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

Jan 2, 2024 – 12:55 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 5A0U |
| Title | : | Structure of CutC choline lyase choline bound form from Klebsiella pneumoniae. |
| Authors | : | Kalnins, G.; Tars, K. |
| Deposited on | : | 2015-04-23 |
| Resolution | : | 2.40 Å(reported) |

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

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

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

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

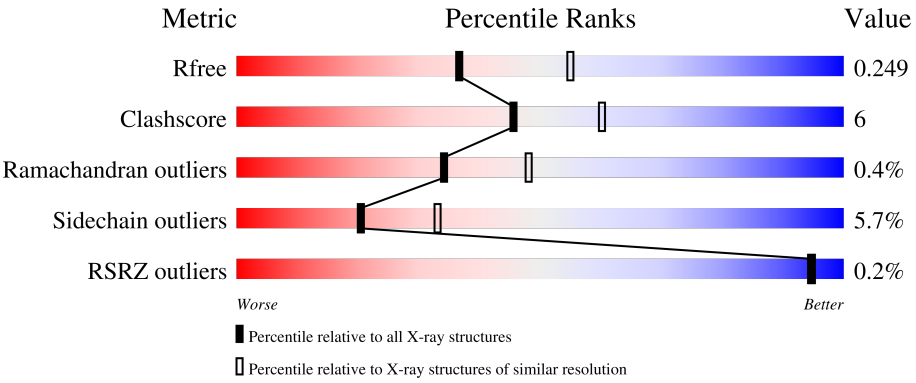
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 3907 (2.40-2.40) |
| Clashscore | 141614 | 4398 (2.40-2.40) |
| Ramachandran outliers | 138981 | 4318 (2.40-2.40) |
| Sidechain outliers | 138945 | 4319 (2.40-2.40) |
| RSRZ outliers | 127900 | 3811 (2.40-2.40) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 795 | 83% 14% . |
| 1 | B | 795 | 83% 15% . |
| 1 | C | 795 | 81% 17% . |
| 1 | D | 795 | 84% 14% . |
| 1 | E | 795 | 78% 19% . |

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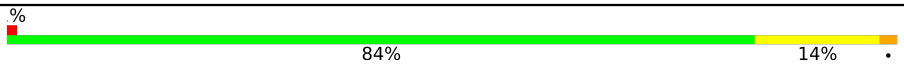
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 795 |   |
| 1 | G | 795 |   |
| 1 | H | 795 |   |

## 2 Entry composition (i)

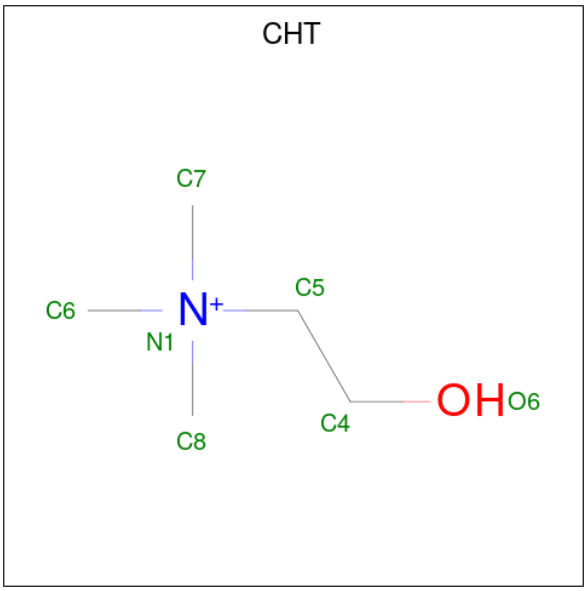
There are 3 unique types of molecules in this entry. The entry contains 52127 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CHOLINE TRIMETHYLAMINE LYASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 792 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6254 | 3954 | 1077 | 1181 | 42 | | | |
| 1 | B | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | C | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | D | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | E | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | F | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | G | 793 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6261 | 3959 | 1078 | 1182 | 42 | | | |
| 1 | H | 795 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6275 | 3968 | 1080 | 1185 | 42 | | | |

- Molecule 2 is CHOLINE ION (three-letter code: CHT) (formula: $C_5H_{14}NO$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | B | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | C | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | D | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | E | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | F | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | G | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |
| 2 | H | 1 | Total C N O<br>7 5 1 1 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 344 | Total O<br>344 344 | 0 | 0 |
| 3 | B | 294 | Total O<br>294 294 | 0 | 0 |
| 3 | C | 297 | Total O<br>297 297 | 0 | 0 |
| 3 | D | 307 | Total O<br>307 307 | 0 | 0 |

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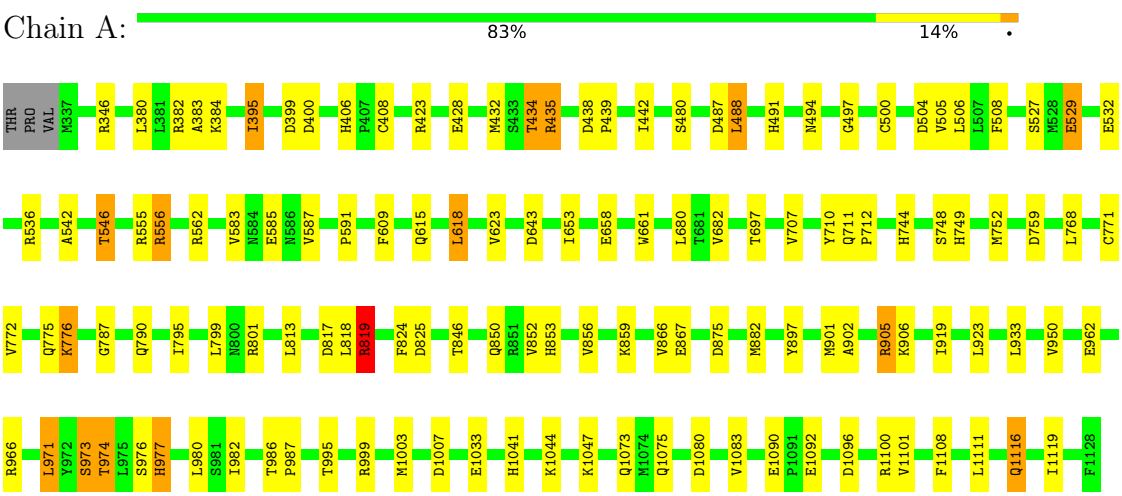
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | E | 163 | Total O<br>163 163 | 0 | 0 |
| 3 | F | 152 | Total O<br>152 152 | 0 | 0 |
| 3 | G | 217 | Total O<br>217 217 | 0 | 0 |
| 3 | H | 202 | Total O<br>202 202 | 0 | 0 |

# 3 Residue-property plots (i)

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

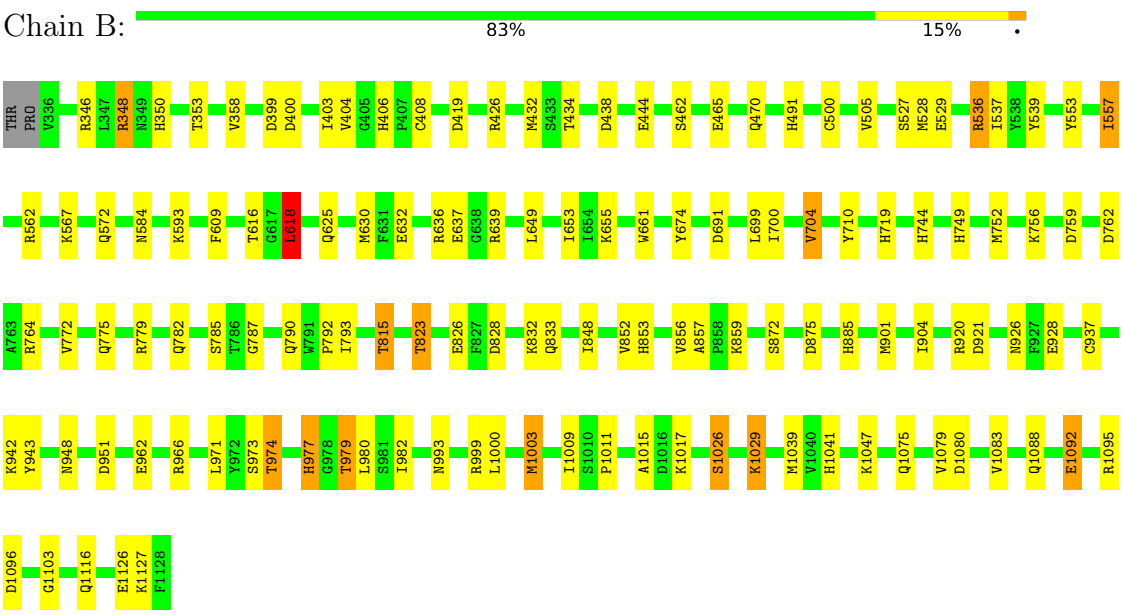
• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain A:



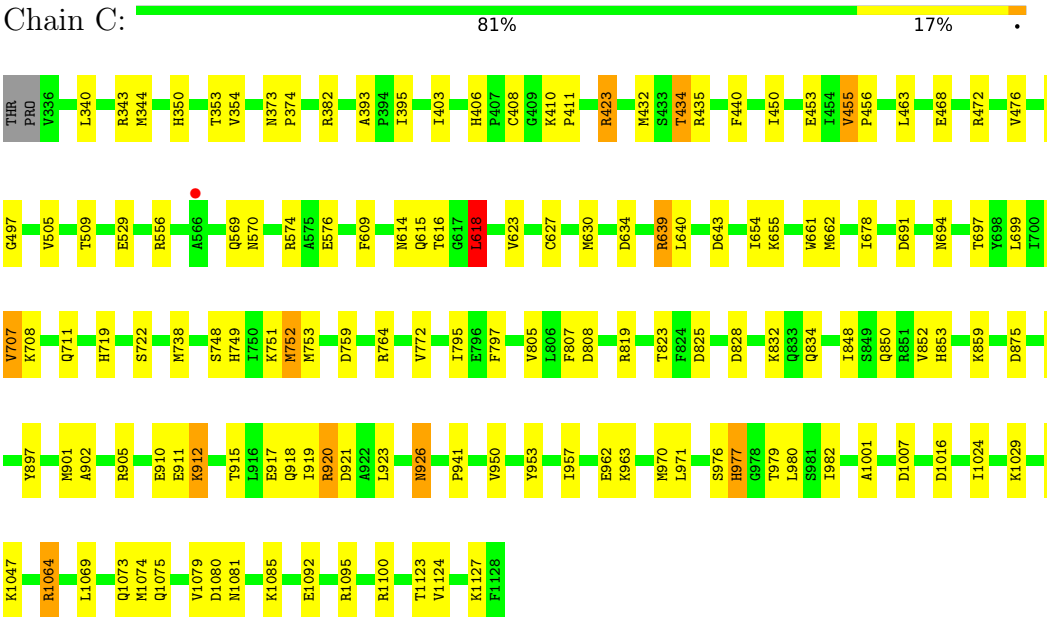

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain B:



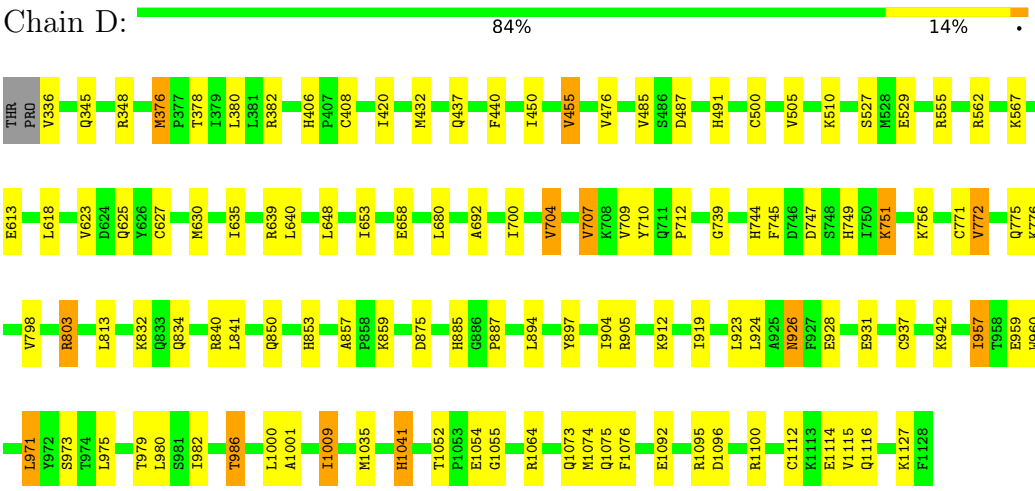

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain C:



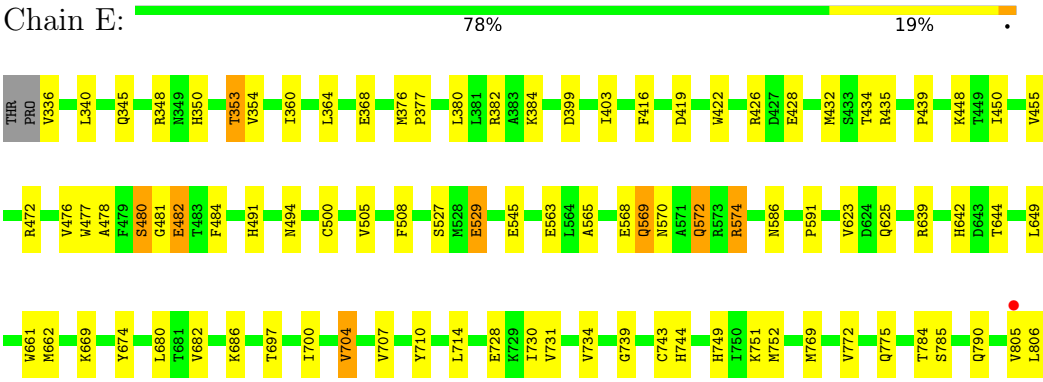

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain D:



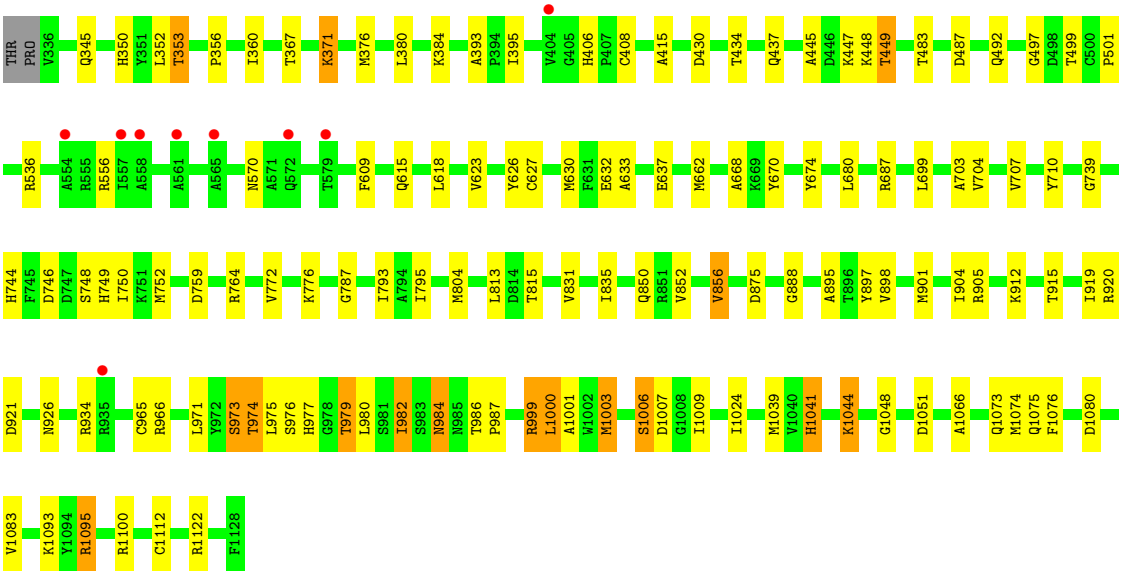

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain E:



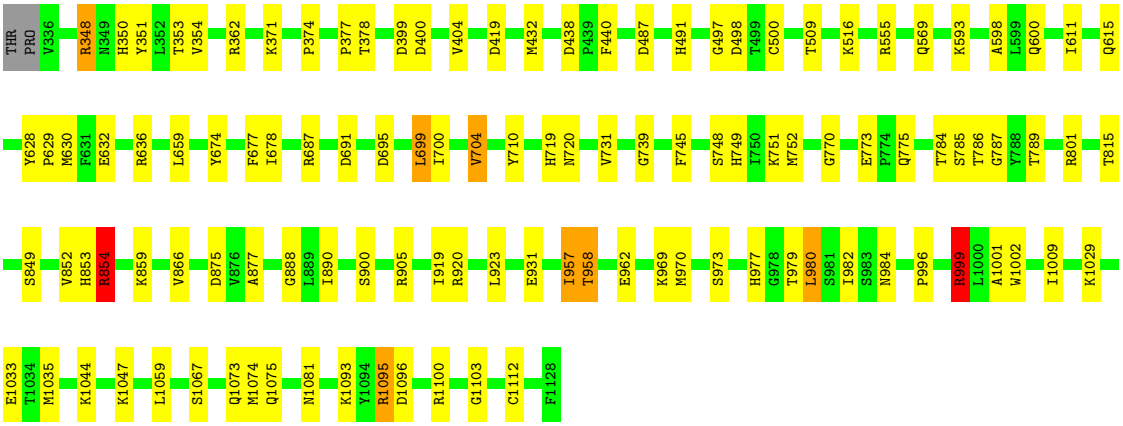

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain F:

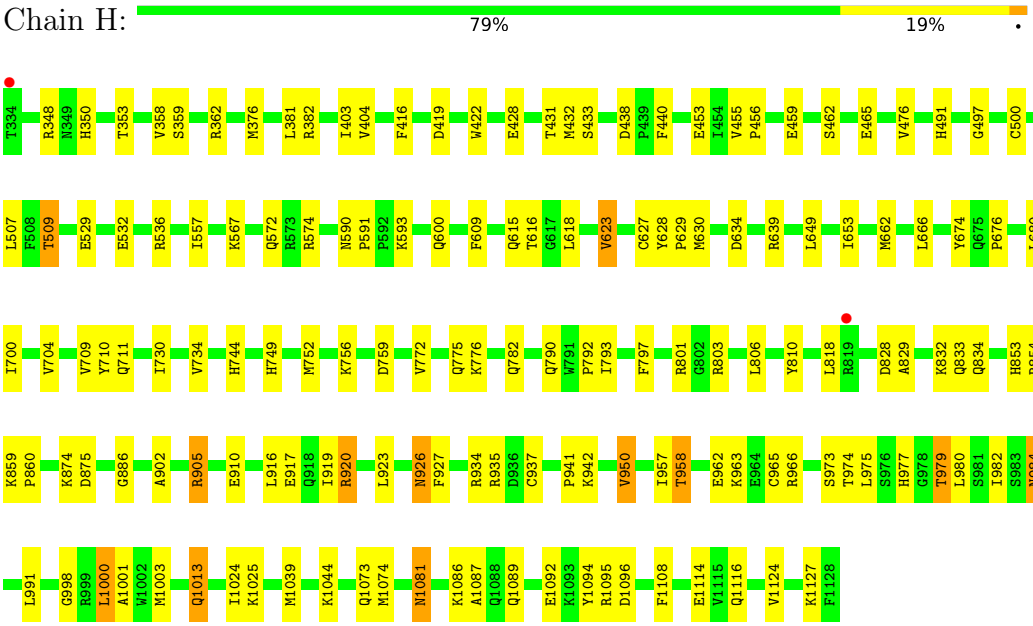

• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain G:


• Molecule 1: CHOLINE TRIMETHYLAMINE LYASE

Chain H:


79%
19%
T334 R348 N349 H350 T353 V358 S359 R362 M376 L381 R382 I403 V404 F416 D419 W422 E428 T431 M432 S433 D438 P439 F440 E453 I454 V455 P456 E459 S462 E465 V476 H491 G497 C500 Y503 D504 V505 L506
L507 F508 T509 E529 E532 R536 I557 K567 Q572 R573 R574 N590 P591 P592 K593 Q600 F609 Q615 T616 G617 L618 V623 C627 Y628 P629 M630 D634 R639 L649 I653 M662 L666 Y674 Q675 P676 L680 T681 L696
I700 V704 V709 Y710 Q711 I730 V734 H744 H749 M752 K756 D759 V772 Q775 K776 Q782 Q790 W791 P792 I793 F797 R801 G802 R803 L806 Y810 L818 R819 D828 A829 K832 Q833 Q834 H853 R854 D855 V856 A857 P858
K859 P860 K874 D875 G886 A902 R905 E910 L916 E917 Q918 I919 R920 L923 N926 F927 R934 R935 D936 C937 P941 K942 V950 I957 T958 E962 K963 E964 C965 R966 S973 T974 L975 S976 H977 G978 T979 L980 S981 I982 S983 N984 N985 T986 P987 I988
L991 G998 R999 L1000 A1001 W1002 M1003 Q1013 I1024 K1025 M1039 K1044 Q1073 M1074 N1081 K1086 A1087 Q1088 Q1089 E1092 K1093 Y1094 R1095 D1096 F1108 E1114 V1115 Q1116 V1124 K1127 F1128

