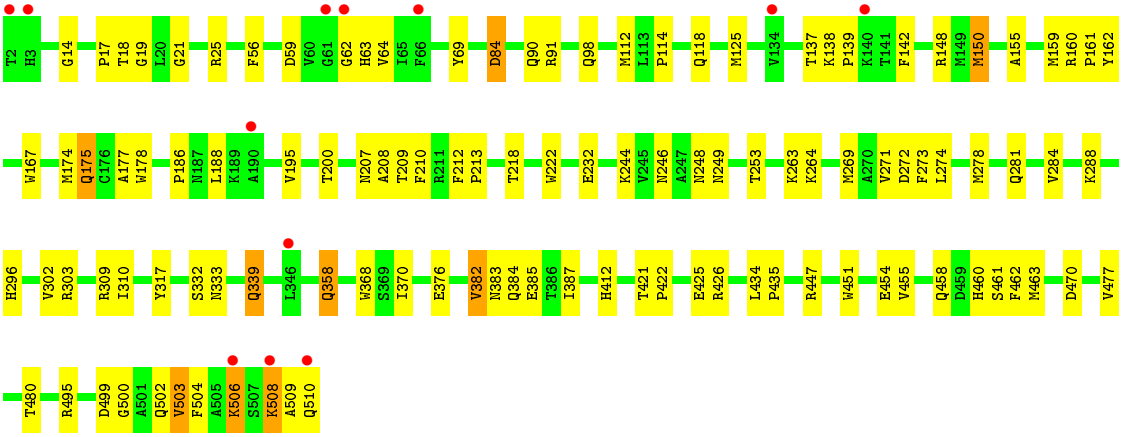

- Molecule 1: UDP-galactopyranose mutase

Chain B:



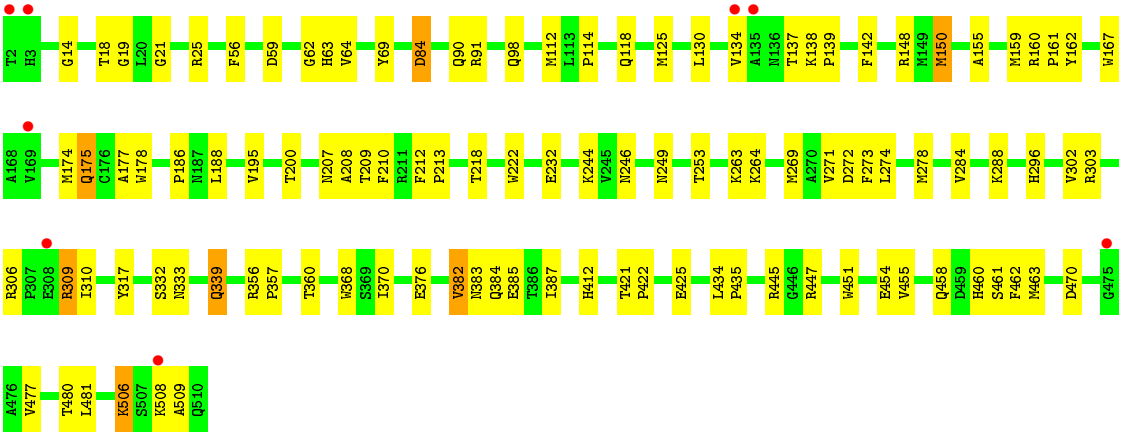

- Molecule 1: UDP-galactopyranose mutase

Chain C:



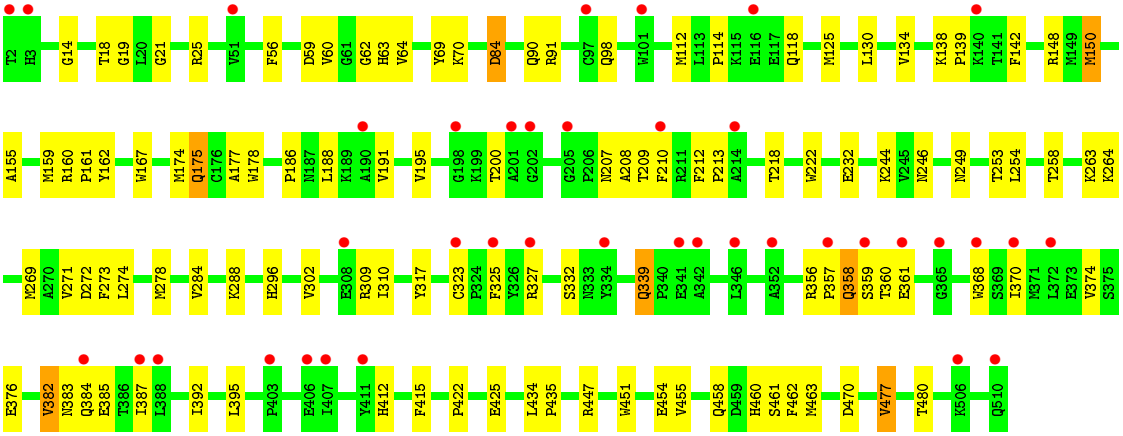

• Molecule 1: UDP-galactopyranose mutase

Chain D:

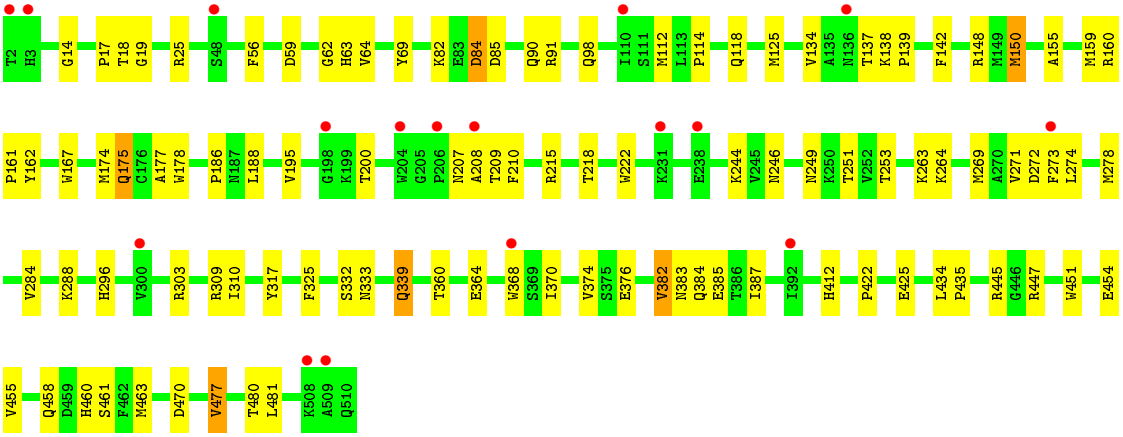

• Molecule 1: UDP-galactopyranose mutase

Chain E:

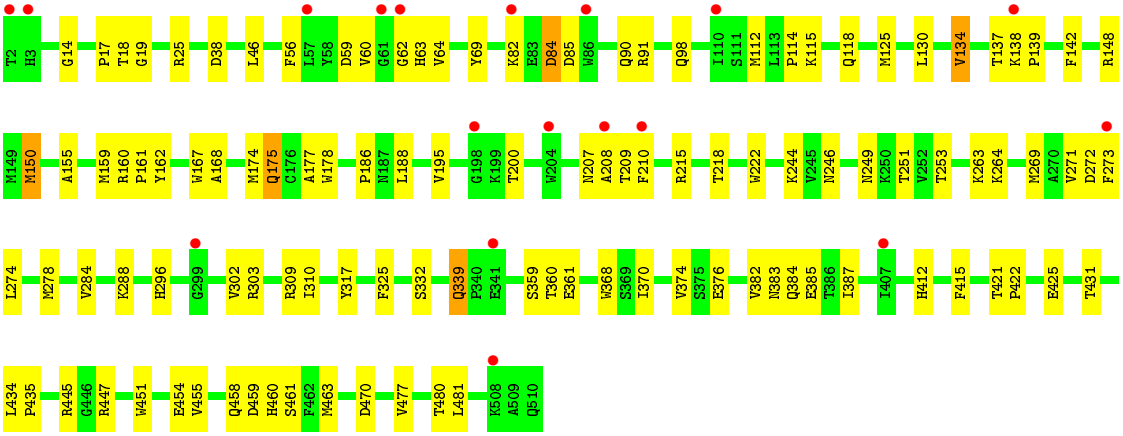

• Molecule 1: UDP-galactopyranose mutase

Chain F:



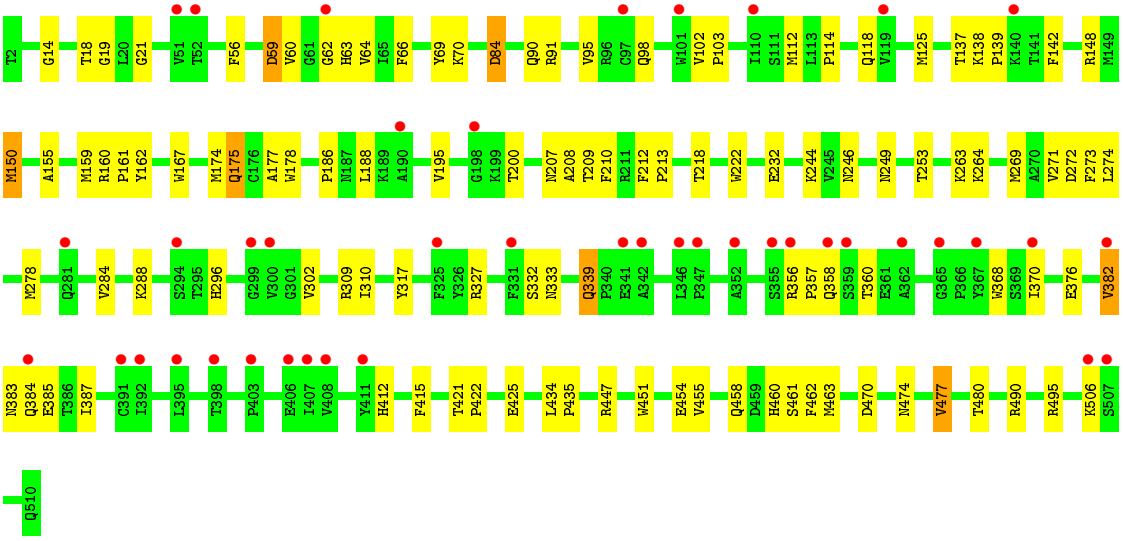

• Molecule 1: UDP-galactopyranose mutase

Chain G:


• Molecule 1: UDP-galactopyranose mutase

Chain H:

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 72.08Å 129.34Å 175.08Å<br>89.97° 103.61° 90.14° | Depositor |
| Resolution (Å) | 20.00 – 2.50<br>20.00 – 2.40 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.7 (20.00-2.50)<br>96.5 (20.00-2.40) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | 0.11 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.94 (at 2.41Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.1_743) | Depositor |
| R, $R_{free}$ | 0.250 , 0.293<br>0.246 , 0.288 | Depositor<br>DCC |
| $R_{free}$ test set | 10355 reflections (5.25%) | DCC |
| Wilson B-factor (Å$^2$) | 54.4 | Xtriage |
| Anisotropy | 0.329 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 47.8 | EDS |
| Estimated twinning fraction | 0.000 for h,-k,-h-l<br>0.399 for -h,k,-l<br>0.000 for -h,-k,h+l | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Outliers | 0 of 233082 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 33444 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 70.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FDA, GDU, CL

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 | 0.22 | 0/4081 | 0.41 | 0/5523 |
| 1 | B | 0.23 | 0/4081 | 0.41 | 0/5523 |
| 1 | C | 0.22 | 0/4081 | 0.40 | 0/5523 |
| 1 | D | 0.22 | 0/4081 | 0.40 | 0/5523 |
| 1 | E | 0.22 | 0/4081 | 0.40 | 0/5523 |
| 1 | F | 0.22 | 0/4081 | 0.41 | 0/5523 |
| 1 | G | 0.22 | 0/4081 | 0.41 | 0/5523 |
| 1 | H | 0.22 | 0/4081 | 0.40 | 0/5523 |
| All | All | 0.22 | 0/32648 | 0.40 | 0/44184 |

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

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 | 3996 | 0 | 3914 | 81 | 0 |
| 1 | B | 3996 | 0 | 3914 | 81 | 0 |
| 1 | C | 3996 | 0 | 3914 | 90 | 0 |
| 1 | D | 3996 | 0 | 3914 | 79 | 0 |
| 1 | E | 3996 | 0 | 3914 | 80 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | F | 3996 | 0 | 3914 | 70 | 0 |
| 1 | G | 3996 | 0 | 3914 | 88 | 0 |
| 1 | H | 3996 | 0 | 3914 | 87 | 0 |
| 2 | A | 36 | 0 | 22 | 2 | 0 |
| 2 | B | 36 | 0 | 22 | 1 | 0 |
| 2 | C | 36 | 0 | 22 | 2 | 0 |
| 2 | D | 36 | 0 | 22 | 2 | 0 |
| 2 | E | 36 | 0 | 22 | 1 | 0 |
| 2 | F | 36 | 0 | 22 | 0 | 0 |
| 2 | G | 36 | 0 | 22 | 2 | 0 |
| 2 | H | 36 | 0 | 22 | 3 | 0 |
| 3 | A | 53 | 0 | 32 | 1 | 0 |
| 3 | B | 53 | 0 | 32 | 1 | 0 |
| 3 | C | 53 | 0 | 32 | 1 | 0 |
| 3 | D | 53 | 0 | 32 | 1 | 0 |
| 3 | E | 53 | 0 | 32 | 1 | 0 |
| 3 | F | 53 | 0 | 32 | 2 | 0 |
| 3 | G | 53 | 0 | 32 | 6 | 0 |
| 3 | H | 53 | 0 | 32 | 1 | 0 |
| 4 | A | 2 | 0 | 0 | 1 | 0 |
| 4 | B | 2 | 0 | 0 | 2 | 0 |
| 4 | E | 1 | 0 | 0 | 1 | 0 |
| 4 | F | 1 | 0 | 0 | 1 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | H | 1 | 0 | 0 | 1 | 0 |
| 5 | A | 109 | 0 | 0 | 7 | 0 |
| 5 | B | 122 | 0 | 0 | 5 | 0 |
| 5 | C | 71 | 0 | 0 | 5 | 0 |
| 5 | D | 104 | 0 | 0 | 5 | 0 |
| 5 | E | 90 | 0 | 0 | 4 | 0 |
| 5 | F | 78 | 0 | 0 | 3 | 0 |
| 5 | G | 97 | 0 | 0 | 8 | 0 |
| 5 | H | 85 | 0 | 0 | 7 | 0 |
| All | All | 33444 | 0 | 31744 | 650 | 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 10.