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 89.41Å 221.87Å 419.48Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 209.74 – 2.40<br>76.21 – 2.40 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 93.6 (209.74-2.40)<br>93.6 (76.21-2.40) | Depositor<br>EDS |
| $R_{merge}$ | 0.17 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.68 (at 2.40Å) | Xtriage |
| Refinement program | REFMAC 5.8.0049 | Depositor |
| R, $R_{free}$ | 0.188 , 0.247<br>0.194 , 0.249 | Depositor<br>DCC |
| $R_{free}$ test set | 15197 reflections (4.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 26.0 | Xtriage |
| Anisotropy | 0.382 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.32 , 30.3 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.45$, $< L^2 > = 0.28$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 52127 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 28.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.65 | 0/6385 | 0.84 | 10/8640 (0.1%) |
| 1 | B | 0.61 | 0/6392 | 0.80 | 7/8650 (0.1%) |
| 1 | C | 0.62 | 0/6392 | 0.82 | 7/8650 (0.1%) |
| 1 | D | 0.65 | 0/6392 | 0.82 | 6/8650 (0.1%) |
| 1 | E | 0.57 | 0/6392 | 0.76 | 1/8650 (0.0%) |
| 1 | F | 0.58 | 0/6392 | 0.75 | 1/8650 (0.0%) |
| 1 | G | 0.59 | 0/6392 | 0.78 | 6/8650 (0.1%) |
| 1 | H | 0.60 | 0/6407 | 0.77 | 3/8672 (0.0%) |
| All | All | 0.61 | 0/51144 | 0.79 | 41/69212 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | E | 0 | 1 |
| 1 | G | 0 | 2 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (41) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | C | 764 | ARG | NE-CZ-NH2 | -10.52 | 115.04 | 120.30 |
| 1 | A | 382 | ARG | NE-CZ-NH2 | -9.14 | 115.73 | 120.30 |
| 1 | C | 764 | ARG | NE-CZ-NH1 | 8.02 | 124.31 | 120.30 |
| 1 | A | 382 | ARG | NE-CZ-NH1 | 7.98 | 124.29 | 120.30 |
| 1 | C | 753 | MET | CG-SD-CE | -7.57 | 88.08 | 100.20 |
| 1 | H | 362 | ARG | NE-CZ-NH1 | 7.56 | 124.08 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 536 | ARG | NE-CZ-NH1 | 7.37 | 123.98 | 120.30 |
| 1 | G | 980 | LEU | CA-CB-CG | 7.29 | 132.07 | 115.30 |
| 1 | G | 854 | ARG | NE-CZ-NH2 | -6.86 | 116.87 | 120.30 |
| 1 | B | 536 | ARG | NE-CZ-NH2 | -6.81 | 116.89 | 120.30 |
| 1 | A | 556 | ARG | NE-CZ-NH2 | -6.46 | 117.07 | 120.30 |
| 1 | D | 803 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | D | 487 | ASP | CB-CG-OD1 | 6.12 | 123.81 | 118.30 |
| 1 | B | 779 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | A | 536 | ARG | NE-CZ-NH1 | 5.77 | 123.18 | 120.30 |
| 1 | F | 536 | ARG | NE-CZ-NH1 | 5.75 | 123.17 | 120.30 |
| 1 | G | 348 | ARG | NE-CZ-NH1 | 5.73 | 123.16 | 120.30 |
| 1 | B | 779 | ARG | NE-CZ-NH2 | -5.67 | 117.47 | 120.30 |
| 1 | G | 1095 | ARG | NE-CZ-NH1 | 5.59 | 123.10 | 120.30 |
| 1 | C | 382 | ARG | NE-CZ-NH1 | 5.59 | 123.09 | 120.30 |
| 1 | A | 423 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | H | 854 | ARG | NE-CZ-NH2 | -5.56 | 117.52 | 120.30 |
| 1 | C | 1080 | ASP | CB-CG-OD1 | 5.54 | 123.29 | 118.30 |
| 1 | E | 382 | ARG | NE-CZ-NH1 | 5.53 | 123.07 | 120.30 |
| 1 | A | 556 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 1 | B | 618 | LEU | CA-CB-CG | -5.38 | 102.94 | 115.30 |
| 1 | H | 536 | ARG | NE-CZ-NH2 | -5.34 | 117.63 | 120.30 |
| 1 | A | 643 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 1 | A | 825 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |
| 1 | C | 618 | LEU | CA-CB-CG | -5.27 | 103.17 | 115.30 |
| 1 | D | 382 | ARG | NE-CZ-NH2 | -5.21 | 117.69 | 120.30 |
| 1 | D | 382 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | A | 819 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | D | 376 | MET | CG-SD-CE | -5.16 | 91.95 | 100.20 |
| 1 | A | 1096 | ASP | CB-CG-OD1 | 5.14 | 122.92 | 118.30 |
| 1 | B | 762 | ASP | CB-CG-OD2 | -5.12 | 113.69 | 118.30 |
| 1 | B | 764 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | G | 854 | ARG | CG-CD-NE | -5.08 | 101.13 | 111.80 |
| 1 | G | 999 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | C | 643 | ASP | CB-CG-OD1 | 5.05 | 122.85 | 118.30 |
| 1 | D | 803 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | E | 480 | SER | Peptide |
| 1 | G | 377 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | G | 789 | THR | Peptide |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 6254 | 0 | 6171 | 73 | 0 |
| 1 | B | 6261 | 0 | 6180 | 75 | 0 |
| 1 | C | 6261 | 0 | 6180 | 94 | 0 |
| 1 | D | 6261 | 0 | 6180 | 71 | 0 |
| 1 | E | 6261 | 0 | 6180 | 88 | 0 |
| 1 | F | 6261 | 0 | 6180 | 85 | 0 |
| 1 | G | 6261 | 0 | 6180 | 66 | 0 |
| 1 | H | 6275 | 0 | 6194 | 90 | 0 |
| 2 | A | 7 | 0 | 14 | 1 | 0 |
| 2 | B | 7 | 0 | 14 | 0 | 0 |
| 2 | C | 7 | 0 | 14 | 1 | 0 |
| 2 | D | 7 | 0 | 14 | 0 | 0 |
| 2 | E | 7 | 0 | 14 | 0 | 0 |
| 2 | F | 7 | 0 | 14 | 0 | 0 |
| 2 | G | 7 | 0 | 14 | 2 | 0 |
| 2 | H | 7 | 0 | 14 | 0 | 0 |
| 3 | A | 344 | 0 | 0 | 5 | 0 |
| 3 | B | 294 | 0 | 0 | 7 | 0 |
| 3 | C | 297 | 0 | 0 | 4 | 0 |
| 3 | D | 307 | 0 | 0 | 6 | 0 |
| 3 | E | 163 | 0 | 0 | 1 | 0 |
| 3 | F | 152 | 0 | 0 | 10 | 0 |
| 3 | G | 217 | 0 | 0 | 6 | 0 |
| 3 | H | 202 | 0 | 0 | 4 | 0 |
| All | All | 52127 | 0 | 49557 | 642 | 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 6.

All (642) 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:G:979:THR:HG21 | 1:G:1009:ILE:HD11 | 1.44 | 0.97 |
| 1:C:722:SER:O | 1:C:1064:ARG:NH2 | 2.01 | 0.92 |
| 1:E:999:ARG:NH2 | 1:E:1003:MET:O | 2.03 | 0.92 |
| 1:F:999:ARG:NH1 | 1:F:1003:MET:O | 2.02 | 0.91 |
| 1:E:568:GLU:O | 1:E:574:ARG:NH1 | 2.04 | 0.89 |
| 1:H:497:GLY:H | 1:H:615:GLN:HE21 | 1.22 | 0.87 |
| 1:D:376:MET:HE1 | 1:D:380:LEU:HG | 1.56 | 0.85 |
| 1:E:477:TRP:O | 1:E:481:GLY:HA3 | 1.77 | 0.84 |
| 1:C:941:PRO:O | 1:C:950:VAL:HG11 | 1.80 | 0.81 |
| 1:H:350:HIS:O | 1:H:353:THR:HB | 1.79 | 0.80 |
| 1:C:795:ILE:HD11 | 1:C:901:MET:HE2 | 1.62 | 0.80 |
| 1:G:784:THR:HG22 | 3:G:2148:HOH:O | 1.81 | 0.80 |
| 1:B:637:GLU:OE1 | 1:B:639:ARG:NH2 | 2.17 | 0.77 |
| 1:G:979:THR:CG2 | 1:G:1009:ILE:HD11 | 2.14 | 0.76 |
| 1:A:966:ARG:HH11 | 1:A:974:THR:HG22 | 1.50 | 0.76 |
| 1:A:897:TYR:CZ | 1:A:901:MET:HE3 | 2.21 | 0.75 |
| 1:C:902:ALA:CB | 1:C:950:VAL:HG12 | 2.17 | 0.75 |
| 1:B:1075:GLN:HE22 | 1:B:1103:GLY:H | 1.34 | 0.74 |
| 1:G:497:GLY:H | 1:G:615:GLN:HE21 | 1.34 | 0.74 |
| 1:A:999:ARG:NH1 | 1:A:1003:MET:O | 2.21 | 0.73 |
| 1:G:962:GLU:OE1 | 1:G:977:HIS:HD2 | 1.71 | 0.73 |
| 1:F:897:TYR:CZ | 1:F:901:MET:HE3 | 2.23 | 0.72 |
| 1:G:432:MET:HE3 | 1:G:440:PHE:HB2 | 1.70 | 0.72 |
| 1:B:350:HIS:O | 1:B:353:THR:HB | 1.89 | 0.72 |
| 1:E:478:ALA:HA | 1:E:482:GLU:HG3 | 1.72 | 0.72 |
| 1:C:1024:ILE:HD11 | 1:C:1074:MET:HE1 | 1.72 | 0.72 |
| 1:H:984:ASN:C | 1:H:984:ASN:HD22 | 1.91 | 0.72 |
| 1:B:999:ARG:NH1 | 1:B:1003:MET:O | 2.23 | 0.72 |
| 1:A:744:HIS:HD2 | 1:A:749:HIS:CE1 | 2.09 | 0.71 |
| 1:E:805:VAL:HG11 | 1:E:993:ASN:HB2 | 1.73 | 0.69 |
| 1:E:682:VAL:CG2 | 1:E:697:THR:HG23 | 2.22 | 0.69 |
| 1:D:527:SER:HB2 | 1:D:529:GLU:OE2 | 1.91 | 0.69 |
| 1:A:682:VAL:HG13 | 1:A:697:THR:HG23 | 1.75 | 0.69 |
| 1:A:711:GLN:NE2 | 3:A:2173:HOH:O | 2.25 | 0.69 |
| 1:E:572:GLN:HE21 | 1:E:572:GLN:HA | 1.58 | 0.69 |
| 1:A:795:ILE:HD11 | 1:A:901:MET:HE2 | 1.74 | 0.68 |
| 1:F:430:ASP:OD1 | 1:F:447:LYS:NZ | 2.26 | 0.68 |
| 1:G:509:THR:HG21 | 3:G:2072:HOH:O | 1.92 | 0.68 |
| 1:E:813:LEU:N | 1:E:834:GLN:OE1 | 2.27 | 0.68 |
| 1:C:1024:ILE:HD11 | 1:C:1074:MET:CE | 2.24 | 0.68 |
| 1:H:491:HIS:O | 1:H:853:HIS:HE1 | 1.76 | 0.68 |
| 1:A:380:LEU:O | 1:A:384:LYS:HG2 | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:759:ASP:HB3 | 3:A:2212:HOH:O | 1.95 | 0.66 |
| 1:F:979:THR:HG22 | 1:F:1039:MET:HA | 1.78 | 0.66 |
| 1:G:773:GLU:OE2 | 1:G:784:THR:HG21 | 1.95 | 0.66 |
| 1:F:895:ALA:HB3 | 1:F:1006:SER:OG | 1.95 | 0.66 |
| 1:G:1009:ILE:O | 1:G:1009:ILE:HG22 | 1.95 | 0.66 |
| 1:H:627:CYS:HA | 1:H:630:MET:HE2 | 1.78 | 0.66 |
| 1:D:1052:THR:CG2 | 1:D:1054:GLU:CD | 2.64 | 0.66 |
| 1:E:731:VAL:HG22 | 1:E:1059:LEU:HD23 | 1.77 | 0.66 |
| 1:E:743:CYS:HB2 | 1:E:1074:MET:O | 1.95 | 0.66 |
| 1:H:431:THR:HG23 | 3:H:2037:HOH:O | 1.96 | 0.66 |
| 1:B:1080:ASP:HB3 | 1:B:1083:VAL:HG23 | 1.76 | 0.66 |
| 1:H:1108:PHE:CZ | 1:H:1116:GLN:HB2 | 2.31 | 0.66 |
| 1:D:894:LEU:HD22 | 1:D:1009:ILE:CD1 | 2.26 | 0.65 |
| 1:F:395:ILE:HD11 | 1:F:556:ARG:HB3 | 1.78 | 0.65 |
| 1:F:746:ASP:O | 1:F:750:ILE:HG12 | 1.97 | 0.65 |
| 1:B:920:ARG:NH1 | 1:B:921:ASP:OD1 | 2.30 | 0.65 |
| 1:C:748:SER:O | 1:C:752:MET:HG2 | 1.96 | 0.65 |
| 1:F:966:ARG:HH11 | 1:F:974:THR:HG22 | 1.62 | 0.65 |
| 1:A:897:TYR:CE1 | 1:A:901:MET:CE | 2.80 | 0.64 |
| 1:D:627:CYS:HA | 1:D:630:MET:CE | 2.27 | 0.64 |
| 1:F:497:GLY:H | 1:F:615:GLN:HE21 | 1.43 | 0.64 |
| 1:E:1073:GLN:HE22 | 1:E:1075:GLN:HE21 | 1.43 | 0.64 |
| 1:E:857:ALA:O | 1:E:859:LYS:NZ | 2.28 | 0.64 |
| 1:H:404:VAL:H | 1:H:600:GLN:HE22 | 1.44 | 0.64 |
| 1:A:497:GLY:H | 1:A:615:GLN:HE21 | 1.45 | 0.64 |
| 1:E:682:VAL:HG22 | 1:E:697:THR:HG23 | 1.80 | 0.64 |
| 1:H:627:CYS:HA | 1:H:630:MET:CE | 2.28 | 0.64 |
| 1:E:902:ALA:HB2 | 1:E:950:VAL:HG23 | 1.79 | 0.64 |
| 1:B:419:ASP:OD1 | 1:B:419:ASP:N | 2.30 | 0.63 |
| 1:C:423:ARG:NH2 | 1:C:468:GLU:OE1 | 2.31 | 0.63 |
| 1:A:962:GLU:OE2 | 1:A:976:SER:HB2 | 1.97 | 0.63 |
| 1:E:1048:GLY:HA2 | 1:E:1051:ASP:OD2 | 1.98 | 0.63 |
| 1:C:491:HIS:O | 1:C:853:HIS:HE1 | 1.82 | 0.63 |
| 1:A:542:ALA:O | 1:A:546:THR:HG23 | 1.99 | 0.63 |
| 1:A:795:ILE:HD11 | 1:A:901:MET:CE | 2.29 | 0.63 |
| 1:B:346:ARG:NH1 | 1:B:400:ASP:OD1 | 2.31 | 0.63 |
| 1:D:1073:GLN:HE22 | 1:D:1075:GLN:HE21 | 1.45 | 0.63 |
| 1:E:700:ILE:O | 1:E:704:VAL:HG12 | 1.99 | 0.62 |
| 1:B:691:ASP:OD1 | 1:B:719:HIS:HE1 | 1.82 | 0.62 |
| 1:H:979:THR:HG22 | 1:H:1039:MET:HA | 1.81 | 0.62 |
| 1:C:627:CYS:HA | 1:C:630:MET:CE | 2.30 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:395:ILE:HD11 | 1:C:556:ARG:HB3 | 1.80 | 0.62 |
| 1:F:350:HIS:O | 1:F:353:THR:HB | 2.00 | 0.61 |
| 1:H:984:ASN:O | 1:H:988:ILE:HG12 | 2.00 | 0.61 |
| 1:A:487:ASP:O | 1:A:787:GLY:HA2 | 2.01 | 0.61 |
| 1:A:406:HIS:HD2 | 1:A:408:CYS:H | 1.49 | 0.61 |
| 1:A:682:VAL:CG1 | 1:A:697:THR:HG23 | 2.29 | 0.60 |
| 1:B:966:ARG:HH11 | 1:B:974:THR:CG2 | 2.14 | 0.60 |
| 1:E:478:ALA:HA | 1:E:482:GLU:CG | 2.31 | 0.60 |
| 1:B:744:HIS:HD2 | 1:B:749:HIS:CE1 | 2.19 | 0.60 |
| 1:E:954:ALA:HA | 1:E:957:ILE:HD11 | 1.83 | 0.60 |
| 1:F:966:ARG:HH11 | 1:F:974:THR:CG2 | 2.13 | 0.60 |
| 1:H:358:VAL:HG21 | 1:H:432:MET:HE3 | 1.84 | 0.60 |
| 1:B:942:LYS:HG2 | 1:B:1015:ALA:HB1 | 1.84 | 0.60 |
| 1:E:569:GLN:HA | 1:E:569:GLN:OE1 | 2.01 | 0.60 |
| 1:E:984:ASN:C | 1:E:984:ASN:HD22 | 2.05 | 0.60 |
| 1:G:350:HIS:O | 1:G:353:THR:HB | 2.01 | 0.60 |
| 1:C:627:CYS:HA | 1:C:630:MET:HE1 | 1.84 | 0.60 |
| 1:F:483:THR:HB | 1:F:804:MET:HE1 | 1.83 | 0.60 |
| 1:H:382:ARG:HD2 | 3:H:2017:HOH:O | 2.02 | 0.60 |
| 1:E:979:THR:HG21 | 1:E:1035:MET:SD | 2.41 | 0.59 |
| 1:F:926:ASN:HD21 | 1:F:1001:ALA:H | 1.50 | 0.59 |
| 1:D:432:MET:HE3 | 1:D:440:PHE:HB2 | 1.83 | 0.59 |
| 1:F:1024:ILE:HD11 | 1:F:1074:MET:HE2 | 1.83 | 0.59 |
| 1:H:696:LEU:HD12 | 1:H:700:ILE:HG13 | 1.84 | 0.59 |
| 1:B:885:HIS:HE2 | 1:B:966:ARG:HH12 | 1.49 | 0.59 |
| 1:H:358:VAL:HG21 | 1:H:432:MET:CE | 2.31 | 0.59 |
| 1:A:897:TYR:CE1 | 1:A:901:MET:HE1 | 2.38 | 0.59 |
| 1:D:406:HIS:HD2 | 1:D:408:CYS:H | 1.48 | 0.59 |
| 1:D:623:VAL:HG22 | 1:D:680:LEU:HD21 | 1.85 | 0.59 |
| 1:D:897:TYR:CE1 | 1:D:957:ILE:HG12 | 2.38 | 0.59 |
| 1:A:383:ALA:HB1 | 1:A:546:THR:HG22 | 1.84 | 0.58 |
| 1:E:1099:VAL:HG11 | 1:E:1108:PHE:CD1 | 2.37 | 0.58 |
| 1:D:857:ALA:O | 1:D:859:LYS:NZ | 2.35 | 0.58 |
| 1:E:913:LYS:HD3 | 1:E:914:TYR:CZ | 2.38 | 0.58 |
| 1:C:614:ASN:HD21 | 1:C:662:MET:H | 1.51 | 0.58 |
| 1:H:934:ARG:NH1 | 1:H:1000:LEU:HD13 | 2.19 | 0.58 |
| 1:G:404:VAL:H | 1:G:600:GLN:HE22 | 1.52 | 0.58 |
| 1:E:403:ILE:HD13 | 1:E:652:PHE:HB2 | 1.85 | 0.58 |
| 1:E:744:HIS:HD2 | 1:E:749:HIS:CE1 | 2.22 | 0.57 |
| 1:F:627:CYS:HA | 1:F:630:MET:CE | 2.34 | 0.57 |
| 1:F:973:SER:OG | 1:F:974:THR:N | 2.34 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:934:ARG:NH1 | 1:H:998:GLY:O | 2.36 | 0.57 |