All (650) 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:E:323:CYS:SG | 5:E:542:HOH:O | 2.26 | 0.94 |
| 1:G:69:TYR:HE2 | 5:G:729:HOH:O | 1.55 | 0.87 |
| 1:F:125:MSE:HE2 | 1:F:188:LEU:HA | 1.58 | 0.84 |
| 1:D:125:MSE:HE2 | 1:D:188:LEU:HA | 1.59 | 0.84 |
| 1:G:125:MSE:HE2 | 1:G:188:LEU:HA | 1.59 | 0.83 |
| 1:H:125:MSE:HE2 | 1:H:188:LEU:HA | 1.60 | 0.82 |
| 1:A:125:MSE:HE2 | 1:A:188:LEU:HA | 1.60 | 0.82 |
| 1:C:125:MSE:HE2 | 1:C:188:LEU:HA | 1.60 | 0.82 |
| 1:B:125:MSE:HE2 | 1:B:188:LEU:HA | 1.60 | 0.82 |
| 1:E:125:MSE:HE2 | 1:E:188:LEU:HA | 1.61 | 0.81 |
| 1:G:360:THR:HG22 | 1:G:360:THR:O | 1.83 | 0.77 |
| 1:G:125:MSE:HB2 | 5:G:553:HOH:O | 1.85 | 0.75 |
| 1:B:477:VAL:HG12 | 4:B:511:CL:CL | 2.25 | 0.73 |
| 1:D:134:VAL:HG22 | 1:E:134:VAL:HG22 | 1.70 | 0.73 |
| 1:C:508:LYS:HG2 | 1:C:509:ALA:N | 2.04 | 0.72 |
| 1:D:112:MSE:HE3 | 1:D:200:THR:HG23 | 1.72 | 0.71 |
| 1:D:91:ARG:HH11 | 1:D:207:ASN:HB2 | 1.55 | 0.71 |
| 1:B:91:ARG:HH11 | 1:B:207:ASN:HB2 | 1.56 | 0.71 |
| 1:C:112:MSE:HE3 | 1:C:200:THR:HG23 | 1.73 | 0.71 |
| 1:G:112:MSE:HE3 | 1:G:200:THR:HG23 | 1.73 | 0.71 |
| 1:G:91:ARG:HH11 | 1:G:207:ASN:HB2 | 1.56 | 0.71 |
| 1:A:91:ARG:HH11 | 1:A:207:ASN:HB2 | 1.56 | 0.70 |
| 1:A:327:ARG:N | 5:A:660:HOH:O | 2.20 | 0.70 |
| 1:E:112:MSE:HE3 | 1:E:200:THR:HG23 | 1.74 | 0.70 |
| 1:F:112:MSE:HE3 | 1:F:200:THR:HG23 | 1.72 | 0.70 |
| 1:A:455:VAL:HG21 | 1:A:480:THR:HG23 | 1.74 | 0.69 |
| 1:F:91:ARG:HH11 | 1:F:207:ASN:HB2 | 1.56 | 0.69 |
| 1:C:296:HIS:HD2 | 1:C:412:HIS:HE1 | 1.40 | 0.69 |
| 1:C:358:GLN:CD | 1:C:358:GLN:H | 1.95 | 0.69 |
| 1:E:274:LEU:HD11 | 1:E:278:MSE:HE3 | 1.75 | 0.69 |
| 1:H:477:VAL:HG12 | 4:H:511:CL:CL | 2.30 | 0.69 |
| 1:D:138:LYS:HG3 | 1:D:139:PRO:HD2 | 1.75 | 0.69 |
| 1:H:112:MSE:HE3 | 1:H:200:THR:HG23 | 1.75 | 0.69 |
| 1:E:138:LYS:HG3 | 1:E:139:PRO:HD2 | 1.76 | 0.68 |
| 1:C:91:ARG:HH11 | 1:C:207:ASN:HB2 | 1.59 | 0.68 |
| 1:C:138:LYS:HG3 | 1:C:139:PRO:HD2 | 1.76 | 0.68 |
| 1:H:91:ARG:HH11 | 1:H:207:ASN:HB2 | 1.58 | 0.68 |
| 1:D:455:VAL:HG21 | 1:D:480:THR:HG23 | 1.75 | 0.67 |
| 1:C:455:VAL:HG21 | 1:C:480:THR:HG23 | 1.75 | 0.67 |
| 1:A:159:MSE:HE1 | 2:A:802:GDU:O2 | 1.94 | 0.67 |
| 1:B:112:MSE:HE3 | 1:B:200:THR:HG23 | 1.77 | 0.67 |
| 1:G:138:LYS:HG3 | 1:G:139:PRO:HD2 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:296:HIS:HD2 | 1:D:412:HIS:HE1 | 1.40 | 0.67 |
| 1:E:91:ARG:HH11 | 1:E:207:ASN:HB2 | 1.60 | 0.67 |
| 1:H:274:LEU:HD11 | 1:H:278:MSE:HE3 | 1.76 | 0.67 |
| 1:H:138:LYS:HG3 | 1:H:139:PRO:HD2 | 1.77 | 0.67 |
| 1:E:455:VAL:HG21 | 1:E:480:THR:HG23 | 1.77 | 0.66 |
| 1:F:138:LYS:HG3 | 1:F:139:PRO:HD2 | 1.76 | 0.66 |
| 1:G:296:HIS:HD2 | 1:G:412:HIS:HE1 | 1.44 | 0.66 |
| 1:C:455:VAL:HG22 | 1:C:460:HIS:HB3 | 1.78 | 0.66 |
| 1:E:455:VAL:HG22 | 1:E:460:HIS:HB3 | 1.78 | 0.66 |
| 1:H:296:HIS:HD2 | 1:H:412:HIS:HE1 | 1.43 | 0.66 |
| 1:F:360:THR:HG22 | 1:F:360:THR:O | 1.94 | 0.66 |
| 1:B:274:LEU:HD11 | 1:B:278:MSE:HE3 | 1.78 | 0.66 |
| 1:G:455:VAL:HG21 | 1:G:480:THR:HG23 | 1.78 | 0.65 |
| 1:F:455:VAL:HG21 | 1:F:480:THR:HG23 | 1.78 | 0.65 |
| 1:A:477:VAL:HG12 | 4:A:511:CL:CL | 2.33 | 0.65 |
| 1:E:296:HIS:HD2 | 1:E:412:HIS:HE1 | 1.45 | 0.65 |
| 1:F:455:VAL:HG22 | 1:F:460:HIS:HB3 | 1.77 | 0.65 |
| 1:A:138:LYS:HG3 | 1:A:139:PRO:HD2 | 1.77 | 0.65 |
| 1:A:296:HIS:HD2 | 1:A:412:HIS:HE1 | 1.43 | 0.65 |
| 1:D:137:THR:HG23 | 5:D:724:HOH:O | 1.97 | 0.64 |
| 1:H:455:VAL:HG22 | 1:H:460:HIS:HB3 | 1.78 | 0.64 |
| 1:E:477:VAL:HG12 | 4:E:511:CL:CL | 2.34 | 0.64 |
| 1:A:112:MSE:HE3 | 1:A:200:THR:HG23 | 1.78 | 0.64 |
| 1:D:455:VAL:HG22 | 1:D:460:HIS:HB3 | 1.78 | 0.64 |
| 1:A:274:LEU:HD11 | 1:A:278:MSE:HE3 | 1.79 | 0.64 |
| 1:G:455:VAL:HG22 | 1:G:460:HIS:HB3 | 1.77 | 0.64 |
| 1:B:138:LYS:HG3 | 1:B:139:PRO:HD2 | 1.79 | 0.64 |
| 1:C:232:GLU:HG3 | 1:H:232:GLU:CG | 2.28 | 0.63 |
| 1:B:359:SER:OG | 1:B:361:GLU:HG2 | 1.98 | 0.63 |
| 1:F:296:HIS:HD2 | 1:F:412:HIS:HE1 | 1.44 | 0.63 |
| 1:B:455:VAL:HG21 | 1:B:480:THR:HG23 | 1.80 | 0.62 |
| 1:G:17:PRO:HD2 | 3:G:600:FDA:O5' | 1.99 | 0.62 |
| 1:E:359:SER:HB3 | 1:E:361:GLU:HG2 | 1.79 | 0.62 |
| 1:B:178:TRP:CB | 1:B:454:GLU:HG3 | 2.28 | 0.62 |
| 1:H:455:VAL:HG21 | 1:H:480:THR:HG23 | 1.80 | 0.62 |
| 1:A:178:TRP:CB | 1:A:454:GLU:HG3 | 2.30 | 0.62 |
| 1:C:232:GLU:CG | 1:H:232:GLU:HG3 | 2.30 | 0.62 |
| 1:C:232:GLU:HG3 | 1:H:232:GLU:HG2 | 1.80 | 0.62 |
| 1:B:296:HIS:HD2 | 1:B:412:HIS:HE1 | 1.45 | 0.62 |
| 1:B:159:MSE:HE1 | 2:B:802:GDU:O2 | 2.00 | 0.61 |
| 1:F:178:TRP:CB | 1:F:454:GLU:HG3 | 2.31 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:455:VAL:HG22 | 1:B:460:HIS:HB3 | 1.82 | 0.60 |
| 1:G:178:TRP:CB | 1:G:454:GLU:HG3 | 2.30 | 0.60 |
| 1:A:455:VAL:HG22 | 1:A:460:HIS:HB3 | 1.82 | 0.60 |
| 1:G:460:HIS:CD2 | 5:G:729:HOH:O | 2.53 | 0.60 |
| 1:A:175:GLN:NE2 | 1:A:177:ALA:H | 2.00 | 0.60 |
| 1:B:178:TRP:HB2 | 1:B:454:GLU:HG3 | 1.83 | 0.60 |
| 1:H:178:TRP:CB | 1:H:454:GLU:HG3 | 2.31 | 0.60 |
| 1:H:178:TRP:HB2 | 1:H:454:GLU:HG3 | 1.84 | 0.60 |
| 1:E:178:TRP:CB | 1:E:454:GLU:HG3 | 2.32 | 0.60 |
| 1:F:178:TRP:HB2 | 1:F:454:GLU:HG3 | 1.84 | 0.59 |
| 1:F:17:PRO:HD2 | 3:F:600:FDA:O5' | 2.01 | 0.59 |
| 1:H:125:MSE:HG2 | 1:H:188:LEU:HD13 | 1.84 | 0.59 |
| 1:G:91:ARG:NH1 | 1:G:207:ASN:HB2 | 2.17 | 0.59 |
| 1:G:207:ASN:ND2 | 5:G:563:HOH:O | 2.35 | 0.59 |
| 1:F:91:ARG:NH1 | 1:F:207:ASN:HB2 | 2.17 | 0.59 |
| 1:D:178:TRP:CB | 1:D:454:GLU:HG3 | 2.33 | 0.59 |
| 1:E:18:THR:OG1 | 1:E:461:SER:HB3 | 2.03 | 0.59 |
| 1:C:137:THR:HG23 | 5:C:543:HOH:O | 2.01 | 0.58 |
| 1:C:232:GLU:HG2 | 1:H:232:GLU:HG3 | 1.83 | 0.58 |
| 1:G:178:TRP:HB2 | 1:G:454:GLU:HG3 | 1.84 | 0.58 |
| 1:D:274:LEU:HD11 | 1:D:278:MSE:HE3 | 1.84 | 0.58 |
| 1:A:178:TRP:HB2 | 1:A:454:GLU:HG3 | 1.85 | 0.58 |
| 1:A:303:ARG:NH1 | 5:A:567:HOH:O | 2.23 | 0.58 |
| 1:A:91:ARG:NH1 | 1:A:207:ASN:HB2 | 2.18 | 0.58 |
| 1:F:18:THR:OG1 | 1:F:461:SER:HB3 | 2.04 | 0.58 |
| 1:H:18:THR:OG1 | 1:H:461:SER:HB3 | 2.04 | 0.58 |
| 1:E:274:LEU:CD1 | 1:E:278:MSE:HE3 | 2.33 | 0.57 |
| 1:H:274:LEU:CD1 | 1:H:278:MSE:HE3 | 2.33 | 0.57 |
| 1:B:222:TRP:HE1 | 1:B:458:GLN:NE2 | 2.02 | 0.57 |
| 1:E:178:TRP:HB2 | 1:E:454:GLU:HG3 | 1.86 | 0.57 |
| 1:D:91:ARG:NH1 | 1:D:207:ASN:HB2 | 2.17 | 0.57 |
| 1:C:178:TRP:CB | 1:C:454:GLU:HG3 | 2.34 | 0.57 |
| 1:F:125:MSE:HG2 | 1:F:188:LEU:HD13 | 1.86 | 0.57 |
| 1:F:222:TRP:HE1 | 1:F:458:GLN:NE2 | 2.02 | 0.57 |
| 1:H:91:ARG:NH1 | 1:H:207:ASN:HB2 | 2.19 | 0.57 |
| 1:G:274:LEU:HD11 | 1:G:278:MSE:HE3 | 1.87 | 0.57 |
| 1:C:159:MSE:HE1 | 2:C:802:GDU:O2 | 2.04 | 0.56 |
| 1:B:358:GLN:NE2 | 1:C:84:ASP:HA | 2.20 | 0.56 |
| 1:E:317:TYR:N | 5:E:530:HOH:O | 2.38 | 0.56 |
| 1:A:18:THR:OG1 | 1:A:461:SER:HB3 | 2.05 | 0.56 |
| 1:B:91:ARG:NH1 | 1:B:207:ASN:HB2 | 2.18 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:434:LEU:HB2 | 1:B:435:PRO:HD3 | 1.88 | 0.56 |
| 1:F:477:VAL:HG12 | 4:F:511:CL:CL | 2.42 | 0.56 |
| 1:B:425:GLU:OE2 | 1:B:425:GLU:N | 2.39 | 0.56 |
| 1:B:125:MSE:HG2 | 1:B:188:LEU:HD13 | 1.87 | 0.56 |
| 1:E:91:ARG:NH1 | 1:E:207:ASN:HB2 | 2.20 | 0.56 |
| 1:F:274:LEU:HD11 | 1:F:278:MSE:HE3 | 1.88 | 0.56 |
| 1:B:18:THR:OG1 | 1:B:461:SER:HB3 | 2.06 | 0.55 |
| 1:D:125:MSE:HG2 | 1:D:188:LEU:HD13 | 1.88 | 0.55 |
| 1:D:178:TRP:HB2 | 1:D:454:GLU:HG3 | 1.87 | 0.55 |
| 1:D:175:GLN:NE2 | 1:D:177:ALA:H | 2.04 | 0.55 |
| 1:D:222:TRP:HE1 | 1:D:458:GLN:NE2 | 2.04 | 0.55 |
| 1:C:499:ASP:O | 1:C:503:VAL:HG12 | 2.07 | 0.55 |
| 1:C:178:TRP:HB2 | 1:C:454:GLU:HG3 | 1.89 | 0.55 |
| 1:G:159:MSE:HE1 | 2:G:802:GDU:O2 | 2.07 | 0.55 |
| 1:H:159:MSE:HE1 | 2:H:802:GDU:O2 | 2.07 | 0.55 |
| 1:E:222:TRP:HE1 | 1:E:458:GLN:NE2 | 2.05 | 0.55 |
| 1:D:506:LYS:N | 1:D:506:LYS:HE3 | 2.22 | 0.55 |
| 1:B:274:LEU:CD1 | 1:B:278:MSE:HE3 | 2.37 | 0.55 |
| 1:G:459:ASP:CG | 5:G:729:HOH:O | 2.45 | 0.55 |
| 1:C:125:MSE:HG2 | 1:C:188:LEU:HD13 | 1.88 | 0.55 |
| 1:B:360:THR:HG22 | 1:B:360:THR:O | 2.06 | 0.55 |
| 1:G:434:LEU:HB2 | 1:G:435:PRO:HD3 | 1.89 | 0.55 |
| 1:E:383:ASN:OD1 | 1:E:385:GLU:HG2 | 2.07 | 0.55 |
| 1:C:222:TRP:HE1 | 1:C:458:GLN:NE2 | 2.03 | 0.55 |
| 1:E:434:LEU:HB2 | 1:E:435:PRO:HD3 | 1.88 | 0.54 |
| 1:G:18:THR:OG1 | 1:G:461:SER:HB3 | 2.07 | 0.54 |
| 1:D:508:LYS:HG2 | 1:D:509:ALA:N | 2.21 | 0.54 |
| 1:H:383:ASN:OD1 | 1:H:385:GLU:HG2 | 2.07 | 0.54 |
| 1:A:222:TRP:HE1 | 1:A:458:GLN:NE2 | 2.04 | 0.54 |
| 1:G:222:TRP:HE1 | 1:G:458:GLN:NE2 | 2.05 | 0.54 |
| 1:A:359:SER:OG | 1:A:361:GLU:HG2 | 2.07 | 0.54 |
| 1:C:91:ARG:NH1 | 1:C:207:ASN:HB2 | 2.21 | 0.54 |
| 1:D:162:TYR:HH | 1:D:317:TYR:HD1 | 1.53 | 0.54 |
| 1:A:425:GLU:OE2 | 1:A:425:GLU:N | 2.39 | 0.54 |
| 1:G:118:GLN:NE2 | 1:G:195:VAL:HG13 | 2.22 | 0.54 |
| 1:D:18:THR:OG1 | 1:D:461:SER:HB3 | 2.08 | 0.54 |
| 1:H:222:TRP:HE1 | 1:H:458:GLN:NE2 | 2.06 | 0.54 |
| 1:G:460:HIS:N | 5:G:729:HOH:O | 2.41 | 0.54 |
| 1:G:125:MSE:HG2 | 1:G:188:LEU:HD13 | 1.88 | 0.54 |
| 1:E:125:MSE:HG2 | 1:E:188:LEU:HD13 | 1.88 | 0.54 |
| 1:H:118:GLN:NE2 | 1:H:195:VAL:HG13 | 2.23 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:246:ASN:ND2 | 1:A:249:ASN:HD21 | 2.06 | 0.53 |
| 1:B:56:PHE:CE1 | 1:B:339:GLN:HB3 | 2.43 | 0.53 |
| 1:G:84:ASP:OD1 | 1:G:84:ASP:N | 2.40 | 0.53 |
| 1:F:118:GLN:NE2 | 1:F:195:VAL:HG13 | 2.23 | 0.53 |
| 1:C:248:ASN:ND2 | 5:C:528:HOH:O | 2.40 | 0.53 |
| 1:B:269:MSE:HE2 | 1:B:273:PHE:HB3 | 1.90 | 0.53 |
| 1:A:125:MSE:HG2 | 1:A:188:LEU:HD13 | 1.91 | 0.53 |
| 1:A:434:LEU:HB2 | 1:A:435:PRO:HD3 | 1.89 | 0.53 |
| 1:H:246:ASN:ND2 | 1:H:249:ASN:HD21 | 2.07 | 0.53 |
| 1:C:274:LEU:HD11 | 1:C:278:MSE:HE3 | 1.90 | 0.53 |
| 1:A:274:LEU:CD1 | 1:A:278:MSE:HE3 | 2.37 | 0.53 |
| 1:D:383:ASN:OD1 | 1:D:385:GLU:HG2 | 2.07 | 0.53 |
| 1:D:434:LEU:HB2 | 1:D:435:PRO:HD3 | 1.90 | 0.53 |
| 1:C:502:GLN:O | 1:C:506:LYS:HE2 | 2.08 | 0.53 |
| 1:C:434:LEU:HB2 | 1:C:435:PRO:HD3 | 1.91 | 0.53 |
| 1:F:174:MSE:HB2 | 1:F:422:PRO:O | 2.09 | 0.53 |
| 1:C:383:ASN:OD1 | 1:C:385:GLU:HG2 | 2.09 | 0.52 |
| 1:H:434:LEU:HB2 | 1:H:435:PRO:HD3 | 1.92 | 0.52 |
| 1:D:455:VAL:HG21 | 1:D:480:THR:CG2 | 2.40 | 0.52 |
| 1:B:175:GLN:NE2 | 1:B:177:ALA:H | 2.07 | 0.52 |
| 1:A:207:ASN:ND2 | 5:A:559:HOH:O | 2.43 | 0.52 |
| 1:B:246:ASN:ND2 | 1:B:249:ASN:HD21 | 2.08 | 0.52 |
| 1:C:175:GLN:NE2 | 1:C:177:ALA:H | 2.06 | 0.52 |
| 1:G:162:TYR:HH | 1:G:317:TYR:HD1 | 1.57 | 0.52 |
| 1:G:175:GLN:NE2 | 1:G:177:ALA:H | 2.07 | 0.52 |
| 1:C:18:THR:OG1 | 1:C:461:SER:HB3 | 2.09 | 0.52 |
| 1:G:56:PHE:CE1 | 1:G:339:GLN:HB3 | 2.44 | 0.52 |
| 1:A:269:MSE:HE2 | 1:A:273:PHE:HB3 | 1.90 | 0.52 |
| 1:G:174:MSE:HB2 | 1:G:422:PRO:O | 2.10 | 0.52 |
| 1:H:84:ASP:OD1 | 1:H:84:ASP:N | 2.42 | 0.52 |
| 1:E:455:VAL:HG21 | 1:E:480:THR:CG2 | 2.40 | 0.52 |
| 1:F:303:ARG:NH1 | 5:F:531:HOH:O | 2.27 | 0.52 |
| 1:B:96:ARG:NH2 | 5:B:568:HOH:O | 2.22 | 0.52 |
| 1:H:64:VAL:HG13 | 1:H:210:PHE:CD1 | 2.45 | 0.52 |
| 1:F:56:PHE:CE1 | 1:F:339:GLN:HB3 | 2.45 | 0.52 |
| 1:D:368:TRP:CZ3 | 1:D:370:ILE:HD11 | 2.45 | 0.52 |
| 1:D:274:LEU:CD1 | 1:D:278:MSE:HE3 | 2.40 | 0.51 |
| 1:F:269:MSE:HE2 | 1:F:273:PHE:HB3 | 1.92 | 0.51 |
| 1:C:17:PRO:HD2 | 3:C:600:FDA:O5' | 2.10 | 0.51 |
| 1:A:175:GLN:HE21 | 1:A:177:ALA:H | 1.58 | 0.51 |
| 1:E:118:GLN:NE2 | 1:E:195:VAL:HG13 | 2.25 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:70:LYS:NZ | 5:E:561:HOH:O | 2.39 | 0.51 |
| 1:B:383:ASN:OD1 | 1:B:385:GLU:HG2 | 2.11 | 0.51 |
| 1:H:327:ARG:NH1 | 2:H:802:GDU:H5' | 2.25 | 0.51 |
| 1:H:356:ARG:HB3 | 1:H:357:PRO:HD2 | 1.92 | 0.51 |
| 1:H:368:TRP:CZ3 | 1:H:370:ILE:HD11 | 2.46 | 0.51 |
| 1:B:84:ASP:N | 1:B:84:ASP:OD1 | 2.42 | 0.51 |
| 3:B:600:FDA:H9 | 3:B:600:FDA:O2' | 2.11 | 0.51 |
| 1:F:434:LEU:HB2 | 1:F:435:PRO:HD3 | 1.91 | 0.51 |
| 1:G:360:THR:O | 1:G:360:THR:CG2 | 2.54 | 0.51 |
| 1:H:56:PHE:CE1 | 1:H:339:GLN:HB3 | 2.46 | 0.51 |
| 1:A:383:ASN:OD1 | 1:A:385:GLU:HG2 | 2.11 | 0.51 |
| 1:E:162:TYR:HH | 1:E:317:TYR:HD1 | 1.58 | 0.51 |
| 1:D:175:GLN:HE21 | 1:D:177:ALA:H | 1.58 | 0.51 |
| 1:F:175:GLN:NE2 | 1:F:177:ALA:H | 2.09 | 0.51 |
| 1:C:56:PHE:CE1 | 1:C:339:GLN:HB3 | 2.46 | 0.51 |
| 1:H:269:MSE:HE2 | 1:H:273:PHE:HB3 | 1.92 | 0.51 |
| 1:F:246:ASN:ND2 | 1:F:249:ASN:HD21 | 2.09 | 0.51 |
| 1:C:246:ASN:ND2 | 1:C:249:ASN:HD21 | 2.08 | 0.51 |
| 1:G:368:TRP:CZ3 | 1:G:370:ILE:HD11 | 2.46 | 0.51 |
| 1:D:269:MSE:HE2 | 1:D:273:PHE:HB3 | 1.92 | 0.51 |
| 1:D:112:MSE:HE3 | 1:D:200:THR:CG2 | 2.41 | 0.51 |
| 1:D:56:PHE:CE1 | 1:D:339:GLN:HB3 | 2.46 | 0.51 |
| 1:D:425:GLU:OE2 | 1:D:425:GLU:N | 2.44 | 0.51 |
| 1:A:455:VAL:HG21 | 1:A:480:THR:CG2 | 2.40 | 0.50 |
| 1:D:455:VAL:O | 1:D:455:VAL:HG13 | 2.11 | 0.50 |
| 1:E:64:VAL:HG13 | 1:E:210:PHE:CD1 | 2.45 | 0.50 |
| 1:C:455:VAL:HG21 | 1:C:480:THR:CG2 | 2.40 | 0.50 |
| 1:F:162:TYR:HH | 1:F:317:TYR:HD1 | 1.57 | 0.50 |
| 1:A:21:GLY:HA2 | 1:A:462:PHE:CE1 | 2.47 | 0.50 |
| 1:C:269:MSE:HE2 | 1:C:273:PHE:HB3 | 1.94 | 0.50 |
| 1:C:84:ASP:OD1 | 1:C:84:ASP:N | 2.40 | 0.50 |
| 1:A:64:VAL:HG13 | 1:A:210:PHE:CD1 | 2.47 | 0.50 |
| 1:H:382:VAL:HG22 | 5:H:557:HOH:O | 2.11 | 0.50 |
| 1:E:246:ASN:ND2 | 1:E:249:ASN:HD21 | 2.10 | 0.50 |
| 1:E:356:ARG:HB3 | 1:E:357:PRO:HD2 | 1.94 | 0.50 |
| 1:E:327:ARG:NH1 | 2:E:802:GDU:H5' | 2.27 | 0.50 |
| 1:D:159:MSE:HE1 | 2:D:802:GDU:O2 | 2.12 | 0.50 |
| 1:F:167:TRP:HB3 | 1:F:174:MSE:HE1 | 1.93 | 0.50 |
| 1:A:56:PHE:CE1 | 1:A:339:GLN:HB3 | 2.47 | 0.50 |
| 1:E:368:TRP:CZ3 | 1:E:370:ILE:HD11 | 2.46 | 0.50 |
| 1:B:118:GLN:NE2 | 1:B:195:VAL:HG13 | 2.27 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:303:ARG:NH1 | 5:B:549:HOH:O | 2.22 | 0.50 |
| 1:C:64:VAL:HG13 | 1:C:210:PHE:CD1 | 2.47 | 0.50 |
| 1:A:150:MSE:HG3 | 1:A:186:PRO:HG3 | 1.93 | 0.50 |
| 1:H:317:TYR:N | 5:H:524:HOH:O | 2.45 | 0.49 |
| 1:E:167:TRP:HB3 | 1:E:174:MSE:HE1 | 1.93 | 0.49 |
| 1:H:384:GLN:O | 1:H:387:ILE:HG22 | 2.12 | 0.49 |
| 1:B:368:TRP:CZ3 | 1:B:370:ILE:HD11 | 2.47 | 0.49 |
| 1:D:167:TRP:HB3 | 1:D:174:MSE:HE1 | 1.93 | 0.49 |
| 1:A:162:TYR:HH | 1:A:317:TYR:HD1 | 1.59 | 0.49 |
| 1:F:425:GLU:OE2 | 1:F:425:GLU:N | 2.44 | 0.49 |
| 1:A:155:ALA:HA | 1:A:159:MSE:HB2 | 1.94 | 0.49 |
| 1:C:495:ARG:HB2 | 5:F:544:HOH:O | 2.12 | 0.49 |
| 1:E:56:PHE:CE1 | 1:E:339:GLN:HB3 | 2.47 | 0.49 |
| 1:H:69:TYR:CG | 1:H:463:MSE:HG3 | 2.47 | 0.49 |
| 1:G:296:HIS:CE1 | 1:G:382:VAL:HG21 | 2.48 | 0.49 |
| 1:G:269:MSE:HE2 | 1:G:273:PHE:HB3 | 1.94 | 0.49 |
| 1:D:84:ASP:N | 1:D:84:ASP:OD1 | 2.41 | 0.49 |
| 1:B:359:SER:HB3 | 4:B:512:CL:CL | 2.50 | 0.49 |
| 1:B:296:HIS:CE1 | 1:B:382:VAL:HG21 | 2.48 | 0.49 |
| 1:G:246:ASN:ND2 | 1:G:249:ASN:HD21 | 2.11 | 0.49 |
| 1:A:303:ARG:NH2 | 5:A:567:HOH:O | 2.39 | 0.49 |
| 1:E:332:SER:HA | 1:E:339:GLN:HE21 | 1.78 | 0.49 |
| 1:F:64:VAL:HG13 | 1:F:210:PHE:CD1 | 2.48 | 0.49 |
| 1:E:84:ASP:N | 1:E:84:ASP:OD1 | 2.41 | 0.49 |
| 1:E:425:GLU:OE2 | 1:E:425:GLU:N | 2.46 | 0.49 |
| 1:G:112:MSE:HE3 | 1:G:200:THR:CG2 | 2.42 | 0.49 |
| 1:F:69:TYR:CG | 1:F:463:MSE:HG3 | 2.47 | 0.49 |
| 1:B:134:VAL:HG22 | 1:G:134:VAL:HG22 | 1.93 | 0.49 |
| 1:H:91:ARG:HD3 | 1:H:207:ASN:HB3 | 1.94 | 0.49 |
| 1:G:175:GLN:HE21 | 1:G:177:ALA:H | 1.61 | 0.49 |
| 1:F:383:ASN:OD1 | 1:F:385:GLU:HG2 | 2.13 | 0.49 |
| 1:A:142:PHE:HB2 | 1:A:174:MSE:HG3 | 1.95 | 0.49 |
| 1:C:167:TRP:HB3 | 1:C:174:MSE:HE1 | 1.94 | 0.49 |
| 1:C:160:ARG:N | 1:C:161:PRO:HD2 | 2.28 | 0.49 |
| 1:G:425:GLU:OE2 | 1:G:425:GLU:N | 2.45 | 0.49 |
| 1:C:232:GLU:CG | 1:H:232:GLU:CG | 2.90 | 0.48 |
| 1:E:160:ARG:N | 1:E:161:PRO:HD2 | 2.27 | 0.48 |
| 1:F:84:ASP:OD1 | 1:F:84:ASP:N | 2.40 | 0.48 |
| 1:A:91:ARG:HD3 | 1:A:207:ASN:HB3 | 1.95 | 0.48 |
| 1:C:118:GLN:NE2 | 1:C:195:VAL:HG13 | 2.28 | 0.48 |
| 1:H:495:ARG:HB2 | 5:H:533:HOH:O | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:175:GLN:NE2 | 1:E:177:ALA:H | 2.11 | 0.48 |
| 1:G:69:TYR:CG | 1:G:463:MSE:HG3 | 2.48 | 0.48 |
| 1:F:455:VAL:HG21 | 1:F:480:THR:CG2 | 2.43 | 0.48 |
| 1:G:274:LEU:CD1 | 1:G:278:MSE:HE3 | 2.43 | 0.48 |
| 1:G:284:VAL:HG12 | 1:G:288:LYS:HE2 | 1.95 | 0.48 |
| 1:H:455:VAL:HG21 | 1:H:480:THR:CG2 | 2.43 | 0.48 |
| 1:C:332:SER:HA | 1:C:339:GLN:HE21 | 1.79 | 0.48 |
| 1:D:118:GLN:NE2 | 1:D:195:VAL:HG13 | 2.28 | 0.48 |
| 1:A:118:GLN:NE2 | 1:A:195:VAL:HG13 | 2.29 | 0.48 |
| 1:E:112:MSE:HE3 | 1:E:200:THR:CG2 | 2.42 | 0.48 |
| 1:E:91:ARG:HD3 | 1:E:207:ASN:HB3 | 1.95 | 0.48 |
| 1:H:274:LEU:CG | 1:H:278:MSE:HE3 | 2.43 | 0.48 |
| 1:B:358:GLN:HE22 | 1:C:84:ASP:HA | 1.78 | 0.48 |
| 1:B:56:PHE:CD1 | 1:B:339:GLN:HB3 | 2.48 | 0.48 |
| 1:E:69:TYR:CG | 1:E:463:MSE:HG3 | 2.48 | 0.48 |
| 3:H:600:FDA:H9 | 3:H:600:FDA:H1'1 | 1.56 | 0.48 |
| 1:E:269:MSE:HE2 | 1:E:273:PHE:HB3 | 1.95 | 0.48 |
| 1:C:112:MSE:HE3 | 1:C:200:THR:CG2 | 2.42 | 0.48 |
| 1:F:274:LEU:CD1 | 1:F:278:MSE:HE3 | 2.44 | 0.48 |
| 1:C:425:GLU:N | 1:C:425:GLU:OE2 | 2.44 | 0.48 |
| 1:C:510:GLN:HE21 | 1:H:506:LYS:HB3 | 1.79 | 0.48 |
| 1:B:199:LYS:NZ | 5:B:750:HOH:O | 2.47 | 0.48 |
| 1:C:368:TRP:CZ3 | 1:C:370:ILE:HD11 | 2.49 | 0.48 |
| 1:D:64:VAL:HG13 | 1:D:210:PHE:CD1 | 2.47 | 0.48 |
| 1:H:160:ARG:N | 1:H:161:PRO:HD2 | 2.28 | 0.48 |
| 1:H:174:MSE:HB2 | 1:H:422:PRO:O | 2.14 | 0.48 |
| 1:G:150:MSE:HG3 | 1:G:186:PRO:HG3 | 1.96 | 0.48 |
| 1:D:91:ARG:HD3 | 1:D:207:ASN:HB3 | 1.96 | 0.48 |
| 1:C:175:GLN:HE21 | 1:C:177:ALA:H | 1.62 | 0.48 |
| 1:B:64:VAL:HG13 | 1:B:210:PHE:CD1 | 2.48 | 0.48 |
| 1:B:91:ARG:HD3 | 1:B:207:ASN:HB3 | 1.94 | 0.48 |
| 1:E:296:HIS:HE1 | 1:E:376:GLU:OE2 | 1.97 | 0.48 |
| 1:E:384:GLN:O | 1:E:387:ILE:HG22 | 2.12 | 0.48 |
| 1:A:447:ARG:O | 1:A:451:TRP:HA | 2.14 | 0.47 |
| 1:G:64:VAL:HG13 | 1:G:210:PHE:CD1 | 2.49 | 0.47 |
| 1:D:356:ARG:HB3 | 1:D:357:PRO:HD2 | 1.96 | 0.47 |
| 1:F:455:VAL:O | 1:F:455:VAL:HG13 | 2.13 | 0.47 |
| 1:F:332:SER:HA | 1:F:339:GLN:HE21 | 1.79 | 0.47 |
| 1:D:309:ARG:HB3 | 5:D:642:HOH:O | 2.13 | 0.47 |
| 1:D:272:ASP:N | 1:D:272:ASP:OD1 | 2.47 | 0.47 |
| 1:C:69:TYR:CG | 1:C:463:MSE:HG3 | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:455:VAL:HG21 | 1:B:480:THR:CG2 | 2.44 | 0.47 |