| 1:F:759:ASP:HB3 | 3:F:2080:HOH:O | 2.03 | 0.57 |
| 1:H:966:ARG:HH11 | 1:H:974:THR:CG2 | 2.16 | 0.57 |
| 1:D:926:ASN:HD21 | 1:D:1000:LEU:HB2 | 1.69 | 0.57 |
| 1:H:680:LEU:HD23 | 1:H:681:THR:N | 2.20 | 0.57 |
| 1:C:823:THR:HG22 | 1:C:825:ASP:N | 2.19 | 0.57 |
| 1:C:406:HIS:HD2 | 1:C:408:CYS:H | 1.52 | 0.57 |
| 1:B:785:SER:HB3 | 3:B:2202:HOH:O | 2.03 | 0.56 |
| 1:C:902:ALA:HB2 | 1:C:950:VAL:HG12 | 1.87 | 0.56 |
| 1:D:813:LEU:H | 1:D:834:GLN:HE22 | 1.52 | 0.56 |
| 1:D:500:CYS:H | 1:D:775:GLN:HE22 | 1.53 | 0.56 |
| 1:H:730:ILE:O | 1:H:734:VAL:HG23 | 2.05 | 0.56 |
| 1:H:965:CYS:O | 1:H:975:LEU:HB3 | 2.06 | 0.56 |
| 1:H:1013:GLN:H | 1:H:1013:GLN:HE21 | 1.51 | 0.56 |
| 1:E:491:HIS:O | 1:E:853:HIS:HE1 | 1.87 | 0.56 |
| 1:G:785:SER:HA | 1:G:888:GLY:O | 2.05 | 0.56 |
| 1:F:356:PRO:HG2 | 1:F:674:TYR:CE2 | 2.40 | 0.56 |
| 1:F:850:GLN:HB3 | 1:F:971:LEU:HD22 | 1.88 | 0.56 |
| 1:D:894:LEU:HD22 | 1:D:1009:ILE:HD13 | 1.87 | 0.56 |
| 1:G:362:ARG:NH2 | 1:G:419:ASP:OD1 | 2.38 | 0.56 |
| 1:H:902:ALA:CB | 1:H:950:VAL:HG12 | 2.35 | 0.56 |
| 1:E:348:ARG:NH1 | 1:E:707:VAL:O | 2.40 | 0.55 |
| 1:H:1013:GLN:H | 1:H:1013:GLN:NE2 | 2.04 | 0.55 |
| 1:E:650:GLN:HB3 | 1:E:707:VAL:HG21 | 1.89 | 0.55 |
| 1:H:416:PHE:HA | 1:H:662:MET:HE1 | 1.89 | 0.55 |
| 1:C:905:ARG:HD2 | 1:C:953:TYR:OH | 2.07 | 0.55 |
| 1:F:749:HIS:HA | 1:F:752:MET:HG2 | 1.87 | 0.55 |
| 1:C:897:TYR:CZ | 1:C:901:MET:HE3 | 2.39 | 0.55 |
| 1:C:639:ARG:O | 1:C:640:LEU:HD23 | 2.06 | 0.55 |
| 1:H:497:GLY:H | 1:H:615:GLN:NE2 | 2.00 | 0.55 |
| 1:E:376:MET:HE1 | 1:E:380:LEU:HG | 1.87 | 0.55 |
| 1:F:934:ARG:HH12 | 1:F:1000:LEU:HG | 1.70 | 0.55 |
| 2:G:2000:CHT:O6 | 2:G:2000:CHT:H82 | 2.07 | 0.55 |
| 1:D:627:CYS:HA | 1:D:630:MET:HE1 | 1.87 | 0.54 |
| 1:E:1080:ASP:HB3 | 1:E:1083:VAL:HG23 | 1.88 | 0.54 |
| 1:C:1074:MET:CE | 3:C:2280:HOH:O | 2.55 | 0.54 |
| 1:G:399:ASP:O | 1:G:400:ASP:HB2 | 2.07 | 0.54 |
| 1:D:1041:HIS:HD2 | 3:D:2294:HOH:O | 1.89 | 0.54 |
| 1:E:749:HIS:HA | 1:E:752:MET:HG2 | 1.89 | 0.54 |
| 1:B:462:SER:OG | 1:B:465:GLU:OE1 | 2.24 | 0.54 |
| 1:B:974:THR:HG21 | 3:B:2186:HOH:O | 2.06 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1073:GLN:HE22 | 1:C:1075:GLN:HE21 | 1.55 | 0.54 |
| 1:D:450:ILE:O | 1:D:455:VAL:HG13 | 2.07 | 0.54 |
| 1:C:897:TYR:CE1 | 1:C:901:MET:CE | 2.90 | 0.54 |
| 1:G:931:GLU:H | 1:G:931:GLU:CD | 2.11 | 0.54 |
| 1:B:700:ILE:O | 1:B:704:VAL:HG13 | 2.06 | 0.54 |
| 1:B:749:HIS:HA | 1:B:752:MET:HG2 | 1.89 | 0.54 |
| 1:D:609:PHE:CG | 1:D:618:LEU:HD22 | 2.43 | 0.54 |
| 1:B:404:VAL:CG2 | 1:B:557:ILE:HD13 | 2.37 | 0.54 |
| 1:G:785:SER:HB3 | 1:G:890:ILE:HD12 | 1.90 | 0.54 |
| 1:H:1044:LYS:NZ | 1:H:1081:ASN:HD21 | 2.06 | 0.54 |
| 1:F:437:GLN:HG3 | 1:F:668:ALA:HB1 | 1.89 | 0.53 |
| 1:G:739:GLY:HA3 | 1:G:1100:ARG:HB2 | 1.90 | 0.53 |
| 1:B:609:PHE:CD2 | 1:B:618:LEU:HD22 | 2.43 | 0.53 |
| 1:E:416:PHE:HA | 1:E:662:MET:HE1 | 1.91 | 0.53 |
| 1:H:937:CYS:O | 1:H:942:LYS:NZ | 2.41 | 0.53 |
| 1:A:609:PHE:HB3 | 1:A:618:LEU:HD21 | 1.91 | 0.53 |
| 1:B:404:VAL:HG23 | 1:B:557:ILE:HD13 | 1.89 | 0.53 |
| 1:C:697:THR:HG22 | 1:C:701:MET:CE | 2.39 | 0.53 |
| 1:E:1073:GLN:HE22 | 1:E:1075:GLN:NE2 | 2.06 | 0.53 |
| 1:H:962:GLU:OE1 | 1:H:977:HIS:HD2 | 1.91 | 0.53 |
| 1:C:1075:GLN:HE22 | 1:C:1100:ARG:HH21 | 1.57 | 0.53 |
| 1:A:749:HIS:HA | 1:A:752:MET:HG2 | 1.90 | 0.53 |
| 1:F:850:GLN:OE1 | 1:F:971:LEU:HB2 | 2.09 | 0.53 |
| 1:B:399:ASP:O | 1:B:400:ASP:HB2 | 2.08 | 0.53 |
| 1:D:437:GLN:HE22 | 1:D:1112:CYS:H | 1.57 | 0.53 |
| 1:A:432:MET:HA | 1:A:435:ARG:HD3 | 1.90 | 0.53 |
| 1:A:434:THR:HB | 3:A:2062:HOH:O | 2.09 | 0.53 |
| 1:B:979:THR:HG21 | 1:B:1009:ILE:CG2 | 2.39 | 0.53 |
| 1:A:395:ILE:CD1 | 1:A:556:ARG:CZ | 2.87 | 0.53 |
| 1:H:428:GLU:HA | 1:H:431:THR:HG22 | 1.91 | 0.53 |
| 1:H:790:GLN:HG2 | 1:H:792:PRO:HD2 | 1.90 | 0.53 |
| 1:F:445:ALA:O | 1:F:449:THR:HG22 | 2.09 | 0.53 |
| 1:G:749:HIS:HA | 1:G:752:MET:HG2 | 1.90 | 0.53 |
| 1:H:966:ARG:HH11 | 1:H:974:THR:HG23 | 1.74 | 0.53 |
| 1:B:823:THR:HG22 | 1:B:826:GLU:H | 1.74 | 0.52 |
| 1:D:850:GLN:HB3 | 1:D:971:LEU:HD22 | 1.92 | 0.52 |
| 1:A:497:GLY:H | 1:A:615:GLN:NE2 | 2.07 | 0.52 |
| 1:C:828:ASP:OD2 | 1:C:832:LYS:HE2 | 2.09 | 0.52 |
| 1:A:1075:GLN:NE2 | 1:A:1100:ARG:HH21 | 2.07 | 0.52 |
| 1:E:476:VAL:HG12 | 1:E:841:LEU:HD12 | 1.90 | 0.52 |
| 1:G:1044:LYS:NZ | 1:G:1081:ASN:HD21 | 2.07 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:557:ILE:HD11 | 1:B:584:ASN:CG | 2.30 | 0.52 |
| 1:F:449:THR:HG21 | 3:F:2021:HOH:O | 2.09 | 0.52 |
| 1:H:505:VAL:O | 1:H:509:THR:HG21 | 2.10 | 0.52 |
| 1:B:426:ARG:HD2 | 1:B:426:ARG:C | 2.30 | 0.52 |
| 1:B:979:THR:CG2 | 1:B:1009:ILE:HG23 | 2.40 | 0.52 |
| 1:F:750:ILE:CD1 | 1:F:764:ARG:HA | 2.40 | 0.52 |
| 1:G:700:ILE:O | 1:G:704:VAL:HG13 | 2.10 | 0.52 |
| 1:F:1048:GLY:HA2 | 1:F:1051:ASP:OD2 | 2.10 | 0.52 |
| 1:H:634:ASP:OD1 | 1:H:639:ARG:NH1 | 2.39 | 0.52 |
| 1:C:902:ALA:HB1 | 1:C:950:VAL:HG12 | 1.89 | 0.52 |
| 1:C:1074:MET:HE2 | 3:C:2280:HOH:O | 2.10 | 0.52 |
| 1:F:915:THR:HG21 | 3:F:2117:HOH:O | 2.09 | 0.52 |
| 1:A:933:LEU:C | 1:A:933:LEU:HD23 | 2.31 | 0.51 |
| 1:F:395:ILE:CD1 | 1:F:556:ARG:HB3 | 2.41 | 0.51 |
| 1:B:491:HIS:O | 1:B:853:HIS:HE1 | 1.94 | 0.51 |
| 1:E:966:ARG:HH11 | 1:E:974:THR:CG2 | 2.24 | 0.51 |
| 1:F:609:PHE:CG | 1:F:618:LEU:HD22 | 2.46 | 0.51 |
| 1:H:615:GLN:HG3 | 1:H:618:LEU:HD11 | 1.93 | 0.51 |
| 1:F:483:THR:HB | 1:F:804:MET:CE | 2.41 | 0.51 |
| 1:G:498:ASP:OD1 | 2:G:2000:CHT:H61 | 2.11 | 0.51 |
| 1:C:823:THR:HG22 | 1:C:825:ASP:H | 1.76 | 0.51 |
| 1:A:428:GLU:O | 1:A:432:MET:HB2 | 2.11 | 0.51 |
| 1:C:403:ILE:HG22 | 1:C:655:LYS:HG3 | 1.92 | 0.51 |
| 1:E:1099:VAL:HG11 | 1:E:1108:PHE:HD1 | 1.76 | 0.51 |
| 1:G:1009:ILE:HD11 | 1:G:1035:MET:HE2 | 1.92 | 0.51 |
| 1:G:632:GLU:OE2 | 1:G:636:ARG:NH1 | 2.44 | 0.51 |
| 1:G:854:ARG:HB2 | 1:G:877:ALA:O | 2.11 | 0.51 |
| 1:G:1009:ILE:CB | 3:G:2130:HOH:O | 2.59 | 0.51 |
| 1:F:920:ARG:NH1 | 1:F:921:ASP:OD1 | 2.43 | 0.50 |
| 1:A:897:TYR:CZ | 1:A:901:MET:CE | 2.94 | 0.50 |
| 1:C:797:PHE:HB2 | 1:C:834:GLN:HG2 | 1.93 | 0.50 |
| 1:F:965:CYS:O | 1:F:975:LEU:HB3 | 2.11 | 0.50 |
| 1:D:609:PHE:CD2 | 1:D:618:LEU:HD22 | 2.46 | 0.50 |
| 1:H:759:ASP:HB3 | 3:H:2134:HOH:O | 2.11 | 0.50 |
| 1:E:468:GLU:O | 1:E:472:ARG:HG2 | 2.11 | 0.50 |
| 1:B:948:ASN:HD22 | 1:B:1029:LYS:HE2 | 1.76 | 0.50 |
| 1:F:1041:HIS:HD2 | 3:F:2150:HOH:O | 1.93 | 0.50 |
| 1:H:497:GLY:N | 1:H:615:GLN:HE21 | 2.01 | 0.50 |
| 1:C:915:THR:HG22 | 1:C:918:GLN:OE1 | 2.11 | 0.50 |
| 1:F:497:GLY:N | 1:F:615:GLN:HE21 | 2.07 | 0.50 |
| 1:B:553:TYR:O | 1:B:557:ILE:HG23 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:759:ASP:HB3 | 3:B:2191:HOH:O | 2.12 | 0.50 |
| 1:H:348:ARG:NH2 | 1:H:1096:ASP:OD2 | 2.44 | 0.50 |
| 1:C:609:PHE:CG | 1:C:618:LEU:HD22 | 2.46 | 0.49 |
| 1:E:848:ILE:O | 1:E:852:VAL:HG13 | 2.11 | 0.49 |
| 1:B:632:GLU:OE1 | 1:B:636:ARG:NH2 | 2.44 | 0.49 |