| 1:A:84:ASP:OD1 | 1:A:84:ASP:N | 2.42 | 0.47 |
| 1:H:70:LYS:NZ | 5:H:553:HOH:O | 2.47 | 0.47 |
| 1:E:274:LEU:CG | 1:E:278:MSE:HE3 | 2.45 | 0.47 |
| 1:G:167:TRP:HB3 | 1:G:174:MSE:HE1 | 1.96 | 0.47 |
| 1:F:91:ARG:HD3 | 1:F:207:ASN:HB3 | 1.96 | 0.47 |
| 1:D:246:ASN:ND2 | 1:D:249:ASN:HD21 | 2.11 | 0.47 |
| 1:D:160:ARG:N | 1:D:161:PRO:HD2 | 2.29 | 0.47 |
| 1:G:455:VAL:HG21 | 1:G:480:THR:CG2 | 2.44 | 0.47 |
| 1:D:69:TYR:CG | 1:D:463:MSE:HG3 | 2.49 | 0.47 |
| 1:A:69:TYR:CG | 1:A:463:MSE:HG3 | 2.49 | 0.47 |
| 1:A:384:GLN:O | 1:A:387:ILE:HG22 | 2.14 | 0.47 |
| 1:G:91:ARG:HD3 | 1:G:207:ASN:HB3 | 1.97 | 0.47 |
| 1:C:91:ARG:HD3 | 1:C:207:ASN:HB3 | 1.96 | 0.47 |
| 1:F:303:ARG:NH2 | 5:F:531:HOH:O | 2.44 | 0.47 |
| 1:H:167:TRP:HB3 | 1:H:174:MSE:HE1 | 1.97 | 0.47 |
| 1:B:162:TYR:HH | 1:B:317:TYR:HD1 | 1.61 | 0.47 |
| 1:C:303:ARG:NH1 | 5:C:524:HOH:O | 2.28 | 0.47 |
| 1:G:160:ARG:N | 1:G:161:PRO:HD2 | 2.30 | 0.47 |
| 1:F:447:ARG:O | 1:F:451:TRP:HA | 2.15 | 0.47 |
| 1:A:368:TRP:CZ3 | 1:A:370:ILE:HD11 | 2.50 | 0.47 |
| 1:B:69:TYR:CG | 1:B:463:MSE:HG3 | 2.50 | 0.47 |
| 1:H:425:GLU:OE2 | 1:H:425:GLU:N | 2.47 | 0.47 |
| 1:B:174:MSE:HB2 | 1:B:422:PRO:O | 2.14 | 0.47 |
| 1:B:384:GLN:O | 1:B:387:ILE:HG22 | 2.14 | 0.47 |
| 1:C:426:ARG:NH2 | 1:C:454:GLU:OE1 | 2.39 | 0.47 |
| 1:D:458:GLN:HG3 | 3:D:600:FDA:HN1 | 1.80 | 0.47 |
| 1:D:302:VAL:HG11 | 1:D:368:TRP:CE2 | 2.49 | 0.47 |
| 1:A:160:ARG:N | 1:A:161:PRO:HD2 | 2.30 | 0.47 |
| 1:F:150:MSE:HG3 | 1:F:186:PRO:HG3 | 1.97 | 0.47 |
| 1:D:384:GLN:O | 1:D:387:ILE:HG22 | 2.15 | 0.47 |
| 1:C:455:VAL:O | 1:C:455:VAL:HG13 | 2.15 | 0.47 |
| 1:B:160:ARG:N | 1:B:161:PRO:HD2 | 2.30 | 0.47 |
| 1:H:284:VAL:HG12 | 1:H:288:LYS:HE2 | 1.97 | 0.47 |
| 1:C:272:ASP:OD1 | 1:C:272:ASP:N | 2.48 | 0.47 |
| 1:F:175:GLN:HE21 | 1:F:177:ALA:H | 1.63 | 0.46 |
| 1:A:69:TYR:CD2 | 1:A:463:MSE:HG3 | 2.50 | 0.46 |
| 1:C:504:PHE:HE1 | 1:F:263:LYS:HD2 | 1.81 | 0.46 |
| 1:A:296:HIS:HE1 | 1:A:376:GLU:OE2 | 1.98 | 0.46 |
| 1:B:360:THR:HG21 | 5:C:519:HOH:O | 2.14 | 0.46 |
| 1:H:332:SER:HA | 1:H:339:GLN:HE21 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:384:GLN:O | 1:G:387:ILE:HG22 | 2.15 | 0.46 |
| 1:A:98:GLN:NE2 | 1:A:114:PRO:HG2 | 2.31 | 0.46 |
| 1:B:155:ALA:HA | 1:B:159:MSE:HB2 | 1.97 | 0.46 |
| 1:C:274:LEU:HG | 1:C:278:MSE:HE3 | 1.97 | 0.46 |
| 1:A:296:HIS:CE1 | 1:A:382:VAL:HG21 | 2.51 | 0.46 |
| 1:C:274:LEU:CD1 | 1:C:278:MSE:HE3 | 2.45 | 0.46 |
| 1:B:142:PHE:HB2 | 1:B:174:MSE:HG3 | 1.98 | 0.46 |
| 1:F:368:TRP:CZ3 | 1:F:370:ILE:HD11 | 2.51 | 0.46 |
| 1:E:14:GLY:O | 1:E:19:GLY:HA3 | 2.16 | 0.46 |
| 1:D:284:VAL:HG12 | 1:D:288:LYS:HE2 | 1.97 | 0.46 |
| 1:F:160:ARG:N | 1:F:161:PRO:HD2 | 2.30 | 0.46 |
| 1:A:274:LEU:CG | 1:A:278:MSE:HE3 | 2.46 | 0.46 |
| 1:F:284:VAL:HG12 | 1:F:288:LYS:HE2 | 1.97 | 0.46 |
| 1:E:130:LEU:HD23 | 1:G:130:LEU:HD23 | 1.97 | 0.46 |
| 1:B:455:VAL:HG13 | 1:B:455:VAL:O | 2.16 | 0.46 |
| 1:F:274:LEU:CG | 1:F:278:MSE:HE3 | 2.45 | 0.46 |
| 1:F:263:LYS:O | 1:F:264:LYS:HD3 | 2.16 | 0.46 |
| 1:C:284:VAL:HG12 | 1:C:288:LYS:HE2 | 1.98 | 0.46 |
| 1:B:21:GLY:HA2 | 1:B:462:PHE:CE1 | 2.50 | 0.46 |
| 1:G:383:ASN:OD1 | 1:G:385:GLU:HG2 | 2.15 | 0.46 |
| 1:F:112:MSE:HE3 | 1:F:200:THR:CG2 | 2.41 | 0.46 |
| 1:D:447:ARG:O | 1:D:451:TRP:HA | 2.15 | 0.46 |
| 1:A:272:ASP:OD1 | 1:A:272:ASP:N | 2.45 | 0.46 |
| 1:C:384:GLN:O | 1:C:387:ILE:HG22 | 2.16 | 0.46 |
| 1:C:296:HIS:CE1 | 1:C:382:VAL:HG21 | 2.51 | 0.46 |
| 1:H:272:ASP:N | 1:H:272:ASP:OD1 | 2.46 | 0.46 |
| 1:H:490:ARG:NH2 | 5:H:530:HOH:O | 2.47 | 0.46 |
| 1:H:296:HIS:HE1 | 1:H:376:GLU:OE2 | 1.99 | 0.46 |
| 1:B:274:LEU:CG | 1:B:278:MSE:HE3 | 2.46 | 0.46 |
| 1:G:274:LEU:HG | 1:G:278:MSE:HE3 | 1.98 | 0.46 |
| 1:G:142:PHE:HB2 | 1:G:174:MSE:HG3 | 1.98 | 0.46 |
| 1:D:303:ARG:NH1 | 5:D:539:HOH:O | 2.31 | 0.46 |
| 1:H:14:GLY:O | 1:H:19:GLY:HA3 | 2.16 | 0.46 |
| 1:G:274:LEU:CG | 1:G:278:MSE:HE3 | 2.46 | 0.45 |
| 1:C:175:GLN:HE22 | 1:C:177:ALA:HB3 | 1.81 | 0.45 |
| 1:G:332:SER:HA | 1:G:339:GLN:HE21 | 1.81 | 0.45 |
| 1:D:332:SER:HA | 1:D:339:GLN:HE21 | 1.80 | 0.45 |
| 1:F:384:GLN:O | 1:F:387:ILE:HG22 | 2.16 | 0.45 |
| 1:B:112:MSE:HE3 | 1:B:200:THR:CG2 | 2.44 | 0.45 |
| 1:F:296:HIS:CE1 | 1:F:382:VAL:HG21 | 2.50 | 0.45 |
| 1:H:142:PHE:HB2 | 1:H:174:MSE:HG3 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:244:LYS:HB3 | 1:E:253:THR:HB | 1.99 | 0.45 |
| 1:B:447:ARG:O | 1:B:451:TRP:HA | 2.15 | 0.45 |
| 1:E:383:ASN:HA | 5:E:552:HOH:O | 2.15 | 0.45 |
| 1:C:274:LEU:CG | 1:C:278:MSE:HE3 | 2.46 | 0.45 |
| 1:E:155:ALA:HA | 1:E:159:MSE:HB2 | 1.99 | 0.45 |
| 1:H:175:GLN:NE2 | 1:H:177:ALA:H | 2.13 | 0.45 |
| 1:G:455:VAL:HG13 | 1:G:455:VAL:O | 2.17 | 0.45 |
| 1:D:445:ARG:NE | 1:D:481:LEU:HD22 | 2.32 | 0.45 |
| 1:G:272:ASP:OD1 | 1:G:272:ASP:N | 2.45 | 0.45 |
| 1:D:274:LEU:CG | 1:D:278:MSE:HE3 | 2.46 | 0.45 |
| 1:C:155:ALA:HA | 1:C:159:MSE:HB2 | 1.97 | 0.45 |
| 1:C:150:MSE:SE | 1:C:159:MSE:HE3 | 2.66 | 0.45 |
| 1:F:142:PHE:HB2 | 1:F:174:MSE:HG3 | 1.97 | 0.45 |
| 2:D:802:GDU:O2B | 2:D:802:GDU:O2' | 2.29 | 0.45 |
| 1:E:212:PHE:CG | 1:E:213:PRO:HD2 | 2.51 | 0.45 |
| 1:G:115:LYS:HD2 | 5:G:558:HOH:O | 2.15 | 0.45 |
| 1:D:360:THR:O | 1:D:360:THR:HG22 | 2.16 | 0.45 |
| 1:G:38:ASP:OD1 | 3:G:600:FDA:O3B | 2.31 | 0.45 |
| 1:G:46:LEU:HB2 | 3:G:600:FDA:O4' | 2.16 | 0.45 |
| 1:G:56:PHE:CD1 | 1:G:339:GLN:HB3 | 2.52 | 0.45 |
| 1:C:281:GLN:HG2 | 5:C:552:HOH:O | 2.15 | 0.45 |
| 1:G:447:ARG:O | 1:G:451:TRP:HA | 2.17 | 0.45 |
| 1:H:455:VAL:O | 1:H:455:VAL:HG13 | 2.16 | 0.45 |
| 1:A:112:MSE:HE3 | 1:A:200:THR:CG2 | 2.45 | 0.45 |
| 1:C:244:LYS:HB3 | 1:C:253:THR:HB | 1.98 | 0.45 |
| 1:B:150:MSE:HG3 | 1:B:186:PRO:HG3 | 1.97 | 0.45 |
| 1:B:284:VAL:HG12 | 1:B:288:LYS:HE2 | 1.98 | 0.45 |
| 1:C:138:LYS:HG3 | 1:C:139:PRO:CD | 2.45 | 0.45 |
| 1:F:155:ALA:HA | 1:F:159:MSE:HB2 | 1.97 | 0.45 |
| 1:H:112:MSE:HE3 | 1:H:200:THR:CG2 | 2.43 | 0.45 |
| 1:F:138:LYS:HG3 | 1:F:139:PRO:CD | 2.46 | 0.45 |
| 1:A:175:GLN:HE22 | 1:A:177:ALA:HB3 | 1.82 | 0.45 |
| 1:E:310:ILE:HD13 | 1:E:368:TRP:CZ3 | 2.52 | 0.45 |
| 1:A:174:MSE:HB2 | 1:A:422:PRO:O | 2.17 | 0.45 |
| 1:C:447:ARG:O | 1:C:451:TRP:HA | 2.17 | 0.45 |
| 1:H:212:PHE:CG | 1:H:213:PRO:HD2 | 2.52 | 0.45 |
| 1:D:296:HIS:CE1 | 1:D:382:VAL:HG21 | 2.52 | 0.44 |
| 1:H:274:LEU:HG | 1:H:278:MSE:HE3 | 2.00 | 0.44 |
| 1:H:69:TYR:CD2 | 1:H:463:MSE:HG3 | 2.51 | 0.44 |
| 1:F:274:LEU:HG | 1:F:278:MSE:HE3 | 1.99 | 0.44 |
| 1:D:69:TYR:CD2 | 1:D:463:MSE:HG3 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:98:GLN:NE2 | 1:E:114:PRO:HG2 | 2.32 | 0.44 |
| 1:E:263:LYS:O | 1:E:264:LYS:HD3 | 2.18 | 0.44 |
| 1:E:138:LYS:HG3 | 1:E:139:PRO:CD | 2.46 | 0.44 |
| 1:D:175:GLN:HE22 | 1:D:177:ALA:HB3 | 1.81 | 0.44 |
| 1:C:500:GLY:HA2 | 1:C:503:VAL:HG13 | 1.99 | 0.44 |
| 1:C:142:PHE:HB2 | 1:C:174:MSE:HG3 | 1.98 | 0.44 |
| 1:C:302:VAL:HG11 | 1:C:368:TRP:CE2 | 2.50 | 0.44 |
| 1:E:284:VAL:HG12 | 1:E:288:LYS:HE2 | 1.99 | 0.44 |
| 1:A:302:VAL:HG11 | 1:A:368:TRP:CE2 | 2.52 | 0.44 |
| 1:G:263:LYS:O | 1:G:264:LYS:HD3 | 2.17 | 0.44 |
| 1:B:310:ILE:HD13 | 1:B:368:TRP:CZ3 | 2.52 | 0.44 |
| 1:C:21:GLY:HA2 | 1:C:462:PHE:CE1 | 2.52 | 0.44 |
| 1:C:150:MSE:HG3 | 1:C:186:PRO:HG3 | 1.99 | 0.44 |
| 1:B:332:SER:HA | 1:B:339:GLN:HE21 | 1.82 | 0.44 |
| 1:D:56:PHE:CD1 | 1:D:339:GLN:HB3 | 2.52 | 0.44 |
| 1:B:302:VAL:HG11 | 1:B:368:TRP:CE2 | 2.53 | 0.44 |
| 1:C:69:TYR:CD2 | 1:C:463:MSE:HG3 | 2.53 | 0.44 |
| 1:F:244:LYS:HB3 | 1:F:253:THR:HB | 1.99 | 0.44 |
| 1:G:155:ALA:HA | 1:G:159:MSE:HB2 | 1.99 | 0.44 |
| 1:D:421:THR:HA | 1:D:422:PRO:HD3 | 1.86 | 0.44 |
| 1:B:167:TRP:HB3 | 1:B:174:MSE:HE1 | 2.00 | 0.44 |
| 1:D:263:LYS:O | 1:D:264:LYS:HD3 | 2.17 | 0.44 |
| 1:C:296:HIS:HE1 | 1:C:376:GLU:OE2 | 2.01 | 0.44 |
| 1:D:142:PHE:HB2 | 1:D:174:MSE:HG3 | 1.99 | 0.44 |
| 1:G:244:LYS:HB3 | 1:G:253:THR:HB | 1.98 | 0.44 |
| 1:E:272:ASP:OD1 | 1:E:272:ASP:N | 2.46 | 0.44 |
| 1:E:207:ASN:O | 1:E:208:ALA:C | 2.57 | 0.44 |
| 1:E:174:MSE:HB2 | 1:E:422:PRO:O | 2.17 | 0.44 |
| 1:B:82:LYS:HB2 | 1:B:85:ASP:OD1 | 2.18 | 0.44 |
| 1:B:296:HIS:HE1 | 1:B:376:GLU:OE2 | 2.01 | 0.43 |
| 1:D:274:LEU:HG | 1:D:278:MSE:HE3 | 2.00 | 0.43 |
| 1:E:150:MSE:SE | 1:E:159:MSE:HE3 | 2.68 | 0.43 |
| 1:A:25:ARG:HD2 | 1:A:466:VAL:HG13 | 2.00 | 0.43 |
| 1:A:332:SER:HA | 1:A:339:GLN:HE21 | 1.82 | 0.43 |
| 1:E:69:TYR:CD2 | 1:E:463:MSE:HG3 | 2.53 | 0.43 |
| 1:A:310:ILE:HD13 | 1:A:368:TRP:CZ3 | 2.54 | 0.43 |
| 1:B:60:VAL:HG13 | 1:B:415:PHE:CE2 | 2.53 | 0.43 |
| 1:C:98:GLN:NE2 | 1:C:114:PRO:HG2 | 2.33 | 0.43 |
| 1:F:445:ARG:NE | 1:F:481:LEU:HD22 | 2.34 | 0.43 |
| 1:F:98:GLN:NE2 | 1:F:114:PRO:HG2 | 2.34 | 0.43 |
| 1:G:359:SER:OG | 1:G:361:GLU:HB3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:63:HIS:HB2 | 1:F:218:THR:HG21 | 2.00 | 0.43 |
| 1:B:207:ASN:O | 1:B:208:ALA:C | 2.57 | 0.43 |
| 1:F:207:ASN:O | 1:F:208:ALA:C | 2.57 | 0.43 |
| 1:G:167:TRP:O | 1:G:168:ALA:HB3 | 2.18 | 0.43 |
| 1:H:162:TYR:HH | 1:H:317:TYR:HD1 | 1.65 | 0.43 |
| 1:A:167:TRP:HB3 | 1:A:174:MSE:HE1 | 2.01 | 0.43 |
| 1:H:98:GLN:NE2 | 1:H:114:PRO:HG2 | 2.32 | 0.43 |
| 1:H:310:ILE:HD13 | 1:H:368:TRP:CZ3 | 2.54 | 0.43 |
| 1:A:244:LYS:HB3 | 1:A:253:THR:HB | 2.00 | 0.43 |
| 1:D:150:MSE:HG3 | 1:D:186:PRO:HG3 | 2.00 | 0.43 |
| 1:A:60:VAL:HG13 | 1:A:415:PHE:CE2 | 2.53 | 0.43 |
| 1:E:63:HIS:HB2 | 1:E:218:THR:HG21 | 2.00 | 0.43 |
| 1:G:63:HIS:HB2 | 1:G:218:THR:HG21 | 2.01 | 0.43 |
| 1:H:360:THR:O | 1:H:360:THR:HG22 | 2.19 | 0.43 |
| 1:F:296:HIS:HE1 | 1:F:376:GLU:OE2 | 2.01 | 0.43 |
| 1:B:175:GLN:HE21 | 1:B:177:ALA:H | 1.65 | 0.43 |
| 1:E:150:MSE:HG3 | 1:E:186:PRO:HG3 | 1.99 | 0.43 |
| 1:G:207:ASN:O | 1:G:208:ALA:C | 2.57 | 0.43 |
| 1:H:155:ALA:HA | 1:H:159:MSE:HB2 | 2.00 | 0.43 |
| 1:F:249:ASN:O | 1:F:251:THR:HG23 | 2.19 | 0.43 |
| 1:B:303:ARG:NH2 | 5:B:549:HOH:O | 2.45 | 0.43 |
| 1:A:284:VAL:HG12 | 1:A:288:LYS:HE2 | 1.99 | 0.43 |
| 1:E:60:VAL:HG13 | 1:E:415:PHE:CE2 | 2.53 | 0.43 |
| 1:A:207:ASN:O | 1:A:208:ALA:C | 2.57 | 0.43 |
| 1:C:56:PHE:CD1 | 1:C:339:GLN:HB3 | 2.53 | 0.43 |
| 1:B:196:ILE:HG21 | 1:D:118:GLN:HB3 | 2.00 | 0.43 |
| 1:H:60:VAL:HG13 | 1:H:415:PHE:CE2 | 2.54 | 0.43 |
| 3:A:600:FDA:O2' | 3:A:600:FDA:H9 | 2.19 | 0.43 |
| 1:C:207:ASN:O | 1:C:208:ALA:C | 2.57 | 0.42 |
| 1:H:56:PHE:CD1 | 1:H:339:GLN:HB3 | 2.54 | 0.42 |
| 1:E:21:GLY:HA2 | 1:E:462:PHE:CE1 | 2.54 | 0.42 |
| 1:G:421:THR:HA | 1:G:422:PRO:HD3 | 1.87 | 0.42 |
| 1:C:212:PHE:CG | 1:C:213:PRO:HD2 | 2.54 | 0.42 |
| 1:H:447:ARG:O | 1:H:451:TRP:HA | 2.19 | 0.42 |
| 1:B:272:ASP:OD1 | 1:B:272:ASP:N | 2.45 | 0.42 |
| 1:D:296:HIS:HE1 | 1:D:376:GLU:OE2 | 2.01 | 0.42 |
| 1:F:56:PHE:CD1 | 1:F:339:GLN:HB3 | 2.54 | 0.42 |
| 1:E:56:PHE:CD1 | 1:E:339:GLN:HB3 | 2.54 | 0.42 |
| 1:G:249:ASN:O | 1:G:251:THR:HG23 | 2.19 | 0.42 |
| 1:C:310:ILE:HD13 | 1:C:368:TRP:CZ3 | 2.53 | 0.42 |
| 1:D:98:GLN:NE2 | 1:D:114:PRO:HG2 | 2.34 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:66:PHE:CD2 | 1:H:66:PHE:N | 2.88 | 0.42 |
| 1:F:333:ASN:HA | 1:F:333:ASN:HD22 | 1.72 | 0.42 |
| 1:H:333:ASN:HD22 | 1:H:333:ASN:HA | 1.71 | 0.42 |
| 1:B:98:GLN:NE2 | 1:B:114:PRO:HG2 | 2.34 | 0.42 |
| 1:H:63:HIS:HB2 | 1:H:218:THR:HG21 | 2.01 | 0.42 |
| 1:H:207:ASN:O | 1:H:208:ALA:C | 2.57 | 0.42 |
| 2:C:802:GDU:O2' | 2:C:802:GDU:O2B | 2.29 | 0.42 |
| 1:D:244:LYS:HB3 | 1:D:253:THR:HB | 2.01 | 0.42 |
| 1:A:82:LYS:HB2 | 1:A:85:ASP:OD1 | 2.19 | 0.42 |
| 1:A:150:MSE:SE | 1:A:159:MSE:HE3 | 2.69 | 0.42 |
| 1:A:373:GLU:HB2 | 5:A:660:HOH:O | 2.19 | 0.42 |
| 1:G:303:ARG:NH1 | 5:G:519:HOH:O | 2.40 | 0.42 |
| 1:E:296:HIS:CE1 | 1:E:382:VAL:HG21 | 2.54 | 0.42 |
| 1:D:155:ALA:HA | 1:D:159:MSE:HB2 | 2.02 | 0.42 |
| 1:F:69:TYR:CD2 | 1:F:463:MSE:HG3 | 2.54 | 0.42 |
| 1:B:325:PHE:HA | 1:B:374:VAL:HG22 | 2.02 | 0.42 |
| 1:H:474:ASN:ND2 | 5:H:523:HOH:O | 2.52 | 0.42 |
| 1:E:358:GLN:H | 1:E:358:GLN:CD | 2.23 | 0.42 |
| 1:A:212:PHE:CG | 1:A:213:PRO:HD2 | 2.54 | 0.42 |
| 1:B:63:HIS:HB2 | 1:B:218:THR:HG21 | 2.01 | 0.42 |
| 1:D:138:LYS:HG3 | 1:D:139:PRO:CD | 2.45 | 0.42 |
| 1:H:150:MSE:SE | 1:H:159:MSE:HE3 | 2.70 | 0.42 |
| 1:A:421:THR:HA | 1:A:422:PRO:HD3 | 1.87 | 0.42 |
| 1:H:244:LYS:HB3 | 1:H:253:THR:HB | 2.02 | 0.42 |
| 1:A:360:THR:HG21 | 5:D:512:HOH:O | 2.19 | 0.42 |
| 1:D:232:GLU:H | 1:D:232:GLU:CD | 2.22 | 0.42 |
| 1:F:14:GLY:O | 1:F:19:GLY:HA3 | 2.20 | 0.42 |
| 1:G:296:HIS:HE1 | 1:G:376:GLU:OE2 | 2.02 | 0.42 |
| 1:H:296:HIS:CE1 | 1:H:382:VAL:HG21 | 2.55 | 0.42 |
| 1:B:138:LYS:HG3 | 1:B:139:PRO:CD | 2.48 | 0.42 |
| 1:E:302:VAL:HG11 | 1:E:368:TRP:CE2 | 2.55 | 0.42 |
| 1:A:455:VAL:HG13 | 1:A:455:VAL:O | 2.18 | 0.42 |
| 1:G:14:GLY:O | 1:G:19:GLY:HA3 | 2.20 | 0.42 |
| 1:B:244:LYS:HB3 | 1:B:253:THR:HB | 2.02 | 0.42 |
| 1:A:445:ARG:NE | 1:A:481:LEU:HD22 | 2.34 | 0.42 |
| 1:E:447:ARG:O | 1:E:451:TRP:HA | 2.19 | 0.42 |
| 1:G:60:VAL:HG13 | 1:G:415:PHE:CE2 | 2.54 | 0.41 |
| 1:E:360:THR:O | 1:E:360:THR:HG22 | 2.20 | 0.41 |
| 1:A:235:ARG:NH1 | 5:A:550:HOH:O | 2.52 | 0.41 |
| 1:D:382:VAL:HG22 | 5:D:658:HOH:O | 2.19 | 0.41 |
| 1:H:150:MSE:HG3 | 1:H:186:PRO:HG3 | 2.00 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:455:VAL:HG23 | 1:G:460:HIS:CD2 | 2.54 | 0.41 |
| 1:D:207:ASN:O | 1:D:208:ALA:C | 2.58 | 0.41 |
| 1:E:455:VAL:O | 1:E:455:VAL:HG13 | 2.20 | 0.41 |
| 1:C:14:GLY:O | 1:C:19:GLY:HA3 | 2.20 | 0.41 |
| 1:G:98:GLN:NE2 | 1:G:114:PRO:HG2 | 2.36 | 0.41 |
| 1:F:310:ILE:HD13 | 1:F:368:TRP:CZ3 | 2.55 | 0.41 |
| 1:H:21:GLY:HA2 | 1:H:462:PHE:CE1 | 2.55 | 0.41 |
| 1:C:162:TYR:HH | 1:C:317:TYR:HD1 | 1.66 | 0.41 |
| 1:C:263:LYS:O | 1:C:264:LYS:HD3 | 2.20 | 0.41 |
| 1:D:21:GLY:HA2 | 1:D:462:PHE:CE1 | 2.55 | 0.41 |
| 1:E:125:MSE:HE1 | 1:E:191:VAL:HG21 | 2.02 | 0.41 |
| 1:A:327:ARG:NH1 | 2:A:802:GDU:H5' | 2.36 | 0.41 |
| 1:B:175:GLN:HE22 | 1:B:177:ALA:HB3 | 1.85 | 0.41 |
| 1:A:360:THR:HG22 | 1:A:360:THR:O | 2.20 | 0.41 |
| 1:A:31:GLY:N | 5:A:513:HOH:O | 2.35 | 0.41 |
| 1:D:310:ILE:HD13 | 1:D:368:TRP:CZ3 | 2.55 | 0.41 |
| 1:C:174:MSE:HB2 | 1:C:422:PRO:O | 2.21 | 0.41 |
| 1:A:306:ARG:HH11 | 1:A:333:ASN:HD21 | 1.67 | 0.41 |
| 1:D:63:HIS:HB2 | 1:D:218:THR:HG21 | 2.01 | 0.41 |
| 1:B:130:LEU:HD23 | 1:D:130:LEU:HD23 | 2.03 | 0.41 |
| 3:E:600:FDA:H9 | 3:E:600:FDA:H1'1 | 1.72 | 0.41 |
| 1:A:274:LEU:HG | 1:A:278:MSE:HE3 | 2.02 | 0.41 |
| 3:G:600:FDA:O2' | 3:G:600:FDA:H9 | 2.21 | 0.41 |
| 1:F:332:SER:HA | 1:F:339:GLN:NE2 | 2.36 | 0.41 |
| 1:G:302:VAL:HG11 | 1:G:368:TRP:CE2 | 2.56 | 0.41 |
| 1:D:174:MSE:HB2 | 1:D:422:PRO:O | 2.20 | 0.41 |
| 1:C:421:THR:HA | 1:C:422:PRO:HD3 | 1.85 | 0.41 |
| 1:A:262:TYR:CE1 | 1:A:265:LEU:HB2 | 2.55 | 0.41 |
| 1:G:69:TYR:CD2 | 1:G:463:MSE:HG3 | 2.55 | 0.41 |
| 1:E:274:LEU:HG | 1:E:278:MSE:HE3 | 2.02 | 0.41 |
| 1:B:361:GLU:O | 5:B:536:HOH:O | 2.22 | 0.41 |
| 2:G:802:GDU:O2B | 2:G:802:GDU:O2' | 2.31 | 0.41 |
| 1:F:325:PHE:HA | 1:F:374:VAL:HG22 | 2.02 | 0.41 |
| 1:G:82:LYS:HB2 | 1:G:85:ASP:OD1 | 2.20 | 0.41 |
| 1:H:327:ARG:HH12 | 2:H:802:GDU:H5' | 1.84 | 0.41 |
| 1:G:431:THR:O | 1:G:435:PRO:HG2 | 2.21 | 0.41 |
| 1:H:59:ASP:HB3 | 1:H:60:VAL:H | 1.78 | 0.41 |
| 1:E:325:PHE:HA | 1:E:374:VAL:HG22 | 2.02 | 0.41 |
| 1:C:63:HIS:HB2 | 1:C:218:THR:HG21 | 2.03 | 0.41 |
| 1:G:138:LYS:HG3 | 1:G:139:PRO:CD | 2.47 | 0.41 |
| 1:G:46:LEU:HB2 | 3:G:600:FDA:HO4' | 1.86 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:302:VAL:HG11 | 1:H:368:TRP:CE2 | 2.55 | 0.41 |
| 1:G:310:ILE:HD13 | 1:G:368:TRP:CZ3 | 2.56 | 0.41 |
| 1:B:318:PHE:HA | 1:B:319:PRO:HD2 | 1.93 | 0.41 |
| 1:E:392:ILE:HA | 1:E:395:LEU:HD12 | 2.02 | 0.41 |
| 1:F:82:LYS:HB2 | 1:F:85:ASP:OD1 | 2.20 | 0.41 |
| 1:C:333:ASN:HA | 1:C:333:ASN:HD22 | 1.69 | 0.41 |
| 1:B:69:TYR:CD2 | 1:B:463:MSE:HG3 | 2.56 | 0.40 |
| 1:H:263:LYS:O | 1:H:264:LYS:HD3 | 2.21 | 0.40 |
| 1:G:325:PHE:HA | 1:G:374:VAL:HG22 | 2.03 | 0.40 |
| 1:E:232:GLU:H | 1:E:232:GLU:CD | 2.22 | 0.40 |
| 1:A:138:LYS:HG3 | 1:A:139:PRO:CD | 2.47 | 0.40 |
| 1:G:458:GLN:HG3 | 3:G:600:FDA:HN1 | 1.85 | 0.40 |
| 1:D:306:ARG:HH11 | 1:D:333:ASN:HD21 | 1.70 | 0.40 |
| 1:F:272:ASP:N | 1:F:272:ASP:OD1 | 2.44 | 0.40 |
| 1:C:510:GLN:NE2 | 1:H:506:LYS:HB3 | 2.36 | 0.40 |
| 1:A:14:GLY:O | 1:A:19:GLY:HA3 | 2.20 | 0.40 |
| 1:B:222:TRP:HE1 | 1:B:458:GLN:HE21 | 1.70 | 0.40 |
| 1:C:332:SER:HA | 1:C:339:GLN:NE2 | 2.36 | 0.40 |
| 1:A:56:PHE:CD1 | 1:A:339:GLN:HB3 | 2.55 | 0.40 |
| 1:E:142:PHE:HB2 | 1:E:174:MSE:HG3 | 2.04 | 0.40 |
| 1:E:332:SER:HA | 1:E:339:GLN:NE2 | 2.36 | 0.40 |
| 1:B:306:ARG:HH11 | 1:B:333:ASN:HD21 | 1.68 | 0.40 |
| 1:D:212:PHE:CG | 1:D:213:PRO:HD2 | 2.57 | 0.40 |
| 1:B:483:TYR:N | 1:B:484:PRO:HD3 | 2.37 | 0.40 |
| 1:H:102:VAL:HA | 1:H:103:PRO:HD3 | 1.95 | 0.40 |
| 1:G:296:HIS:HD2 | 1:G:412:HIS:CE1 | 2.32 | 0.40 |
| 1:C:232:GLU:CD | 1:C:232:GLU:H | 2.23 | 0.40 |
| 3:F:600:FDA:H1'1 | 3:F:600:FDA:H9 | 1.78 | 0.40 |
| 1:H:64:VAL:HG13 | 1:H:210:PHE:CG | 2.57 | 0.40 |
| 1:H:95:VAL:HA | 5:H:524:HOH:O | 2.21 | 0.40 |
| 1:H:421:THR:HA | 1:H:422:PRO:HD3 | 1.88 | 0.40 |
| 1:E:254:LEU:HD12 | 1:E:258:THR:HB | 2.02 | 0.40 |
| 1:G:445:ARG:NE | 1:G:481:LEU:HD22 | 2.37 | 0.40 |
| 1:D:14:GLY:O | 1:D:19:GLY:HA3 | 2.22 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 507/509 (100%) | 488 (96%) | 17 (3%) | 2 (0%) | 39 | 61 |
| 1 | B | 507/509 (100%) | 489 (96%) | 16 (3%) | 2 (0%) | 39 | 61 |
| 1 | C | 507/509 (100%) | 486 (96%) | 19 (4%) | 2 (0%) | 39 | 61 |
| 1 | D | 507/509 (100%) | 489 (96%) | 16 (3%) | 2 (0%) | 39 | 61 |
| 1 | E | 507/509 (100%) | 487 (96%) | 18 (4%) | 2 (0%) | 39 | 61 |
| 1 | F | 507/509 (100%) | 488 (96%) | 16 (3%) | 3 (1%) | 30 | 50 |
| 1 | G | 507/509 (100%) | 483 (95%) | 22 (4%) | 2 (0%) | 39 | 61 |
| 1 | H | 507/509 (100%) | 486 (96%) | 19 (4%) | 2 (0%) | 39 | 61 |
| All | All | 4056/4072 (100%) | 3896 (96%) | 143 (4%) | 17 (0%) | 39 | 61 |

All (17) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 59 | ASP |
| 1 | A | 59 | ASP |
| 1 | B | 59 | ASP |
| 1 | C | 59 | ASP |
| 1 | D | 59 | ASP |
| 1 | E | 59 | ASP |
| 1 | G | 59 | ASP |
| 1 | H | 59 | ASP |
| 1 | F | 364 | GLU |
| 1 | E | 62 | GLY |
| 1 | H | 62 | GLY |
| 1 | B | 62 | GLY |
| 1 | C | 62 | GLY |
| 1 | D | 62 | GLY |
| 1 | F | 62 | GLY |
| 1 | A | 62 | GLY |
| 1 | G | 62 | GLY |

### 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 | 431/417 (103%) | 417 (97%) | 14 (3%) | 46 | 74 |
| 1 | B | 431/417 (103%) | 417 (97%) | 14 (3%) | 46 | 74 |
| 1 | C | 431/417 (103%) | 414 (96%) | 17 (4%) | 39 | 66 |
| 1 | D | 431/417 (103%) | 417 (97%) | 14 (3%) | 46 | 74 |
| 1 | E | 431/417 (103%) | 417 (97%) | 14 (3%) | 46 | 74 |
| 1 | F | 431/417 (103%) | 415 (96%) | 16 (4%) | 41 | 68 |
| 1 | G | 431/417 (103%) | 416 (96%) | 15 (4%) | 43 | 70 |
| 1 | H | 431/417 (103%) | 417 (97%) | 14 (3%) | 46 | 74 |
| All | All | 3448/3336 (103%) | 3330 (97%) | 118 (3%) | 44 | 72 |