| 1:D:832:LYS:HB3 | 1:D:960:TRP:CZ2 | 2.46 | 0.49 |
| 1:E:336:VAL:HA | 1:E:345:GLN:HG3 | 1.94 | 0.49 |
| 1:A:434:THR:HG22 | 3:A:2066:HOH:O | 2.13 | 0.49 |
| 1:C:432:MET:HE3 | 1:C:440:PHE:HB2 | 1.95 | 0.49 |
| 1:C:848:ILE:O | 1:C:852:VAL:HG13 | 2.12 | 0.49 |
| 1:F:1024:ILE:HD11 | 1:F:1074:MET:CE | 2.43 | 0.49 |
| 1:G:720:ASN:ND2 | 1:G:1067:SER:OG | 2.45 | 0.49 |
| 1:H:984:ASN:C | 1:H:984:ASN:ND2 | 2.64 | 0.49 |
| 1:E:730:ILE:O | 1:E:734:VAL:HG23 | 2.12 | 0.49 |
| 1:G:1009:ILE:HG13 | 3:G:2130:HOH:O | 2.12 | 0.49 |
| 1:C:920:ARG:HG3 | 1:C:921:ASP:N | 2.28 | 0.49 |
| 1:D:491:HIS:O | 1:D:853:HIS:HE1 | 1.96 | 0.49 |
| 1:C:1075:GLN:NE2 | 1:C:1100:ARG:HH21 | 2.11 | 0.49 |
| 1:F:449:THR:CG2 | 3:F:2021:HOH:O | 2.61 | 0.49 |
| 1:F:497:GLY:H | 1:F:615:GLN:NE2 | 2.08 | 0.49 |
| 1:F:1074:MET:CE | 3:F:2148:HOH:O | 2.60 | 0.49 |
| 1:G:1075:GLN:NE2 | 1:G:1100:ARG:HH21 | 2.10 | 0.49 |
| 1:A:986:THR:HB | 1:A:987:PRO:CD | 2.42 | 0.49 |
| 1:C:850:GLN:HB3 | 1:C:971:LEU:HD22 | 1.93 | 0.49 |
| 1:D:598:ALA:HB2 | 1:D:630:MET:HE3 | 1.95 | 0.49 |
| 1:F:748:SER:O | 1:F:752:MET:HG2 | 2.12 | 0.49 |
| 1:G:497:GLY:N | 1:G:615:GLN:HE21 | 2.07 | 0.49 |
| 1:H:649:LEU:O | 1:H:653:ILE:HG12 | 2.12 | 0.49 |
| 1:A:771:CYS:SG | 2:A:2000:CHT:HC42 | 2.53 | 0.49 |
| 1:B:1088:GLN:HG2 | 1:B:1116:GLN:OE1 | 2.13 | 0.49 |
| 1:D:919:ILE:O | 1:D:923:LEU:HG | 2.13 | 0.49 |
| 1:F:912:LYS:O | 1:F:912:LYS:HD3 | 2.13 | 0.49 |
| 1:B:942:LYS:CG | 1:B:1015:ALA:HB1 | 2.43 | 0.48 |
| 1:E:966:ARG:HH11 | 1:E:974:THR:HG22 | 1.78 | 0.48 |
| 1:G:745:PHE:HZ | 1:G:1074:MET:HE3 | 1.77 | 0.48 |
| 1:A:1080:ASP:HB3 | 1:A:1083:VAL:HG23 | 1.93 | 0.48 |
| 1:D:1052:THR:HG23 | 1:D:1054:GLU:CD | 2.33 | 0.48 |
| 1:B:744:HIS:CD2 | 1:B:749:HIS:CE1 | 3.00 | 0.48 |
| 1:C:897:TYR:CE1 | 1:C:901:MET:HE1 | 2.48 | 0.48 |
| 1:D:700:ILE:O | 1:D:704:VAL:HG13 | 2.13 | 0.48 |
| 1:D:747:ASP:O | 1:D:751:LYS:HG2 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:691:ASP:OD1 | 1:G:719:HIS:HE1 | 1.95 | 0.48 |
| 1:G:745:PHE:CZ | 1:G:1074:MET:CE | 2.96 | 0.48 |
| 1:B:993:ASN:O | 1:B:999:ARG:NH2 | 2.47 | 0.48 |
| 1:E:739:GLY:HA3 | 1:E:1100:ARG:HB2 | 1.95 | 0.48 |
| 1:E:946:ASP:OD1 | 1:E:1029:LYS:NZ | 2.45 | 0.48 |
| 1:B:857:ALA:O | 1:B:859:LYS:NZ | 2.46 | 0.48 |
| 1:C:853:HIS:HD2 | 1:C:859:LYS:NZ | 2.12 | 0.48 |
| 1:C:915:THR:HG23 | 1:C:918:GLN:H | 1.78 | 0.48 |
| 1:C:1073:GLN:HE22 | 1:C:1075:GLN:NE2 | 2.10 | 0.48 |
| 1:E:669:LYS:O | 1:E:983:SER:OG | 2.31 | 0.48 |
| 1:H:797:PHE:HB2 | 1:H:834:GLN:HG2 | 1.94 | 0.48 |
| 1:A:850:GLN:HB3 | 1:A:971:LEU:HD22 | 1.94 | 0.48 |
| 1:E:942:LYS:C | 1:E:950:VAL:HG11 | 2.34 | 0.48 |
| 1:F:1075:GLN:HE22 | 1:F:1100:ARG:HH21 | 1.60 | 0.48 |
| 1:C:1016:ASP:OD2 | 1:C:1123:THR:HG21 | 2.14 | 0.48 |
| 1:E:500:CYS:H | 1:E:775:GLN:HE22 | 1.62 | 0.48 |
| 1:B:962:GLU:OE1 | 1:B:977:HIS:HD2 | 1.96 | 0.48 |
| 1:C:395:ILE:CD1 | 1:C:556:ARG:HB3 | 2.44 | 0.48 |
| 1:C:962:GLU:OE1 | 1:C:977:HIS:HD2 | 1.97 | 0.47 |
| 1:H:680:LEU:HD23 | 1:H:680:LEU:C | 2.34 | 0.47 |
| 1:E:419:ASP:OD1 | 1:E:419:ASP:N | 2.46 | 0.47 |
| 1:A:966:ARG:HH11 | 1:A:974:THR:CG2 | 2.23 | 0.47 |
| 1:H:1087:ALA:HA | 1:H:1094:TYR:CD2 | 2.49 | 0.47 |
| 1:B:406:HIS:HD2 | 1:B:408:CYS:H | 1.62 | 0.47 |
| 1:C:570:ASN:O | 1:C:574:ARG:HB2 | 2.14 | 0.47 |
| 1:B:785:SER:OG | 1:B:787:GLY:O | 2.33 | 0.47 |
| 1:G:739:GLY:HA3 | 1:G:1100:ARG:HD3 | 1.97 | 0.47 |
| 1:G:1009:ILE:HG21 | 3:G:2130:HOH:O | 2.14 | 0.47 |
| 1:H:419:ASP:N | 1:H:419:ASP:OD1 | 2.47 | 0.47 |
| 1:E:428:GLU:OE1 | 1:E:435:ARG:NH1 | 2.47 | 0.47 |
| 1:F:1066:ALA:HB2 | 1:F:1074:MET:HE1 | 1.96 | 0.47 |
| 1:G:628:TYR:N | 1:G:629:PRO:CD | 2.77 | 0.47 |
| 1:A:748:SER:O | 1:A:752:MET:HG2 | 2.15 | 0.47 |
| 1:A:799:LEU:HA | 1:A:818:LEU:HD21 | 1.97 | 0.47 |
| 1:B:358:VAL:CG2 | 1:B:432:MET:HE3 | 2.44 | 0.47 |
| 1:F:1080:ASP:HB3 | 1:F:1083:VAL:HG23 | 1.96 | 0.47 |
| 1:G:371:LYS:O | 1:G:374:PRO:HD3 | 2.14 | 0.47 |
| 1:H:756:LYS:NZ | 1:H:782:GLN:HE22 | 2.12 | 0.47 |
| 1:A:1044:LYS:NZ | 1:A:1119:ILE:O | 2.48 | 0.47 |
| 1:D:745:PHE:CZ | 1:D:1074:MET:CE | 2.98 | 0.47 |
| 1:D:979:THR:HG21 | 1:D:1035:MET:SD | 2.55 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:653:ILE:HG23 | 1:D:712:PRO:HD2 | 1.97 | 0.47 |
| 1:G:438:ASP:HA | 1:G:674:TYR:CZ | 2.50 | 0.47 |
| 1:G:745:PHE:HZ | 1:G:1074:MET:CE | 2.28 | 0.47 |
| 1:F:352:LEU:O | 1:F:1095:ARG:NH1 | 2.47 | 0.47 |
| 1:A:962:GLU:OE1 | 1:A:977:HIS:HD2 | 1.98 | 0.46 |
| 1:F:744:HIS:HD2 | 1:F:749:HIS:CE1 | 2.33 | 0.46 |
| 1:G:491:HIS:O | 1:G:853:HIS:HE1 | 1.97 | 0.46 |
| 1:B:649:LEU:O | 1:B:653:ILE:HG12 | 2.14 | 0.46 |
| 1:C:450:ILE:O | 1:C:455:VAL:HG13 | 2.15 | 0.46 |
| 1:C:627:CYS:HA | 1:C:630:MET:HE2 | 1.97 | 0.46 |
| 1:D:965:CYS:HB3 | 1:D:975:LEU:HB3 | 1.96 | 0.46 |
| 1:F:633:ALA:O | 1:F:637:GLU:HG2 | 2.15 | 0.46 |
| 1:A:432:MET:HE1 | 1:A:442:ILE:HB | 1.96 | 0.46 |
| 1:C:343:ARG:NH2 | 1:C:576:GLU:OE2 | 2.46 | 0.46 |
| 1:C:759:ASP:HB3 | 3:C:2177:HOH:O | 2.14 | 0.46 |
| 1:D:627:CYS:HA | 1:D:630:MET:HE2 | 1.96 | 0.46 |
| 1:G:900:SER:HB2 | 1:G:996:PRO:HD2 | 1.98 | 0.46 |
| 1:A:399:ASP:O | 1:A:400:ASP:HB2 | 2.15 | 0.46 |
| 1:C:694:ASN:O | 1:C:697:THR:HB | 2.15 | 0.46 |
| 2:C:2000:CHT:H82 | 2:C:2000:CHT:O6 | 2.16 | 0.46 |
| 1:D:376:MET:CE | 1:D:380:LEU:HG | 2.39 | 0.46 |
| 1:D:1112:CYS:O | 1:D:1116:GLN:HG3 | 2.16 | 0.46 |
| 1:E:384:LYS:NZ | 1:E:545:GLU:OE2 | 2.37 | 0.46 |
| 1:G:348:ARG:NH2 | 1:G:1096:ASP:OD2 | 2.49 | 0.46 |
| 1:A:480:SER:HB3 | 1:A:488:LEU:HD22 | 1.97 | 0.46 |
| 1:D:926:ASN:HD21 | 1:D:1001:ALA:H | 1.64 | 0.46 |
| 1:F:367:THR:O | 1:F:371:LYS:HB2 | 2.15 | 0.46 |
| 1:F:406:HIS:HD2 | 1:F:408:CYS:H | 1.64 | 0.46 |
| 1:A:902:ALA:HB2 | 1:A:950:VAL:HG23 | 1.97 | 0.46 |
| 1:D:639:ARG:O | 1:D:640:LEU:HD23 | 2.15 | 0.46 |
| 1:F:749:HIS:HA | 1:F:752:MET:CG | 2.46 | 0.46 |
| 1:H:1086:LYS:HA | 1:H:1086:LYS:HE2 | 1.97 | 0.46 |
| 1:A:867:GLU:HB2 | 1:A:882:MET:CE | 2.46 | 0.46 |
| 1:B:966:ARG:HH11 | 1:B:974:THR:HG22 | 1.79 | 0.46 |
| 1:D:959:GLU:CG | 3:D:2252:HOH:O | 2.64 | 0.46 |
| 1:B:951:ASP:OD2 | 1:B:1026:SER:OG | 2.25 | 0.46 |
| 1:C:697:THR:HG22 | 1:C:701:MET:HE2 | 1.98 | 0.46 |
| 1:E:948:ASN:O | 1:E:949:TYR:C | 2.54 | 0.46 |
| 1:H:905:ARG:NH1 | 1:H:910:GLU:OE2 | 2.48 | 0.46 |
| 1:A:346:ARG:NH1 | 1:A:400:ASP:OD1 | 2.50 | 0.46 |
| 1:C:609:PHE:CD2 | 1:C:618:LEU:HD22 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:627:CYS:HA | 1:F:630:MET:HE2 | 1.97 | 0.46 |
| 1:B:848:ILE:O | 1:B:852:VAL:HG13 | 2.16 | 0.45 |
| 1:F:1074:MET:HE2 | 3:F:2148:HOH:O | 2.16 | 0.45 |
| 1:A:406:HIS:HE1 | 1:A:658:GLU:O | 1.98 | 0.45 |
| 1:B:527:SER:HB2 | 3:B:2089:HOH:O | 2.16 | 0.45 |
| 1:D:406:HIS:HE1 | 1:D:658:GLU:O | 2.00 | 0.45 |
| 1:E:527:SER:OG | 1:E:529:GLU:HG2 | 2.17 | 0.45 |
| 1:E:805:VAL:HG13 | 1:E:806:LEU:N | 2.32 | 0.45 |
| 1:H:984:ASN:HD22 | 1:H:985:ASN:N | 2.14 | 0.45 |