All (118) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 84 | ASP |
| 1 | A | 90 | GLN |
| 1 | A | 137 | THR |
| 1 | A | 148 | ARG |
| 1 | A | 150 | MSE |
| 1 | A | 175 | GLN |
| 1 | A | 206 | PRO |
| 1 | A | 209 | THR |
| 1 | A | 271 | VAL |
| 1 | A | 309 | ARG |
| 1 | A | 339 | GLN |
| 1 | A | 382 | VAL |
| 1 | A | 470 | ASP |
| 1 | A | 477 | VAL |
| 1 | B | 84 | ASP |
| 1 | B | 90 | GLN |
| 1 | B | 134 | VAL |
| 1 | B | 137 | THR |
| 1 | B | 148 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 150 | MSE |
| 1 | B | 175 | GLN |
| 1 | B | 206 | PRO |
| 1 | B | 209 | THR |
| 1 | B | 271 | VAL |
| 1 | B | 309 | ARG |
| 1 | B | 339 | GLN |
| 1 | B | 470 | ASP |
| 1 | B | 477 | VAL |
| 1 | C | 25 | ARG |
| 1 | C | 84 | ASP |
| 1 | C | 90 | GLN |
| 1 | C | 148 | ARG |
| 1 | C | 150 | MSE |
| 1 | C | 175 | GLN |
| 1 | C | 209 | THR |
| 1 | C | 271 | VAL |
| 1 | C | 309 | ARG |
| 1 | C | 339 | GLN |
| 1 | C | 358 | GLN |
| 1 | C | 382 | VAL |
| 1 | C | 470 | ASP |
| 1 | C | 477 | VAL |
| 1 | C | 503 | VAL |
| 1 | C | 506 | LYS |
| 1 | C | 508 | LYS |
| 1 | D | 25 | ARG |
| 1 | D | 84 | ASP |
| 1 | D | 90 | GLN |
| 1 | D | 148 | ARG |
| 1 | D | 150 | MSE |
| 1 | D | 175 | GLN |
| 1 | D | 209 | THR |
| 1 | D | 271 | VAL |
| 1 | D | 309 | ARG |
| 1 | D | 339 | GLN |
| 1 | D | 382 | VAL |
| 1 | D | 470 | ASP |
| 1 | D | 477 | VAL |
| 1 | D | 506 | LYS |
| 1 | E | 25 | ARG |
| 1 | E | 84 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 90 | GLN |
| 1 | E | 148 | ARG |
| 1 | E | 150 | MSE |
| 1 | E | 175 | GLN |
| 1 | E | 209 | THR |
| 1 | E | 271 | VAL |
| 1 | E | 309 | ARG |
| 1 | E | 339 | GLN |
| 1 | E | 358 | GLN |
| 1 | E | 382 | VAL |
| 1 | E | 470 | ASP |
| 1 | E | 477 | VAL |
| 1 | F | 25 | ARG |
| 1 | F | 84 | ASP |
| 1 | F | 90 | GLN |
| 1 | F | 134 | VAL |
| 1 | F | 137 | THR |
| 1 | F | 148 | ARG |
| 1 | F | 150 | MSE |
| 1 | F | 175 | GLN |
| 1 | F | 209 | THR |
| 1 | F | 215 | ARG |
| 1 | F | 271 | VAL |
| 1 | F | 309 | ARG |
| 1 | F | 339 | GLN |
| 1 | F | 382 | VAL |
| 1 | F | 470 | ASP |
| 1 | F | 477 | VAL |
| 1 | G | 25 | ARG |
| 1 | G | 84 | ASP |
| 1 | G | 90 | GLN |
| 1 | G | 134 | VAL |
| 1 | G | 137 | THR |
| 1 | G | 148 | ARG |
| 1 | G | 150 | MSE |
| 1 | G | 175 | GLN |
| 1 | G | 209 | THR |
| 1 | G | 215 | ARG |
| 1 | G | 271 | VAL |
| 1 | G | 309 | ARG |
| 1 | G | 339 | GLN |
| 1 | G | 470 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 477 | VAL |
| 1 | H | 84 | ASP |
| 1 | H | 90 | GLN |
| 1 | H | 137 | THR |
| 1 | H | 148 | ARG |
| 1 | H | 150 | MSE |
| 1 | H | 175 | GLN |
| 1 | H | 209 | THR |
| 1 | H | 271 | VAL |
| 1 | H | 309 | ARG |
| 1 | H | 339 | GLN |
| 1 | H | 358 | GLN |
| 1 | H | 382 | VAL |
| 1 | H | 470 | ASP |
| 1 | H | 477 | VAL |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 28 | GLN |
| 1 | A | 98 | GLN |
| 1 | A | 175 | GLN |
| 1 | A | 248 | ASN |
| 1 | A | 249 | ASN |
| 1 | A | 255 | GLN |
| 1 | A | 296 | HIS |
| 1 | A | 333 | ASN |
| 1 | A | 339 | GLN |
| 1 | A | 397 | ASN |
| 1 | A | 412 | HIS |
| 1 | A | 417 | HIS |
| 1 | A | 458 | GLN |
| 1 | A | 474 | ASN |
| 1 | B | 28 | GLN |
| 1 | B | 98 | GLN |
| 1 | B | 175 | GLN |
| 1 | B | 248 | ASN |
| 1 | B | 249 | ASN |
| 1 | B | 255 | GLN |
| 1 | B | 296 | HIS |
| 1 | B | 333 | ASN |
| 1 | B | 339 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 358 | GLN |
| 1 | B | 397 | ASN |
| 1 | B | 417 | HIS |
| 1 | B | 458 | GLN |
| 1 | B | 474 | ASN |
| 1 | C | 28 | GLN |
| 1 | C | 90 | GLN |
| 1 | C | 98 | GLN |
| 1 | C | 175 | GLN |
| 1 | C | 248 | ASN |
| 1 | C | 249 | ASN |
| 1 | C | 255 | GLN |
| 1 | C | 296 | HIS |
| 1 | C | 333 | ASN |
| 1 | C | 339 | GLN |
| 1 | C | 397 | ASN |
| 1 | C | 412 | HIS |
| 1 | C | 417 | HIS |
| 1 | C | 458 | GLN |
| 1 | C | 474 | ASN |
| 1 | C | 510 | GLN |
| 1 | D | 28 | GLN |
| 1 | D | 90 | GLN |
| 1 | D | 98 | GLN |
| 1 | D | 175 | GLN |
| 1 | D | 248 | ASN |
| 1 | D | 249 | ASN |
| 1 | D | 255 | GLN |
| 1 | D | 296 | HIS |
| 1 | D | 333 | ASN |
| 1 | D | 339 | GLN |
| 1 | D | 397 | ASN |
| 1 | D | 412 | HIS |
| 1 | D | 417 | HIS |
| 1 | D | 458 | GLN |
| 1 | D | 474 | ASN |
| 1 | E | 28 | GLN |
| 1 | E | 98 | GLN |
| 1 | E | 175 | GLN |
| 1 | E | 248 | ASN |
| 1 | E | 249 | ASN |
| 1 | E | 255 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 296 | HIS |
| 1 | E | 333 | ASN |
| 1 | E | 339 | GLN |
| 1 | E | 397 | ASN |
| 1 | E | 417 | HIS |
| 1 | E | 458 | GLN |
| 1 | E | 474 | ASN |
| 1 | F | 28 | GLN |
| 1 | F | 98 | GLN |
| 1 | F | 175 | GLN |
| 1 | F | 248 | ASN |
| 1 | F | 249 | ASN |
| 1 | F | 296 | HIS |
| 1 | F | 333 | ASN |
| 1 | F | 339 | GLN |
| 1 | F | 397 | ASN |
| 1 | F | 417 | HIS |
| 1 | F | 458 | GLN |
| 1 | F | 474 | ASN |
| 1 | G | 28 | GLN |
| 1 | G | 98 | GLN |
| 1 | G | 175 | GLN |
| 1 | G | 248 | ASN |
| 1 | G | 249 | ASN |
| 1 | G | 296 | HIS |
| 1 | G | 333 | ASN |
| 1 | G | 339 | GLN |
| 1 | G | 397 | ASN |
| 1 | G | 417 | HIS |
| 1 | G | 458 | GLN |
| 1 | G | 474 | ASN |
| 1 | H | 28 | GLN |
| 1 | H | 98 | GLN |
| 1 | H | 175 | GLN |
| 1 | H | 248 | ASN |
| 1 | H | 249 | ASN |
| 1 | H | 255 | GLN |
| 1 | H | 296 | HIS |
| 1 | H | 333 | ASN |
| 1 | H | 339 | GLN |
| 1 | H | 397 | ASN |
| 1 | H | 417 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 458 | GLN |
| 1 | H | 474 | ASN |