| 1:B:790:GLN:HE21 | 1:B:792:PRO:HB2 | 1.81 | 0.45 |
| 1:D:336:VAL:HA | 1:D:345:GLN:HG3 | 1.97 | 0.45 |
| 1:F:487:ASP:O | 1:F:787:GLY:HA2 | 2.16 | 0.45 |
| 1:A:542:ALA:O | 1:A:546:THR:CG2 | 2.64 | 0.45 |
| 1:C:393:ALA:O | 1:C:556:ARG:NH2 | 2.50 | 0.45 |
| 1:D:1041:HIS:CD2 | 3:D:2294:HOH:O | 2.68 | 0.45 |
| 1:F:623:VAL:HG22 | 1:F:680:LEU:HD21 | 1.98 | 0.45 |
| 1:D:745:PHE:CE2 | 1:D:1074:MET:HE2 | 2.52 | 0.45 |
| 1:H:958:THR:CG2 | 3:H:2174:HOH:O | 2.64 | 0.45 |
| 1:D:1052:THR:HG22 | 1:D:1055:GLY:H | 1.80 | 0.45 |
| 1:B:979:THR:HG23 | 1:B:1009:ILE:HG23 | 1.99 | 0.45 |
| 1:D:510:LYS:HE2 | 3:D:2096:HOH:O | 2.16 | 0.45 |
| 1:D:623:VAL:CG2 | 1:D:680:LEU:HD21 | 2.46 | 0.45 |
| 1:E:823:THR:HG22 | 1:E:826:GLU:H | 1.80 | 0.45 |
| 1:D:420:ILE:HD13 | 1:D:613:GLU:HB2 | 1.98 | 0.45 |
| 1:B:790:GLN:CG | 1:B:792:PRO:HD2 | 2.47 | 0.45 |
| 1:B:853:HIS:HD2 | 1:B:859:LYS:NZ | 2.15 | 0.45 |
| 1:H:853:HIS:HD2 | 1:H:859:LYS:HZ1 | 1.64 | 0.45 |
| 1:H:926:ASN:O | 1:H:927:PHE:HB2 | 2.16 | 0.45 |
| 1:A:749:HIS:HA | 1:A:752:MET:CG | 2.47 | 0.45 |
| 1:B:756:LYS:NZ | 1:B:782:GLN:HE22 | 2.14 | 0.45 |
| 1:B:790:GLN:NE2 | 1:B:793:ILE:N | 2.65 | 0.45 |
| 1:C:494:ASN:ND2 | 1:C:661:TRP:HE1 | 2.15 | 0.45 |
| 1:E:508:PHE:O | 1:E:591:PRO:HB3 | 2.17 | 0.45 |
| 1:G:1075:GLN:HE22 | 1:G:1103:GLY:HA2 | 1.82 | 0.45 |
| 1:C:497:GLY:H | 1:C:615:GLN:NE2 | 2.15 | 0.44 |
| 1:G:999:ARG:CG | 1:G:999:ARG:HH11 | 2.30 | 0.44 |
| 1:H:986:THR:HB | 1:H:987:PRO:CD | 2.46 | 0.44 |
| 1:A:504:ASP:OD2 | 1:A:776:LYS:NZ | 2.49 | 0.44 |
| 1:B:790:GLN:NE2 | 1:B:793:ILE:H | 2.14 | 0.44 |
| 1:E:680:LEU:C | 1:E:680:LEU:HD23 | 2.37 | 0.44 |
| 1:F:1041:HIS:HE1 | 3:F:2141:HOH:O | 2.00 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:1075:GLN:NE2 | 1:F:1100:ARG:HH21 | 2.14 | 0.44 |
| 1:G:695:ASP:O | 1:G:699:LEU:HD12 | 2.16 | 0.44 |
| 1:H:455:VAL:O | 1:H:456:PRO:C | 2.54 | 0.44 |
| 1:H:828:ASP:O | 1:H:832:LYS:HG2 | 2.16 | 0.44 |
| 1:G:984:ASN:OD1 | 1:G:984:ASN:C | 2.56 | 0.44 |
| 1:E:426:ARG:HD2 | 1:E:426:ARG:C | 2.37 | 0.44 |
| 1:E:986:THR:HB | 1:E:987:PRO:HD3 | 2.00 | 0.44 |
| 1:D:885:HIS:HA | 1:D:973:SER:OG | 2.17 | 0.44 |
| 1:E:422:TRP:CZ2 | 1:E:459:GLU:HB2 | 2.52 | 0.44 |
| 1:E:986:THR:HB | 1:E:987:PRO:CD | 2.48 | 0.44 |
| 1:H:744:HIS:HD2 | 1:H:749:HIS:CE1 | 2.35 | 0.44 |
| 1:C:616:THR:HB | 1:C:661:TRP:CG | 2.52 | 0.44 |
| 1:D:744:HIS:HD2 | 1:D:749:HIS:CE1 | 2.35 | 0.44 |
| 1:F:376:MET:HE1 | 1:F:380:LEU:HG | 1.98 | 0.44 |
| 1:B:348:ARG:NH2 | 1:B:1096:ASP:OD2 | 2.51 | 0.44 |
| 1:B:470:GLN:NE2 | 3:B:2059:HOH:O | 2.50 | 0.44 |
| 1:C:350:HIS:O | 1:C:353:THR:HB | 2.17 | 0.44 |
| 1:C:1041:HIS:HD2 | 3:C:2281:HOH:O | 2.00 | 0.44 |
| 1:C:1081:ASN:O | 1:C:1085:LYS:HG3 | 2.17 | 0.44 |
| 1:F:897:TYR:CE2 | 1:F:901:MET:CE | 3.01 | 0.44 |
| 1:G:745:PHE:CZ | 1:G:1074:MET:HE3 | 2.51 | 0.44 |
| 1:C:455:VAL:N | 1:C:456:PRO:CD | 2.81 | 0.44 |
| 1:D:562:ARG:NH2 | 3:D:2112:HOH:O | 2.50 | 0.44 |
| 1:E:984:ASN:C | 1:E:984:ASN:ND2 | 2.71 | 0.44 |
| 1:F:670:TYR:CD2 | 1:F:984:ASN:HB2 | 2.52 | 0.44 |
| 1:F:1044:LYS:NZ | 1:F:1122:ARG:O | 2.43 | 0.44 |
| 1:C:344:MET:CE | 1:C:654:ILE:CD1 | 2.96 | 0.44 |
| 1:D:680:LEU:HD23 | 1:D:680:LEU:C | 2.38 | 0.44 |
| 1:E:350:HIS:O | 1:E:353:THR:HB | 2.18 | 0.44 |
| 1:H:358:VAL:CG2 | 1:H:432:MET:HE3 | 2.48 | 0.44 |
| 1:D:756:LYS:NZ | 1:D:782:GLN:HE22 | 2.15 | 0.43 |
| 1:F:852:VAL:O | 1:F:856:VAL:HG13 | 2.17 | 0.43 |
| 1:H:806:LEU:HD22 | 1:H:991:LEU:HA | 2.00 | 0.43 |
| 1:A:680:LEU:CD2 | 1:A:682:VAL:HG23 | 2.47 | 0.43 |
| 1:B:828:ASP:OD2 | 1:B:832:LYS:HE2 | 2.18 | 0.43 |
| 1:C:941:PRO:HB2 | 1:C:950:VAL:HG13 | 2.00 | 0.43 |
| 1:D:887:PRO:O | 1:D:975:LEU:HD23 | 2.18 | 0.43 |
| 1:G:419:ASP:OD1 | 1:G:419:ASP:N | 2.51 | 0.43 |
| 1:H:917:GLU:O | 1:H:920:ARG:HG3 | 2.18 | 0.43 |
| 1:D:437:GLN:NE2 | 1:D:1112:CYS:H | 2.16 | 0.43 |
| 1:E:586:ASN:N | 1:E:586:ASN:HD22 | 2.15 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:623:VAL:O | 1:F:627:CYS:HB2 | 2.19 | 0.43 |
| 1:G:1001:ALA:HB1 | 1:G:1002:TRP:CE2 | 2.52 | 0.43 |
| 1:A:817:ASP:OD1 | 1:A:819:ARG:HB2 | 2.18 | 0.43 |
| 1:C:463:LEU:HG | 1:C:852:VAL:HG23 | 2.00 | 0.43 |
| 1:H:500:CYS:H | 1:H:775:GLN:HE22 | 1.65 | 0.43 |
| 1:H:941:PRO:HB2 | 1:H:950:VAL:HG13 | 1.99 | 0.43 |
| 1:A:824:PHE:CD1 | 1:A:905:ARG:HG2 | 2.54 | 0.43 |
| 1:C:529:GLU:OE2 | 1:D:840:ARG:NE | 2.44 | 0.43 |
| 1:A:853:HIS:HD2 | 1:A:859:LYS:NZ | 2.16 | 0.43 |
| 1:A:1075:GLN:HE22 | 1:A:1100:ARG:HH21 | 1.66 | 0.43 |
| 1:B:536:ARG:HD3 | 1:B:872:SER:O | 2.19 | 0.43 |
| 1:B:539:TYR:CD1 | 1:B:539:TYR:C | 2.92 | 0.43 |
| 1:C:343:ARG:HH22 | 1:C:576:GLU:CD | 2.22 | 0.43 |
| 1:C:795:ILE:HD11 | 1:C:901:MET:CE | 2.41 | 0.43 |
| 1:D:348:ARG:NH2 | 1:D:1096:ASP:OD2 | 2.44 | 0.43 |
| 1:D:1075:GLN:NE2 | 1:D:1100:ARG:HH21 | 2.17 | 0.43 |
| 1:E:376:MET:O | 1:E:377:PRO:C | 2.55 | 0.43 |
| 1:E:494:ASN:ND2 | 1:E:661:TRP:HE1 | 2.17 | 0.43 |
| 1:H:902:ALA:HB2 | 1:H:950:VAL:HG12 | 2.01 | 0.43 |
| 1:B:403:ILE:HG22 | 1:B:655:LYS:HG3 | 2.00 | 0.43 |
| 1:E:751:LYS:HG3 | 1:E:1033:GLU:HG2 | 2.00 | 0.43 |
| 1:H:966:ARG:HD3 | 1:H:975:LEU:O | 2.18 | 0.43 |
| 1:A:973:SER:OG | 1:A:974:THR:N | 2.50 | 0.43 |
| 1:F:434:THR:HG22 | 1:F:434:THR:O | 2.19 | 0.43 |
| 1:H:858:PRO:O | 1:H:860:PRO:HD3 | 2.18 | 0.43 |
| 1:B:444:GLU:HG2 | 1:E:563:GLU:OE2 | 2.19 | 0.43 |
| 1:B:937:CYS:O | 1:B:942:LYS:NZ | 2.51 | 0.43 |
| 1:C:691:ASP:OD1 | 1:C:719:HIS:HE1 | 2.01 | 0.43 |
| 1:G:677:PHE:O | 1:G:770:GLY:HA2 | 2.19 | 0.43 |
| 1:H:628:TYR:N | 1:H:629:PRO:CD | 2.81 | 0.43 |
| 1:C:888:GLY:HA2 | 1:C:976:SER:O | 2.18 | 0.42 |
| 1:C:1024:ILE:HG23 | 1:C:1069:LEU:HD12 | 2.01 | 0.42 |
| 1:E:432:MET:HB3 | 1:E:432:MET:HE2 | 1.86 | 0.42 |
| 1:E:439:PRO:HD2 | 1:E:674:TYR:OH | 2.19 | 0.42 |
| 1:F:746:ASP:O | 1:F:750:ILE:CG1 | 2.66 | 0.42 |
| 1:F:1000:LEU:O | 1:F:1003:MET:HB2 | 2.18 | 0.42 |
| 1:G:487:ASP:O | 1:G:787:GLY:HA2 | 2.19 | 0.42 |
| 1:G:957:ILE:HD12 | 1:G:958:THR:H | 1.84 | 0.42 |
| 1:A:1108:PHE:CZ | 1:A:1116:GLN:HB3 | 2.54 | 0.42 |
| 3:A:2065:HOH:O | 1:C:434:THR:HB | 2.19 | 0.42 |
| 1:B:528:MET:HE3 | 1:B:537:ILE:HG21 | 2.00 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:373:ASN:N | 1:C:374:PRO:CD | 2.82 | 0.42 |
| 1:C:807:PHE:O | 1:C:808:ASP:C | 2.56 | 0.42 |
| 1:F:986:THR:HB | 1:F:987:PRO:CD | 2.50 | 0.42 |
| 1:F:1041:HIS:CE1 | 3:F:2141:HOH:O | 2.72 | 0.42 |
| 1:H:749:HIS:HA | 1:H:752:MET:HG2 | 2.00 | 0.42 |
| 1:H:941:PRO:O | 1:H:950:VAL:HG11 | 2.19 | 0.42 |
| 1:F:415:ALA:C | 1:F:662:MET:CE | 2.88 | 0.42 |
| 1:A:491:HIS:O | 1:A:853:HIS:HE1 | 2.02 | 0.42 |
| 1:B:562:ARG:NH1 | 3:B:2112:HOH:O | 2.53 | 0.42 |
| 1:C:432:MET:HE3 | 1:C:432:MET:HB3 | 1.92 | 0.42 |
| 1:C:468:GLU:OE2 | 1:C:472:ARG:NH1 | 2.49 | 0.42 |
| 1:E:1007:ASP:O | 1:E:1010:SER:HB3 | 2.20 | 0.42 |
| 1:F:984:ASN:C | 1:F:984:ASN:OD1 | 2.56 | 0.42 |
| 1:H:623:VAL:HG13 | 1:H:680:LEU:HD21 | 2.01 | 0.42 |