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | FDA | A | 600 | - | 48,58,58 | 2.28 | 14 (29%) | 54,89,89 | 2.21 | 14 (25%) |
| 2 | GDU | A | 802 | - | 29,38,38 | 1.72 | 8 (27%) | 43,58,58 | 1.76 | 7 (16%) |
| 3 | FDA | B | 600 | - | 48,58,58 | 2.27 | 14 (29%) | 54,89,89 | 2.21 | 16 (29%) |
| 2 | GDU | B | 802 | - | 29,38,38 | 1.73 | 8 (27%) | 43,58,58 | 1.77 | 7 (16%) |
| 3 | FDA | C | 600 | - | 48,58,58 | 2.27 | 14 (29%) | 54,89,89 | 2.19 | 14 (25%) |
| 2 | GDU | C | 802 | - | 29,38,38 | 1.77 | 8 (27%) | 43,58,58 | 1.78 | 8 (18%) |
| 3 | FDA | D | 600 | - | 48,58,58 | 2.29 | 13 (27%) | 54,89,89 | 2.21 | 15 (27%) |
| 2 | GDU | D | 802 | - | 29,38,38 | 1.76 | 8 (27%) | 43,58,58 | 1.78 | 8 (18%) |
| 3 | FDA | E | 600 | - | 48,58,58 | 2.23 | 13 (27%) | 54,89,89 | 2.15 | 15 (27%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 2 | GDU | E | 802 | - | 29,38,38 | 1.74 | 8 (27%) | 43,58,58 | 1.81 | 6 (13%) |
| 3 | FDA | F | 600 | - | 48,58,58 | 2.30 | 13 (27%) | 54,89,89 | 2.22 | 13 (24%) |
| 2 | GDU | F | 802 | - | 29,38,38 | 1.73 | 8 (27%) | 43,58,58 | 1.81 | 8 (18%) |
| 3 | FDA | G | 600 | - | 48,58,58 | 2.31 | 14 (29%) | 54,89,89 | 2.22 | 13 (24%) |
| 2 | GDU | G | 802 | - | 29,38,38 | 1.75 | 8 (27%) | 43,58,58 | 1.74 | 8 (18%) |
| 3 | FDA | H | 600 | - | 48,58,58 | 2.24 | 13 (27%) | 54,89,89 | 2.13 | 16 (29%) |
| 2 | GDU | H | 802 | - | 29,38,38 | 1.74 | 8 (27%) | 43,58,58 | 1.83 | 7 (16%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | FDA | A | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | A | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | B | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | B | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | C | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | C | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | D | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | D | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | E | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | E | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | F | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | F | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | G | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | G | 802 | - | - | 0/19/59/59 | 0/3/3/3 |
| 3 | FDA | H | 600 | - | - | 0/30/50/50 | 0/6/6/6 |
| 2 | GDU | H | 802 | - | - | 0/19/59/59 | 0/3/3/3 |

All (172) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | G | 600 | FDA | C1'-N10 | -8.24 | 1.39 | 1.48 |
| 3 | D | 600 | FDA | C1'-N10 | -8.04 | 1.39 | 1.48 |
| 3 | F | 600 | FDA | C1'-N10 | -8.01 | 1.40 | 1.48 |
| 3 | C | 600 | FDA | C1'-N10 | -7.89 | 1.40 | 1.48 |
| 3 | B | 600 | FDA | C1'-N10 | -7.83 | 1.40 | 1.48 |
| 3 | A | 600 | FDA | C1'-N10 | -7.78 | 1.40 | 1.48 |
| 3 | E | 600 | FDA | C1'-N10 | -7.63 | 1.40 | 1.48 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | H | 600 | FDA | C1'-N10 | -7.61 | 1.40 | 1.48 |
| 3 | A | 600 | FDA | C2B-C3B | -5.48 | 1.38 | 1.53 |
| 3 | G | 600 | FDA | C2B-C3B | -5.45 | 1.38 | 1.53 |
| 3 | F | 600 | FDA | C2B-C3B | -5.40 | 1.38 | 1.53 |
| 3 | C | 600 | FDA | C2B-C3B | -5.39 | 1.38 | 1.53 |
| 3 | B | 600 | FDA | C2B-C3B | -5.38 | 1.38 | 1.53 |
| 3 | H | 600 | FDA | C2B-C3B | -5.28 | 1.39 | 1.53 |
| 3 | E | 600 | FDA | C2B-C3B | -5.27 | 1.39 | 1.53 |
| 3 | D | 600 | FDA | C2B-C3B | -5.25 | 1.39 | 1.53 |
| 3 | A | 600 | FDA | C9A-C5X | -3.90 | 1.34 | 1.42 |
| 3 | C | 600 | FDA | C9A-C5X | -3.89 | 1.34 | 1.42 |
| 3 | B | 600 | FDA | C9A-C5X | -3.87 | 1.34 | 1.42 |
| 3 | H | 600 | FDA | C9A-C5X | -3.86 | 1.34 | 1.42 |
| 3 | F | 600 | FDA | C9A-C5X | -3.86 | 1.34 | 1.42 |
| 3 | D | 600 | FDA | C9A-C5X | -3.81 | 1.34 | 1.42 |
| 3 | G | 600 | FDA | C9A-C5X | -3.81 | 1.34 | 1.42 |
| 3 | E | 600 | FDA | C9A-C5X | -3.79 | 1.35 | 1.42 |
| 2 | G | 802 | GDU | PB-O3B | -3.69 | 1.50 | 1.60 |
| 2 | F | 802 | GDU | PB-O3B | -3.68 | 1.50 | 1.60 |
| 2 | A | 802 | GDU | PB-O3B | -3.64 | 1.50 | 1.60 |
| 2 | H | 802 | GDU | PB-O3B | -3.64 | 1.50 | 1.60 |
| 2 | B | 802 | GDU | PB-O3B | -3.62 | 1.50 | 1.60 |
| 2 | D | 802 | GDU | PB-O3B | -3.60 | 1.50 | 1.60 |
| 2 | C | 802 | GDU | PB-O3B | -3.57 | 1.50 | 1.60 |
| 2 | E | 802 | GDU | PB-O3B | -3.57 | 1.50 | 1.60 |
| 3 | F | 600 | FDA | O3'-C3' | -3.56 | 1.34 | 1.43 |
| 3 | D | 600 | FDA | O3'-C3' | -3.52 | 1.34 | 1.43 |
| 3 | H | 600 | FDA | O3'-C3' | -3.50 | 1.34 | 1.43 |
| 3 | E | 600 | FDA | O3'-C3' | -3.49 | 1.34 | 1.43 |
| 3 | C | 600 | FDA | O3'-C3' | -3.48 | 1.34 | 1.43 |
| 3 | G | 600 | FDA | O3'-C3' | -3.46 | 1.34 | 1.43 |
| 3 | B | 600 | FDA | O3'-C3' | -3.44 | 1.34 | 1.43 |
| 2 | E | 802 | GDU | C3D-C2D | -3.39 | 1.44 | 1.53 |
| 3 | A | 600 | FDA | O3'-C3' | -3.38 | 1.34 | 1.43 |
| 2 | D | 802 | GDU | C3D-C2D | -3.36 | 1.44 | 1.53 |
| 2 | B | 802 | GDU | C3D-C2D | -3.30 | 1.44 | 1.53 |
| 2 | H | 802 | GDU | C3D-C2D | -3.28 | 1.44 | 1.53 |
| 2 | C | 802 | GDU | C3D-C2D | -3.27 | 1.44 | 1.53 |
| 2 | G | 802 | GDU | C3D-C2D | -3.24 | 1.44 | 1.53 |
| 2 | F | 802 | GDU | C3D-C2D | -3.20 | 1.44 | 1.53 |
| 2 | A | 802 | GDU | C3D-C2D | -3.17 | 1.44 | 1.53 |
| 3 | F | 600 | FDA | C9A-N10 | -3.12 | 1.34 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 600 | FDA | C9A-N10 | -3.09 | 1.34 | 1.38 |
| 3 | B | 600 | FDA | C9A-N10 | -3.09 | 1.34 | 1.38 |
| 3 | D | 600 | FDA | C9A-N10 | -3.05 | 1.34 | 1.38 |
| 3 | G | 600 | FDA | C9A-N10 | -3.04 | 1.34 | 1.38 |
| 3 | F | 600 | FDA | C4'-C3' | -3.04 | 1.47 | 1.53 |
| 3 | C | 600 | FDA | C9A-N10 | -2.99 | 1.34 | 1.38 |
| 2 | G | 802 | GDU | C4'-C3' | -2.98 | 1.44 | 1.52 |
| 2 | A | 802 | GDU | C4'-C3' | -2.97 | 1.44 | 1.52 |
| 2 | H | 802 | GDU | C4'-C3' | -2.97 | 1.44 | 1.52 |
| 2 | C | 802 | GDU | C4'-C3' | -2.97 | 1.44 | 1.52 |
| 3 | H | 600 | FDA | C9A-N10 | -2.97 | 1.34 | 1.38 |
| 2 | D | 802 | GDU | C4'-C3' | -2.97 | 1.44 | 1.52 |
| 2 | B | 802 | GDU | C4'-C3' | -2.94 | 1.44 | 1.52 |
| 2 | E | 802 | GDU | C4'-C3' | -2.94 | 1.44 | 1.52 |
| 2 | F | 802 | GDU | C4'-C3' | -2.94 | 1.44 | 1.52 |
| 3 | G | 600 | FDA | C4'-C3' | -2.92 | 1.47 | 1.53 |
| 3 | E | 600 | FDA | C9A-N10 | -2.92 | 1.34 | 1.38 |
| 3 | B | 600 | FDA | C4'-C3' | -2.89 | 1.47 | 1.53 |
| 3 | A | 600 | FDA | C4'-C3' | -2.83 | 1.47 | 1.53 |
| 3 | E | 600 | FDA | C4'-C3' | -2.78 | 1.47 | 1.53 |
| 3 | C | 600 | FDA | C4'-C3' | -2.77 | 1.47 | 1.53 |
| 3 | H | 600 | FDA | C4'-C3' | -2.74 | 1.47 | 1.53 |
| 2 | C | 802 | GDU | O4D-C1D | -2.74 | 1.37 | 1.41 |
| 2 | C | 802 | GDU | C3D-C4D | -2.73 | 1.45 | 1.53 |
| 2 | G | 802 | GDU | C3D-C4D | -2.70 | 1.45 | 1.53 |
| 2 | D | 802 | GDU | C3D-C4D | -2.69 | 1.45 | 1.53 |
| 2 | B | 802 | GDU | C3D-C4D | -2.66 | 1.45 | 1.53 |
| 3 | D | 600 | FDA | C4'-C3' | -2.65 | 1.48 | 1.53 |
| 2 | A | 802 | GDU | C3D-C4D | -2.64 | 1.45 | 1.53 |
| 2 | E | 802 | GDU | C3D-C4D | -2.64 | 1.45 | 1.53 |
| 2 | F | 802 | GDU | C3D-C4D | -2.61 | 1.46 | 1.53 |
| 2 | D | 802 | GDU | O4D-C1D | -2.61 | 1.37 | 1.41 |
| 2 | H | 802 | GDU | C3D-C4D | -2.57 | 1.46 | 1.53 |
| 2 | F | 802 | GDU | O4D-C1D | -2.56 | 1.38 | 1.41 |
| 2 | G | 802 | GDU | O4D-C1D | -2.54 | 1.38 | 1.41 |
| 3 | G | 600 | FDA | C10-N10 | -2.53 | 1.36 | 1.39 |
| 2 | A | 802 | GDU | O4D-C1D | -2.47 | 1.38 | 1.41 |
| 3 | D | 600 | FDA | O4B-C1B | -2.42 | 1.38 | 1.41 |
| 3 | B | 600 | FDA | O4B-C1B | -2.42 | 1.38 | 1.41 |
| 2 | H | 802 | GDU | O4D-C1D | -2.41 | 1.38 | 1.41 |
| 3 | F | 600 | FDA | O4B-C1B | -2.41 | 1.38 | 1.41 |
| 2 | B | 802 | GDU | O4D-C1D | -2.40 | 1.38 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | E | 802 | GDU | O4D-C1D | -2.34 | 1.38 | 1.41 |
| 2 | C | 802 | GDU | C3'-C2' | -2.33 | 1.46 | 1.52 |
| 3 | G | 600 | FDA | O4B-C1B | -2.29 | 1.38 | 1.41 |
| 3 | A | 600 | FDA | O3B-C3B | -2.29 | 1.37 | 1.43 |
| 2 | D | 802 | GDU | C3'-C2' | -2.28 | 1.46 | 1.52 |
| 2 | A | 802 | GDU | C3'-C2' | -2.28 | 1.46 | 1.52 |
| 2 | E | 802 | GDU | C3'-C2' | -2.27 | 1.46 | 1.52 |
| 2 | B | 802 | GDU | C3'-C2' | -2.26 | 1.46 | 1.52 |
| 3 | D | 600 | FDA | C10-N10 | -2.26 | 1.36 | 1.39 |
| 2 | F | 802 | GDU | C3'-C2' | -2.25 | 1.46 | 1.52 |
| 2 | H | 802 | GDU | C3'-C2' | -2.24 | 1.46 | 1.52 |
| 2 | G | 802 | GDU | C3'-C2' | -2.23 | 1.46 | 1.52 |
| 3 | H | 600 | FDA | O4B-C1B | -2.22 | 1.38 | 1.41 |
| 3 | E | 600 | FDA | O4B-C1B | -2.22 | 1.38 | 1.41 |
| 3 | A | 600 | FDA | O4B-C1B | -2.18 | 1.38 | 1.41 |
| 3 | B | 600 | FDA | O3B-C3B | -2.16 | 1.37 | 1.43 |
| 3 | C | 600 | FDA | C10-N10 | -2.16 | 1.36 | 1.39 |
| 3 | A | 600 | FDA | C10-N10 | -2.14 | 1.36 | 1.39 |
| 3 | C | 600 | FDA | O4B-C1B | -2.09 | 1.38 | 1.41 |
| 3 | F | 600 | FDA | C10-N10 | -2.09 | 1.36 | 1.39 |
| 3 | E | 600 | FDA | O3B-C3B | -2.07 | 1.38 | 1.43 |
| 3 | H | 600 | FDA | O3B-C3B | -2.05 | 1.38 | 1.43 |
| 3 | B | 600 | FDA | C10-N10 | -2.02 | 1.36 | 1.39 |
| 3 | G | 600 | FDA | O3B-C3B | -2.02 | 1.38 | 1.43 |
| 3 | C | 600 | FDA | O3B-C3B | -2.01 | 1.38 | 1.43 |
| 2 | G | 802 | GDU | O5'-C5' | 2.01 | 1.49 | 1.44 |
| 3 | A | 600 | FDA | O4'-C4' | 2.01 | 1.47 | 1.43 |
| 2 | F | 802 | GDU | O5'-C5' | 2.05 | 1.49 | 1.44 |
| 2 | D | 802 | GDU | O5'-C5' | 2.12 | 1.49 | 1.44 |
| 2 | B | 802 | GDU | O5'-C5' | 2.12 | 1.49 | 1.44 |
| 3 | B | 600 | FDA | O4'-C4' | 2.14 | 1.48 | 1.43 |
| 2 | A | 802 | GDU | O5'-C5' | 2.15 | 1.49 | 1.44 |
| 2 | H | 802 | GDU | O5'-C5' | 2.16 | 1.49 | 1.44 |
| 2 | E | 802 | GDU | O5'-C5' | 2.20 | 1.49 | 1.44 |
| 2 | C | 802 | GDU | O5'-C5' | 2.20 | 1.49 | 1.44 |
| 3 | H | 600 | FDA | O4'-C4' | 2.23 | 1.48 | 1.43 |
| 3 | C | 600 | FDA | O4'-C4' | 2.28 | 1.48 | 1.43 |
| 3 | E | 600 | FDA | O4'-C4' | 2.29 | 1.48 | 1.43 |
| 3 | F | 600 | FDA | O4'-C4' | 2.31 | 1.48 | 1.43 |
| 3 | D | 600 | FDA | O4'-C4' | 2.35 | 1.48 | 1.43 |
| 3 | G | 600 | FDA | O4'-C4' | 2.38 | 1.48 | 1.43 |
| 3 | G | 600 | FDA | C4-C4X | 2.79 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | F | 600 | FDA | C4-C4X | 2.83 | 1.46 | 1.41 |
| 3 | H | 600 | FDA | C4-C4X | 2.86 | 1.47 | 1.41 |
| 3 | D | 600 | FDA | C4-C4X | 2.87 | 1.47 | 1.41 |
| 3 | B | 600 | FDA | C4-C4X | 2.88 | 1.47 | 1.41 |
| 3 | C | 600 | FDA | C4-C4X | 2.89 | 1.47 | 1.41 |
| 3 | E | 600 | FDA | C4-C4X | 2.92 | 1.47 | 1.41 |
| 3 | A | 600 | FDA | C4-C4X | 2.97 | 1.47 | 1.41 |
| 2 | A | 802 | GDU | O4-C4 | 3.60 | 1.33 | 1.24 |
| 2 | B | 802 | GDU | O4-C4 | 3.61 | 1.33 | 1.24 |
| 3 | G | 600 | FDA | C7M-C7 | 3.64 | 1.58 | 1.51 |
| 3 | D | 600 | FDA | C7M-C7 | 3.64 | 1.58 | 1.51 |
| 3 | H | 600 | FDA | C7M-C7 | 3.66 | 1.58 | 1.51 |
| 2 | G | 802 | GDU | O4-C4 | 3.66 | 1.33 | 1.24 |
| 3 | C | 600 | FDA | C7M-C7 | 3.68 | 1.58 | 1.51 |
| 3 | E | 600 | FDA | C7M-C7 | 3.68 | 1.58 | 1.51 |
| 2 | F | 802 | GDU | O4-C4 | 3.70 | 1.33 | 1.24 |
| 3 | B | 600 | FDA | C7M-C7 | 3.70 | 1.58 | 1.51 |
| 3 | F | 600 | FDA | C7M-C7 | 3.72 | 1.58 | 1.51 |
| 3 | A | 600 | FDA | C7M-C7 | 3.72 | 1.58 | 1.51 |
| 2 | D | 802 | GDU | O4-C4 | 3.73 | 1.33 | 1.24 |
| 3 | C | 600 | FDA | C4-N3 | 3.74 | 1.40 | 1.33 |
| 2 | E | 802 | GDU | O4-C4 | 3.74 | 1.33 | 1.24 |
| 2 | C | 802 | GDU | O4-C4 | 3.77 | 1.33 | 1.24 |
| 3 | B | 600 | FDA | C4-N3 | 3.78 | 1.40 | 1.33 |
| 3 | E | 600 | FDA | C4-N3 | 3.78 | 1.40 | 1.33 |
| 3 | H | 600 | FDA | C4-N3 | 3.79 | 1.40 | 1.33 |
| 3 | D | 600 | FDA | C4-N3 | 3.79 | 1.40 | 1.33 |
| 2 | H | 802 | GDU | O4-C4 | 3.81 | 1.33 | 1.24 |
| 3 | F | 600 | FDA | C4-N3 | 3.84 | 1.40 | 1.33 |
| 3 | G | 600 | FDA | C4-N3 | 3.86 | 1.40 | 1.33 |
| 3 | A | 600 | FDA | C4-N3 | 3.90 | 1.40 | 1.33 |
| 3 | B | 600 | FDA | C10-N1 | 4.76 | 1.43 | 1.35 |
| 3 | E | 600 | FDA | C10-N1 | 4.79 | 1.43 | 1.35 |
| 3 | G | 600 | FDA | C10-N1 | 4.85 | 1.43 | 1.35 |
| 3 | A | 600 | FDA | C10-N1 | 4.86 | 1.43 | 1.35 |
| 3 | H | 600 | FDA | C10-N1 | 4.91 | 1.43 | 1.35 |
| 3 | C | 600 | FDA | C10-N1 | 4.93 | 1.43 | 1.35 |
| 3 | D | 600 | FDA | C10-N1 | 4.96 | 1.43 | 1.35 |
| 3 | F | 600 | FDA | C10-N1 | 4.98 | 1.43 | 1.35 |

All (175) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | G | 600 | FDA | N3A-C2A-N1A | -9.04 | 121.97 | 128.89 |
| 3 | F | 600 | FDA | N3A-C2A-N1A | -8.95 | 122.04 | 128.89 |
| 3 | C | 600 | FDA | N3A-C2A-N1A | -8.83 | 122.14 | 128.89 |
| 3 | D | 600 | FDA | N3A-C2A-N1A | -8.77 | 122.18 | 128.89 |
| 3 | B | 600 | FDA | N3A-C2A-N1A | -8.72 | 122.22 | 128.89 |
| 3 | E | 600 | FDA | N3A-C2A-N1A | -8.66 | 122.26 | 128.89 |
| 3 | A | 600 | FDA | N3A-C2A-N1A | -8.64 | 122.28 | 128.89 |
| 3 | H | 600 | FDA | N3A-C2A-N1A | -8.44 | 122.43 | 128.89 |
| 3 | B | 600 | FDA | O5B-PA-O1A | -5.04 | 90.07 | 109.62 |
| 3 | A | 600 | FDA | O5B-PA-O1A | -4.87 | 90.70 | 109.62 |
| 3 | D | 600 | FDA | C4X-C10-N10 | -4.84 | 117.67 | 120.52 |
| 3 | D | 600 | FDA | O5B-PA-O1A | -4.79 | 91.01 | 109.62 |
| 3 | C | 600 | FDA | C4X-C10-N10 | -4.76 | 117.71 | 120.52 |
| 3 | G | 600 | FDA | O5B-PA-O1A | -4.76 | 91.16 | 109.62 |
| 3 | F | 600 | FDA | O5B-PA-O1A | -4.65 | 91.56 | 109.62 |
| 3 | C | 600 | FDA | O5B-PA-O1A | -4.60 | 91.75 | 109.62 |
| 3 | B | 600 | FDA | O5'-P-O1P | -4.55 | 91.94 | 109.62 |
| 3 | F | 600 | FDA | C4X-C10-N10 | -4.54 | 117.84 | 120.52 |
| 3 | H | 600 | FDA | O5B-PA-O1A | -4.46 | 92.29 | 109.62 |
| 3 | E | 600 | FDA | O5B-PA-O1A | -4.44 | 92.37 | 109.62 |
| 3 | A | 600 | FDA | O5'-P-O1P | -4.43 | 92.44 | 109.62 |
| 2 | H | 802 | GDU | PB-O3A-PA | -4.39 | 120.40 | 132.73 |
| 2 | E | 802 | GDU | PB-O3A-PA | -4.36 | 120.48 | 132.73 |
| 3 | G | 600 | FDA | C4X-C10-N10 | -4.25 | 118.02 | 120.52 |
| 2 | C | 802 | GDU | PB-O3A-PA | -4.24 | 120.83 | 132.73 |
| 2 | F | 802 | GDU | PB-O3A-PA | -4.22 | 120.89 | 132.73 |
| 3 | E | 600 | FDA | O5'-P-O1P | -3.91 | 94.46 | 109.62 |
| 3 | G | 600 | FDA | C4B-O4B-C1B | -3.85 | 105.49 | 109.72 |
| 3 | A | 600 | FDA | C4X-C10-N10 | -3.82 | 118.27 | 120.52 |
| 3 | H | 600 | FDA | O5'-P-O1P | -3.80 | 94.88 | 109.62 |
| 3 | H | 600 | FDA | C4X-C10-N10 | -3.79 | 118.29 | 120.52 |
| 2 | D | 802 | GDU | C4D-O4D-C1D | -3.77 | 105.58 | 109.72 |
| 3 | D | 600 | FDA | O5'-P-O1P | -3.74 | 95.09 | 109.62 |
| 3 | C | 600 | FDA | O5'-P-O1P | -3.74 | 95.10 | 109.62 |
| 2 | G | 802 | GDU | PB-O3A-PA | -3.74 | 122.23 | 132.73 |
| 3 | F | 600 | FDA | C4B-O4B-C1B | -3.73 | 105.61 | 109.72 |
| 3 | F | 600 | FDA | O5'-P-O1P | -3.70 | 95.24 | 109.62 |
| 2 | D | 802 | GDU | PB-O3A-PA | -3.66 | 122.45 | 132.73 |
| 3 | D | 600 | FDA | C4X-C4-N3 | -3.64 | 118.61 | 123.59 |
| 3 | G | 600 | FDA | O5'-P-O1P | -3.63 | 95.52 | 109.62 |
| 2 | B | 802 | GDU | C4D-O4D-C1D | -3.62 | 105.75 | 109.72 |
| 2 | A | 802 | GDU | PB-O3A-PA | -3.59 | 122.64 | 132.73 |
| 3 | B | 600 | FDA | C4B-O4B-C1B | -3.57 | 105.80 | 109.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 802 | GDU | C4D-O4D-C1D | -3.51 | 105.86 | 109.72 |
| 2 | B | 802 | GDU | PB-O3A-PA | -3.50 | 122.91 | 132.73 |
| 3 | B | 600 | FDA | C4X-C10-N10 | -3.48 | 118.47 | 120.52 |
| 3 | G | 600 | FDA | C4X-C4-N3 | -3.44 | 118.88 | 123.59 |
| 2 | A | 802 | GDU | C4D-O4D-C1D | -3.40 | 105.98 | 109.72 |
| 3 | C | 600 | FDA | C4X-C4-N3 | -3.31 | 119.07 | 123.59 |
| 2 | G | 802 | GDU | C4D-O4D-C1D | -3.30 | 106.09 | 109.72 |
| 3 | F | 600 | FDA | C4X-C4-N3 | -3.26 | 119.14 | 123.59 |
| 3 | H | 600 | FDA | C4X-C4-N3 | -3.21 | 119.20 | 123.59 |
| 3 | A | 600 | FDA | C4B-O4B-C1B | -3.18 | 106.22 | 109.72 |
| 3 | E | 600 | FDA | C4X-C4-N3 | -3.18 | 119.25 | 123.59 |
| 3 | E | 600 | FDA | C4X-C10-N10 | -3.14 | 118.67 | 120.52 |
| 2 | C | 802 | GDU | C4D-O4D-C1D | -3.12 | 106.29 | 109.72 |
| 3 | C | 600 | FDA | C4B-O4B-C1B | -3.11 | 106.31 | 109.72 |
| 3 | D | 600 | FDA | C4B-O4B-C1B | -3.10 | 106.31 | 109.72 |
| 3 | A | 600 | FDA | C4X-C4-N3 | -3.10 | 119.35 | 123.59 |
| 3 | B | 600 | FDA | C4X-C4-N3 | -3.04 | 119.43 | 123.59 |
| 3 | G | 600 | FDA | O2'-C2'-C1' | -2.97 | 102.64 | 109.94 |
| 3 | A | 600 | FDA | O2'-C2'-C1' | -2.89 | 102.84 | 109.94 |
| 3 | C | 600 | FDA | O2'-C2'-C1' | -2.87 | 102.89 | 109.94 |
| 3 | D | 600 | FDA | O2'-C2'-C1' | -2.80 | 103.08 | 109.94 |
| 3 | E | 600 | FDA | C4A-C5A-N7A | -2.79 | 106.91 | 109.48 |
| 3 | E | 600 | FDA | C4B-O4B-C1B | -2.74 | 106.71 | 109.72 |
| 2 | E | 802 | GDU | C4D-O4D-C1D | -2.73 | 106.72 | 109.72 |
| 2 | H | 802 | GDU | C4D-O4D-C1D | -2.68 | 106.77 | 109.72 |
| 3 | H | 600 | FDA | C4B-O4B-C1B | -2.60 | 106.86 | 109.72 |
| 3 | E | 600 | FDA | O2'-C2'-C1' | -2.59 | 103.57 | 109.94 |
| 3 | H | 600 | FDA | C4A-C5A-N7A | -2.58 | 107.10 | 109.48 |
| 3 | C | 600 | FDA | C4A-C5A-N7A | -2.48 | 107.20 | 109.48 |
| 3 | B | 600 | FDA | O2'-C2'-C1' | -2.47 | 103.88 | 109.94 |
| 3 | A | 600 | FDA | C4A-C5A-N7A | -2.45 | 107.22 | 109.48 |
| 3 | G | 600 | FDA | C4A-C5A-N7A | -2.36 | 107.31 | 109.48 |
| 3 | F | 600 | FDA | O2'-C2'-C1' | -2.35 | 104.16 | 109.94 |
| 3 | F | 600 | FDA | C4A-C5A-N7A | -2.25 | 107.41 | 109.48 |
| 3 | D | 600 | FDA | C4A-C5A-N7A | -2.23 | 107.42 | 109.48 |
| 3 | H | 600 | FDA | O2'-C2'-C1' | -2.22 | 104.49 | 109.94 |
| 3 | B | 600 | FDA | C4A-C5A-N7A | -2.15 | 107.50 | 109.48 |
| 3 | H | 600 | FDA | C1'-N10-C9A | -2.03 | 116.58 | 118.86 |
| 2 | C | 802 | GDU | O3A-PA-O5D | 2.01 | 108.26 | 102.94 |
| 3 | H | 600 | FDA | O2A-PA-O5B | 2.01 | 118.58 | 108.46 |
| 3 | D | 600 | FDA | O2P-P-O5' | 2.02 | 118.63 | 108.46 |
| 3 | B | 600 | FDA | O2A-PA-O5B | 2.02 | 118.65 | 108.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | E | 600 | FDA | C4X-N5-C5X | 2.05 | 119.12 | 116.76 |
| 3 | C | 600 | FDA | C1'-C2'-C3' | 2.05 | 115.68 | 109.82 |
| 2 | C | 802 | GDU | O6'-C6'-C5' | 2.05 | 118.12 | 111.33 |
| 2 | F | 802 | GDU | O3B-C1'-C2' | 2.06 | 112.23 | 108.39 |
| 3 | A | 600 | FDA | C4X-N5-C5X | 2.06 | 119.13 | 116.76 |
| 3 | E | 600 | FDA | C1'-C2'-C3' | 2.06 | 115.72 | 109.82 |
| 2 | D | 802 | GDU | O4D-C1D-N1 | 2.09 | 112.50 | 108.08 |
| 2 | F | 802 | GDU | O4D-C1D-N1 | 2.10 | 112.51 | 108.08 |
| 3 | B | 600 | FDA | C1'-C2'-C3' | 2.11 | 115.84 | 109.82 |
| 2 | C | 802 | GDU | O3B-C1'-C2' | 2.13 | 112.37 | 108.39 |
| 3 | B | 600 | FDA | C4X-N5-C5X | 2.15 | 119.23 | 116.76 |
| 3 | C | 600 | FDA | O5B-C5B-C4B | 2.18 | 117.15 | 109.12 |
| 3 | H | 600 | FDA | C4X-N5-C5X | 2.18 | 119.27 | 116.76 |
| 2 | H | 802 | GDU | O3A-PA-O5D | 2.19 | 108.75 | 102.94 |
| 3 | B | 600 | FDA | O5B-C5B-C4B | 2.19 | 117.21 | 109.12 |
| 2 | B | 802 | GDU | O4D-C1D-N1 | 2.21 | 112.75 | 108.08 |
| 2 | G | 802 | GDU | O3B-C1'-C2' | 2.22 | 112.54 | 108.39 |
| 2 | G | 802 | GDU | O4D-C1D-N1 | 2.23 | 112.79 | 108.08 |
| 3 | A | 600 | FDA | O5B-C5B-C4B | 2.27 | 117.49 | 109.12 |
| 2 | D | 802 | GDU | O3B-C1'-C2' | 2.27 | 112.63 | 108.39 |
| 2 | A | 802 | GDU | O4D-C1D-N1 | 2.28 | 112.90 | 108.08 |
| 3 | G | 600 | FDA | O5B-C5B-C4B | 2.29 | 117.56 | 109.12 |
| 3 | F | 600 | FDA | O5B-C5B-C4B | 2.33 | 117.72 | 109.12 |
| 2 | D | 802 | GDU | O5D-C5D-C4D | 2.36 | 117.81 | 109.12 |
| 2 | E | 802 | GDU | O4D-C1D-N1 | 2.38 | 113.11 | 108.08 |
| 3 | C | 600 | FDA | C5X-C9A-N10 | 2.42 | 119.45 | 117.62 |
| 2 | G | 802 | GDU | O5D-C5D-C4D | 2.47 | 118.22 | 109.12 |
| 3 | E | 600 | FDA | O2P-P-O3P | 2.48 | 116.36 | 105.09 |
| 2 | H | 802 | GDU | O4D-C1D-N1 | 2.49 | 113.33 | 108.08 |
| 3 | D | 600 | FDA | C4X-N5-C5X | 2.50 | 119.64 | 116.76 |
| 3 | D | 600 | FDA | O5B-C5B-C4B | 2.53 | 118.43 | 109.12 |
| 3 | A | 600 | FDA | O2P-P-O3P | 2.57 | 116.74 | 105.09 |
| 2 | B | 802 | GDU | O5D-C5D-C4D | 2.57 | 118.61 | 109.12 |
| 3 | G | 600 | FDA | C5X-C9A-N10 | 2.58 | 119.58 | 117.62 |
| 3 | H | 600 | FDA | O5B-C5B-C4B | 2.62 | 118.78 | 109.12 |
| 2 | A | 802 | GDU | O5D-C5D-C4D | 2.65 | 118.90 | 109.12 |
| 3 | E | 600 | FDA | O5B-C5B-C4B | 2.67 | 118.96 | 109.12 |
| 2 | F | 802 | GDU | O5D-C5D-C4D | 2.68 | 119.02 | 109.12 |
| 3 | H | 600 | FDA | O2P-P-O3P | 2.72 | 117.45 | 105.09 |
| 3 | G | 600 | FDA | O2P-P-O3P | 2.74 | 117.54 | 105.09 |
| 3 | B | 600 | FDA | O2P-P-O3P | 2.75 | 117.57 | 105.09 |
| 3 | F | 600 | FDA | O2P-P-O3P | 2.76 | 117.60 | 105.09 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | D | 600 | FDA | O2P-P-O3P | 2.79 | 117.76 | 105.09 |
| 3 | B | 600 | FDA | C5X-C9A-N10 | 2.80 | 119.75 | 117.62 |
| 3 | C | 600 | FDA | O2P-P-O3P | 2.82 | 117.86 | 105.09 |
| 3 | D | 600 | FDA | C5X-C9A-N10 | 2.82 | 119.76 | 117.62 |
| 3 | F | 600 | FDA | C5X-C9A-N10 | 2.84 | 119.78 | 117.62 |
| 3 | E | 600 | FDA | C5X-C9A-N10 | 2.99 | 119.89 | 117.62 |
| 3 | B | 600 | FDA | O2A-PA-O3P | 3.02 | 118.81 | 105.09 |
| 3 | F | 600 | FDA | O2A-PA-O3P | 3.06 | 118.98 | 105.09 |
| 3 | G | 600 | FDA | O2A-PA-O3P | 3.09 | 119.12 | 105.09 |
| 3 | E | 600 | FDA | O2A-PA-O3P | 3.10 | 119.17 | 105.09 |
| 3 | A | 600 | FDA | C5X-C9A-N10 | 3.10 | 119.98 | 117.62 |
| 3 | H | 600 | FDA | O2A-PA-O3P | 3.11 | 119.20 | 105.09 |
| 3 | H | 600 | FDA | C5X-C9A-N10 | 3.19 | 120.05 | 117.62 |
| 2 | G | 802 | GDU | O5'-C5'-C4' | 3.20 | 115.70 | 109.68 |
| 3 | C | 600 | FDA | O2A-PA-O3P | 3.23 | 119.74 | 105.09 |
| 3 | D | 600 | FDA | O2A-PA-O3P | 3.24 | 119.77 | 105.09 |
| 3 | A | 600 | FDA | O2A-PA-O3P | 3.26 | 119.87 | 105.09 |
| 2 | B | 802 | GDU | O5'-C5'-C4' | 3.37 | 116.01 | 109.68 |
| 2 | F | 802 | GDU | O5'-C5'-C4' | 3.48 | 116.21 | 109.68 |
| 2 | A | 802 | GDU | O5'-C5'-C4' | 3.48 | 116.22 | 109.68 |
| 2 | C | 802 | GDU | O5'-C5'-C4' | 3.53 | 116.31 | 109.68 |
| 2 | D | 802 | GDU | O5'-C5'-C4' | 3.69 | 116.61 | 109.68 |
| 2 | A | 802 | GDU | C3'-C4'-C5' | 3.72 | 116.68 | 110.20 |
| 2 | G | 802 | GDU | C3'-C4'-C5' | 3.74 | 116.71 | 110.20 |
| 2 | C | 802 | GDU | C3'-C4'-C5' | 3.83 | 116.88 | 110.20 |
| 2 | B | 802 | GDU | C3'-C4'-C5' | 3.84 | 116.89 | 110.20 |
| 2 | E | 802 | GDU | O5'-C5'-C4' | 3.84 | 116.89 | 109.68 |
| 2 | D | 802 | GDU | C3'-C4'-C5' | 3.86 | 116.93 | 110.20 |
| 2 | H | 802 | GDU | O5'-C5'-C4' | 3.95 | 117.09 | 109.68 |
| 2 | F | 802 | GDU | C3'-C4'-C5' | 4.00 | 117.17 | 110.20 |
| 2 | E | 802 | GDU | C3'-C4'-C5' | 4.07 | 117.28 | 110.20 |
| 3 | D | 600 | FDA | C4-N3-C2 | 4.11 | 118.80 | 115.25 |
| 2 | H | 802 | GDU | C3'-C4'-C5' | 4.20 | 117.51 | 110.20 |
| 3 | C | 600 | FDA | C4-N3-C2 | 4.70 | 119.31 | 115.25 |
| 3 | G | 600 | FDA | C4-N3-C2 | 4.98 | 119.55 | 115.25 |
| 3 | H | 600 | FDA | C4-N3-C2 | 5.00 | 119.57 | 115.25 |
| 3 | B | 600 | FDA | C4-N3-C2 | 5.02 | 119.59 | 115.25 |
| 3 | A | 600 | FDA | C4-N3-C2 | 5.11 | 119.66 | 115.25 |
| 3 | E | 600 | FDA | C4-N3-C2 | 5.18 | 119.72 | 115.25 |
| 3 | F | 600 | FDA | C4-N3-C2 | 5.22 | 119.76 | 115.25 |
| 2 | F | 802 | GDU | C4-N3-C2 | 5.53 | 119.62 | 114.14 |
| 2 | G | 802 | GDU | C4-N3-C2 | 5.55 | 119.64 | 114.14 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | D | 802 | GDU | C4-N3-C2 | 5.55 | 119.64 | 114.14 |
| 2 | E | 802 | GDU | C4-N3-C2 | 5.57 | 119.66 | 114.14 |
| 2 | C | 802 | GDU | C4-N3-C2 | 5.57 | 119.66 | 114.14 |
| 2 | B | 802 | GDU | C4-N3-C2 | 5.58 | 119.67 | 114.14 |
| 2 | H | 802 | GDU | C4-N3-C2 | 5.63 | 119.72 | 114.14 |
| 2 | A | 802 | GDU | C4-N3-C2 | 5.68 | 119.77 | 114.14 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 27 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 3 | A | 600 | FDA | 1 | 0 |
| 2 | A | 802 | GDU | 2 | 0 |
| 3 | B | 600 | FDA | 1 | 0 |
| 2 | B | 802 | GDU | 1 | 0 |
| 3 | C | 600 | FDA | 1 | 0 |
| 2 | C | 802 | GDU | 2 | 0 |
| 3 | D | 600 | FDA | 1 | 0 |
| 2 | D | 802 | GDU | 2 | 0 |
| 3 | E | 600 | FDA | 1 | 0 |
| 2 | E | 802 | GDU | 1 | 0 |
| 3 | F | 600 | FDA | 2 | 0 |
| 3 | G | 600 | FDA | 6 | 0 |
| 2 | G | 802 | GDU | 2 | 0 |
| 3 | H | 600 | FDA | 1 | 0 |
| 2 | H | 802 | GDU | 3 | 0 |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 495/509 (97%) | 0.20 | 3 (0%) 90 91 | 35, 62, 94, 155 | 0 |
| 1 | B | 495/509 (97%) | 0.18 | 6 (1%) 81 83 | 37, 61, 94, 169 | 0 |
| 1 | C | 495/509 (97%) | 0.19 | 12 (2%) 62 66 | 36, 65, 100, 145 | 0 |
| 1 | D | 495/509 (97%) | 0.19 | 8 (1%) 74 78 | 39, 65, 98, 145 | 0 |
| 1 | E | 495/509 (97%) | 0.50 | 39 (7%) 15 17 | 30, 72, 113, 186 | 0 |
| 1 | F | 495/509 (97%) | 0.28 | 17 (3%) 49 54 | 43, 72, 100, 145 | 0 |
| 1 | G | 495/509 (97%) | 0.30 | 18 (3%) 46 51 | 45, 72, 101, 149 | 0 |
| 1 | H | 495/509 (97%) | 0.51 | 42 (8%) 13 14 | 34, 72, 112, 154 | 0 |
| All | All | 3960/4072 (97%) | 0.29 | 145 (3%) 45 50 | 30, 68, 104, 186 | 0 |

All (145) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 342 | ALA | 9.8 |
| 1 | G | 2 | THR | 7.9 |
| 1 | E | 407 | ILE | 6.4 |
| 1 | G | 110 | ILE | 6.4 |
| 1 | A | 2 | THR | 6.0 |
| 1 | D | 2 | THR | 5.9 |
| 1 | B | 2 | THR | 5.9 |
| 1 | E | 384 | GLN | 5.8 |
| 1 | H | 403 | PRO | 5.6 |
| 1 | H | 51 | VAL | 5.6 |
| 1 | G | 208 | ALA | 5.4 |
| 1 | D | 3 | HIS | 5.1 |
| 1 | H | 407 | ILE | 4.7 |
| 1 | G | 508 | LYS | 4.6 |
| 1 | H | 352 | ALA | 4.4 |
| 1 | F | 2 | THR | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 392 | ILE | 4.2 |
| 1 | F | 48 | SER | 4.2 |
| 1 | H | 384 | GLN | 4.2 |
| 1 | G | 57 | LEU | 4.1 |
| 1 | F | 110 | ILE | 4.0 |
| 1 | C | 2 | THR | 3.9 |
| 1 | E | 201 | ALA | 3.9 |
| 1 | G | 3 | HIS | 3.9 |
| 1 | E | 411 | TYR | 3.8 |
| 1 | H | 101 | TRP | 3.8 |
| 1 | G | 62 | GLY | 3.7 |
| 1 | B | 509 | ALA | 3.7 |
| 1 | H | 359 | SER | 3.5 |
| 1 | F | 508 | LYS | 3.5 |
| 1 | F | 509 | ALA | 3.4 |
| 1 | E | 325 | PHE | 3.4 |
| 1 | H | 382 | VAL | 3.4 |
| 1 | C | 508 | LYS | 3.4 |
| 1 | H | 198 | GLY | 3.3 |
| 1 | G | 341 | GLU | 3.3 |
| 1 | C | 140 | LYS | 3.3 |
| 1 | F | 3 | HIS | 3.2 |
| 1 | E | 352 | ALA | 3.1 |
| 1 | H | 119 | VAL | 3.1 |
| 1 | H | 140 | LYS | 3.1 |
| 1 | H | 358 | GLN | 3.1 |
| 1 | F | 368 | TRP | 3.1 |
| 1 | E | 190 | ALA | 3.1 |
| 1 | E | 51 | VAL | 3.0 |
| 1 | E | 342 | ALA | 3.0 |
| 1 | C | 510 | GLN | 3.0 |
| 1 | A | 509 | ALA | 3.0 |
| 1 | F | 198 | GLY | 3.0 |
| 1 | H | 97 | CYS | 3.0 |
| 1 | G | 61 | GLY | 3.0 |
| 1 | H | 346 | LEU | 2.9 |
| 1 | C | 3 | HIS | 2.9 |
| 1 | E | 341 | GLU | 2.9 |
| 1 | E | 116 | GLU | 2.9 |
| 1 | E | 202 | GLY | 2.8 |
| 1 | E | 346 | LEU | 2.7 |
| 1 | G | 204 | TRP | 2.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 387 | ILE | 2.7 |
| 1 | E | 2 | THR | 2.7 |
| 1 | E | 368 | TRP | 2.7 |
| 1 | E | 372 | LEU | 2.7 |
| 1 | H | 355 | SER | 2.7 |
| 1 | C | 190 | ALA | 2.7 |
| 1 | H | 406 | GLU | 2.7 |
| 1 | H | 356 | ARG | 2.6 |
| 1 | E | 210 | PHE | 2.6 |
| 1 | E | 403 | PRO | 2.6 |
| 1 | B | 508 | LYS | 2.6 |
| 1 | H | 506 | LYS | 2.6 |
| 1 | E | 323 | CYS | 2.6 |
| 1 | E | 140 | LYS | 2.6 |
| 1 | C | 61 | GLY | 2.6 |
| 1 | B | 385 | GLU | 2.5 |
| 1 | F | 208 | ALA | 2.5 |
| 1 | H | 52 | THR | 2.5 |
| 1 | H | 294 | SER | 2.5 |
| 1 | H | 190 | ALA | 2.5 |
| 1 | F | 206 | PRO | 2.4 |
| 1 | G | 407 | ILE | 2.4 |
| 1 | H | 411 | TYR | 2.4 |
| 1 | B | 138 | LYS | 2.4 |
| 1 | E | 308 | GLU | 2.4 |
| 1 | E | 357 | PRO | 2.4 |
| 1 | E | 334 | TYR | 2.4 |
| 1 | G | 82 | LYS | 2.4 |
| 1 | E | 214 | ALA | 2.4 |
| 1 | E | 198 | GLY | 2.3 |
| 1 | F | 300 | VAL | 2.3 |
| 1 | H | 398 | THR | 2.3 |
| 1 | D | 475 | GLY | 2.3 |
| 1 | D | 308 | GLU | 2.3 |
| 1 | D | 508 | LYS | 2.3 |
| 1 | E | 406 | GLU | 2.3 |
| 1 | F | 204 | TRP | 2.3 |
| 1 | F | 231 | LYS | 2.3 |
| 1 | D | 135 | ALA | 2.3 |
| 1 | H | 331 | PHE | 2.3 |
| 1 | H | 408 | VAL | 2.3 |
| 1 | H | 341 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 391 | CYS | 2.3 |
| 1 | F | 392 | ILE | 2.3 |
| 1 | H | 347 | PRO | 2.3 |
| 1 | H | 370 | ILE | 2.3 |
| 1 | H | 281 | GLN | 2.3 |
| 1 | H | 299 | GLY | 2.3 |
| 1 | E | 97 | CYS | 2.2 |
| 1 | E | 506 | LYS | 2.2 |
| 1 | H | 367 | TYR | 2.2 |
| 1 | G | 198 | GLY | 2.2 |
| 1 | E | 101 | TRP | 2.2 |
| 1 | H | 300 | VAL | 2.2 |
| 1 | B | 62 | GLY | 2.2 |
| 1 | E | 3 | HIS | 2.1 |
| 1 | H | 362 | ALA | 2.1 |
| 1 | G | 210 | PHE | 2.1 |
| 1 | H | 62 | GLY | 2.1 |
| 1 | E | 359 | SER | 2.1 |
| 1 | F | 238 | GLU | 2.1 |
| 1 | F | 136 | ASN | 2.1 |
| 1 | C | 346 | LEU | 2.1 |
| 1 | G | 273 | PHE | 2.1 |
| 1 | D | 134 | VAL | 2.1 |
| 1 | E | 205 | GLY | 2.1 |
| 1 | A | 116 | GLU | 2.1 |
| 1 | E | 370 | ILE | 2.1 |
| 1 | H | 110 | ILE | 2.1 |
| 1 | E | 327 | ARG | 2.1 |
| 1 | D | 169 | VAL | 2.1 |
| 1 | G | 138 | LYS | 2.1 |
| 1 | H | 395 | LEU | 2.1 |
| 1 | C | 62 | GLY | 2.0 |
| 1 | C | 506 | LYS | 2.0 |
| 1 | E | 365 | GLY | 2.0 |
| 1 | H | 365 | GLY | 2.0 |
| 1 | E | 388 | LEU | 2.0 |
| 1 | E | 361 | GLU | 2.0 |
| 1 | C | 134 | VAL | 2.0 |
| 1 | G | 86 | TRP | 2.0 |
| 1 | C | 66 | PHE | 2.0 |
| 1 | F | 273 | PHE | 2.0 |
| 1 | H | 507 | SER | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | G | 299 | GLY | 2.0 |
| 1 | E | 510 | GLN | 2.0 |
| 1 | H | 325 | PHE | 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 carbohydrates in this entry.

## 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 4 | CL | H | 511 | 1/1 | 0.88 | 0.19 | 0.68 | 92,92,92,92 | 0 |
| 2 | GDU | E | 802 | 36/36 | 0.93 | 0.21 | 0.47 | 36,87,184,204 | 0 |
| 4 | CL | E | 511 | 1/1 | 0.76 | 0.17 | 0.29 | 98,98,98,98 | 0 |
| 4 | CL | B | 512 | 1/1 | 0.94 | 0.15 | 0.00 | 85,85,85,85 | 0 |
| 2 | GDU | C | 802 | 36/36 | 0.95 | 0.17 | -0.18 | 34,83,170,193 | 0 |
| 2 | GDU | F | 802 | 36/36 | 0.93 | 0.16 | -0.21 | 46,101,172,187 | 0 |
| 2 | GDU | G | 802 | 36/36 | 0.94 | 0.17 | -0.32 | 42,96,200,209 | 0 |
| 3 | FDA | E | 600 | 53/53 | 0.96 | 0.15 | -0.33 | 27,56,102,130 | 0 |
| 3 | FDA | D | 600 | 53/53 | 0.97 | 0.14 | -0.51 | 26,64,91,108 | 0 |
| 3 | FDA | C | 600 | 53/53 | 0.97 | 0.14 | -0.67 | 34,66,92,99 | 0 |
| 2 | GDU | A | 802 | 36/36 | 0.97 | 0.16 | -0.68 | 40,66,183,201 | 0 |
| 2 | GDU | B | 802 | 36/36 | 0.95 | 0.16 | -0.73 | 47,68,189,191 | 0 |
| 2 | GDU | H | 802 | 36/36 | 0.94 | 0.15 | -0.75 | 34,83,158,181 | 0 |
| 3 | FDA | H | 600 | 53/53 | 0.96 | 0.14 | -0.76 | 28,55,92,130 | 0 |
| 2 | GDU | D | 802 | 36/36 | 0.95 | 0.15 | -0.83 | 37,80,177,208 | 0 |
| 3 | FDA | G | 600 | 53/53 | 0.95 | 0.12 | -0.85 | 35,67,86,99 | 0 |
| 3 | FDA | F | 600 | 53/53 | 0.96 | 0.13 | -0.87 | 34,62,84,98 | 0 |
| 4 | CL | F | 511 | 1/1 | 0.67 | 0.14 | -1.00 | 127,127,127,127 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | FDA | B | 600 | 53/53 | 0.97 | 0.13 | -1.09 | 31,49,72,95 | 0 |
| 4 | CL | A | 511 | 1/1 | 0.94 | 0.14 | -1.14 | 99,99,99,99 | 0 |
| 3 | FDA | A | 600 | 53/53 | 0.97 | 0.13 | -1.15 | 33,48,67,82 | 0 |
| 4 | CL | B | 511 | 1/1 | 0.91 | 0.13 | -1.37 | 99,99,99,99 | 0 |
| 4 | CL | G | 511 | 1/1 | 0.84 | 0.11 | -1.44 | 91,91,91,91 | 0 |
| 4 | CL | A | 1 | 1/1 | 0.95 | 0.25 | - | 94,94,94,94 | 0 |

## 6.5 Other polymers

There are no such residues in this entry.