| 1:H:829:ALA:O | 1:H:833:GLN:HG3 | 2.18 | 0.42 |
| 1:H:886:GLY:O | 1:H:973:SER:HB3 | 2.20 | 0.42 |
| 1:A:583:VAL:O | 1:A:587:VAL:HG22 | 2.19 | 0.42 |
| 1:A:850:GLN:CB | 1:A:971:LEU:HD22 | 2.49 | 0.42 |
| 1:C:703:ALA:O | 1:C:707:VAL:HG23 | 2.20 | 0.42 |
| 1:D:500:CYS:N | 1:D:775:GLN:HE22 | 2.15 | 0.42 |
| 1:E:360:ILE:HD12 | 1:E:364:LEU:HD21 | 2.01 | 0.42 |
| 1:E:565:ALA:O | 1:E:574:ARG:HD3 | 2.19 | 0.42 |
| 1:E:728:GLU:OE1 | 1:E:1056:ARG:NE | 2.53 | 0.42 |
| 1:G:1009:ILE:CG1 | 3:G:2130:HOH:O | 2.67 | 0.42 |
| 1:H:590:ASN:HB3 | 1:H:591:PRO:HD2 | 2.01 | 0.42 |
| 1:A:529:GLU:H | 1:A:529:GLU:HG2 | 1.66 | 0.42 |
| 1:C:707:VAL:O | 1:C:708:LYS:C | 2.57 | 0.42 |
| 1:E:878:ALA:HA | 1:E:972:TYR:OH | 2.20 | 0.42 |
| 1:E:888:GLY:HA3 | 1:E:1037:ILE:HG13 | 2.01 | 0.42 |
| 1:H:919:ILE:O | 1:H:923:LEU:HG | 2.19 | 0.42 |
| 1:H:986:THR:HB | 1:H:987:PRO:HD3 | 2.02 | 0.42 |
| 1:E:769:MET:SD | 1:E:769:MET:C | 2.98 | 0.42 |
| 1:F:888:GLY:HA2 | 1:F:976:SER:O | 2.19 | 0.42 |
| 1:H:376:MET:HB3 | 1:H:381:LEU:HD13 | 2.01 | 0.42 |
| 1:H:803:ARG:HG3 | 1:H:810:TYR:CE2 | 2.54 | 0.42 |
| 1:A:919:ILE:O | 1:A:923:LEU:HG | 2.20 | 0.42 |
| 1:C:797:PHE:HB2 | 1:C:834:GLN:CG | 2.49 | 0.42 |
| 1:F:986:THR:HB | 1:F:987:PRO:HD3 | 2.02 | 0.42 |
| 1:H:422:TRP:CZ2 | 1:H:459:GLU:HA | 2.55 | 0.42 |
| 1:B:500:CYS:H | 1:B:775:GLN:HE22 | 1.66 | 0.42 |
| 1:D:798:VAL:HG23 | 1:D:834:GLN:HG3 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:897:TYR:CD1 | 1:D:957:ILE:HG12 | 2.55 | 0.42 |
| 1:E:348:ARG:NH2 | 1:E:1096:ASP:OD2 | 2.53 | 0.42 |
| 1:E:888:GLY:HA2 | 1:E:976:SER:O | 2.20 | 0.42 |
| 1:G:749:HIS:HA | 1:G:752:MET:CG | 2.50 | 0.42 |
| 1:H:433:SER:HA | 1:H:440:PHE:O | 2.20 | 0.42 |
| 1:A:562:ARG:NH2 | 1:A:585:GLU:OE2 | 2.53 | 0.42 |
| 1:A:986:THR:HB | 1:A:987:PRO:HD3 | 2.01 | 0.42 |
| 1:B:790:GLN:HG3 | 1:B:792:PRO:HD2 | 2.02 | 0.42 |
| 1:B:1047:LYS:HD3 | 1:B:1047:LYS:HA | 1.98 | 0.42 |
| 1:C:678:ILE:H | 1:C:711:GLN:NE2 | 2.18 | 0.42 |
| 1:E:1001:ALA:HB1 | 1:E:1002:TRP:CE2 | 2.55 | 0.42 |
| 1:F:615:GLN:HG3 | 1:F:618:LEU:HD11 | 2.02 | 0.42 |
| 1:C:850:GLN:HE22 | 1:C:970:MET:HB3 | 1.85 | 0.41 |
| 1:D:739:GLY:HA3 | 1:D:1100:ARG:HB2 | 2.01 | 0.41 |
| 1:D:771:CYS:C | 1:D:772:VAL:HG13 | 2.40 | 0.41 |
| 1:D:986:THR:HG21 | 1:D:1115:VAL:HA | 2.02 | 0.41 |
| 1:E:784:THR:O | 1:E:785:SER:HB3 | 2.20 | 0.41 |
| 1:F:570:ASN:OD1 | 1:F:570:ASN:C | 2.56 | 0.41 |
| 1:G:348:ARG:NH2 | 1:G:1096:ASP:OD1 | 2.53 | 0.41 |
| 1:G:919:ILE:O | 1:G:923:LEU:HG | 2.20 | 0.41 |
| 1:H:438:ASP:HA | 1:H:674:TYR:CZ | 2.55 | 0.41 |
| 1:C:410:LYS:HG2 | 1:C:411:PRO:N | 2.33 | 0.41 |
| 1:D:336:VAL:HG13 | 1:D:345:GLN:HG3 | 2.02 | 0.41 |
| 1:E:416:PHE:HA | 1:E:662:MET:CE | 2.49 | 0.41 |
| 1:E:805:VAL:HG13 | 1:E:1002:TRP:HH2 | 1.85 | 0.41 |
| 1:E:1047:LYS:HG3 | 1:E:1080:ASP:HB2 | 2.02 | 0.41 |
| 1:F:831:VAL:O | 1:F:835:ILE:HG13 | 2.19 | 0.41 |
| 1:H:503:TYR:HA | 1:H:507:LEU:HB3 | 2.03 | 0.41 |
| 1:B:966:ARG:HD3 | 1:B:974:THR:HG23 | 2.01 | 0.41 |
| 1:B:979:THR:HG22 | 1:B:1039:MET:HA | 2.02 | 0.41 |
| 1:E:739:GLY:HA2 | 1:E:1076:PHE:O | 2.20 | 0.41 |
| 1:F:360:ILE:HA | 3:F:2007:HOH:O | 2.20 | 0.41 |
| 1:F:979:THR:O | 1:F:979:THR:HG23 | 2.21 | 0.41 |
| 1:G:748:SER:O | 1:G:752:MET:HG2 | 2.20 | 0.41 |
| 1:H:609:PHE:CG | 1:H:618:LEU:HD22 | 2.55 | 0.41 |
| 1:A:768:LEU:HD22 | 1:A:768:LEU:N | 2.36 | 0.41 |
| 1:D:937:CYS:O | 1:D:942:LYS:NZ | 2.54 | 0.41 |
| 1:H:462:SER:OG | 1:H:465:GLU:HG3 | 2.20 | 0.41 |
| 1:H:627:CYS:HA | 1:H:630:MET:HE1 | 2.01 | 0.41 |
| 1:C:634:ASP:OD1 | 1:C:639:ARG:NH2 | 2.52 | 0.41 |
| 1:C:853:HIS:HD2 | 1:C:859:LYS:HZ1 | 1.66 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:497:GLY:H | 1:G:615:GLN:NE2 | 2.09 | 0.41 |
| 1:H:567:LYS:HG3 | 1:H:567:LYS:O | 2.19 | 0.41 |
| 1:H:793:ILE:HG12 | 1:H:797:PHE:CZ | 2.55 | 0.41 |
| 1:A:653:ILE:HG23 | 1:A:712:PRO:HD2 | 2.02 | 0.41 |
| 1:C:926:ASN:ND2 | 1:C:1001:ALA:H | 2.19 | 0.41 |
| 1:G:351:TYR:O | 1:G:354:VAL:HG12 | 2.20 | 0.41 |
| 1:G:500:CYS:H | 1:G:775:GLN:HE22 | 1.67 | 0.41 |
| 1:H:818:LEU:HD23 | 1:H:916:LEU:HB3 | 2.01 | 0.41 |
| 1:H:1044:LYS:HZ2 | 1:H:1081:ASN:HD21 | 1.69 | 0.41 |
| 1:A:438:ASP:N | 1:A:439:PRO:CD | 2.84 | 0.41 |
| 1:A:500:CYS:H | 1:A:775:GLN:HE22 | 1.69 | 0.41 |
| 1:B:438:ASP:HA | 1:B:674:TYR:CZ | 2.55 | 0.41 |
| 1:A:506:LEU:HD11 | 1:A:867:GLU:HG2 | 2.03 | 0.41 |
| 1:B:815:THR:HG22 | 1:B:833:GLN:HE21 | 1.85 | 0.41 |
| 1:C:882:MET:HG2 | 1:C:883:VAL:HG23 | 2.02 | 0.41 |
| 1:E:450:ILE:O | 1:E:455:VAL:HG13 | 2.20 | 0.41 |
| 1:E:682:VAL:HG11 | 1:E:714:LEU:HD11 | 2.02 | 0.41 |
| 1:G:362:ARG:HD2 | 1:G:611:ILE:O | 2.21 | 0.41 |
| 1:H:1024:ILE:HD12 | 1:H:1074:MET:HE1 | 2.03 | 0.41 |
| 1:A:508:PHE:O | 1:A:591:PRO:HB3 | 2.21 | 0.41 |
| 1:A:846:THR:O | 1:A:850:GLN:HG3 | 2.21 | 0.41 |
| 1:B:1079:VAL:O | 1:B:1079:VAL:HG23 | 2.20 | 0.41 |
| 1:B:1092:GLU:CD | 1:B:1092:GLU:H | 2.24 | 0.41 |
| 1:D:476:VAL:HG23 | 1:D:841:LEU:HB3 | 2.02 | 0.41 |
| 1:F:376:MET:HE1 | 1:F:384:LYS:CE | 2.50 | 0.41 |
| 1:F:393:ALA:O | 1:F:556:ARG:NH2 | 2.54 | 0.41 |
| 1:G:598:ALA:HB2 | 1:G:630:MET:HE3 | 2.03 | 0.41 |
| 1:G:731:VAL:HG22 | 1:G:1059:LEU:HD23 | 2.03 | 0.41 |
| 1:G:853:HIS:HD2 | 1:G:859:LYS:NZ | 2.19 | 0.41 |
| 1:H:926:ASN:HD21 | 1:H:1001:ALA:H | 1.69 | 0.41 |
| 1:A:494:ASN:ND2 | 1:A:661:TRP:HE1 | 2.19 | 0.41 |
| 1:A:623:VAL:HG13 | 1:A:680:LEU:HG | 2.03 | 0.41 |
| 1:C:979:THR:CG2 | 1:C:1039:MET:HA | 2.51 | 0.41 |
| 1:F:499:THR:O | 1:F:501:PRO:HD3 | 2.21 | 0.41 |
| 1:F:739:GLY:HA2 | 1:F:1076:PHE:O | 2.22 | 0.41 |
| 1:B:358:VAL:HG21 | 1:B:432:MET:CE | 2.51 | 0.40 |
| 1:C:699:LEU:HD12 | 1:C:699:LEU:HA | 1.92 | 0.40 |
| 1:C:915:THR:HG22 | 1:C:918:GLN:HG3 | 2.03 | 0.40 |
| 1:D:1052:THR:HG23 | 1:D:1054:GLU:OE1 | 2.21 | 0.40 |
| 1:G:969:LYS:O | 1:G:970:MET:HE2 | 2.21 | 0.40 |
| 1:H:358:VAL:HG21 | 1:H:432:MET:HE1 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:616:THR:OG1 | 1:H:676:PRO:HA | 2.21 | 0.40 |
| 1:A:776:LYS:HD3 | 1:A:776:LYS:C | 2.41 | 0.40 |
| 3:B:2180:HOH:O | 1:C:751:LYS:HE3 | 2.21 | 0.40 |
| 1:C:432:MET:HA | 1:C:435:ARG:HD3 | 2.02 | 0.40 |
| 1:C:708:LYS:HA | 1:C:738:MET:SD | 2.61 | 0.40 |
| 1:C:749:HIS:HA | 1:C:752:MET:CG | 2.51 | 0.40 |
| 1:D:739:GLY:HA2 | 1:D:1076:PHE:O | 2.20 | 0.40 |
| 1:D:1041:HIS:HE1 | 3:D:2277:HOH:O | 2.02 | 0.40 |
| 1:E:434:THR:HG22 | 3:E:2026:HOH:O | 2.22 | 0.40 |
| 1:E:480:SER:O | 1:E:484:PHE:HA | 2.21 | 0.40 |
| 1:G:659:LEU:HD23 | 1:G:678:ILE:HD11 | 2.02 | 0.40 |
| 1:H:700:ILE:O | 1:H:704:VAL:HG23 | 2.21 | 0.40 |
| 1:C:917:GLU:OE1 | 1:C:917:GLU:N | 2.51 | 0.40 |
| 1:C:919:ILE:O | 1:C:923:LEU:HG | 2.21 | 0.40 |
| 1:D:625:GLN:NE2 | 1:D:692:ALA:HB1 | 2.36 | 0.40 |
| 1:F:623:VAL:HA | 1:F:626:TYR:CE1 | 2.56 | 0.40 |
| 1:C:911:GLU:O | 1:C:912:LYS:HB2 | 2.22 | 0.40 |
| 1:D:348:ARG:HD2 | 1:D:707:VAL:O | 2.21 | 0.40 |
| 1:F:376:MET:CE | 1:F:380:LEU:HG | 2.51 | 0.40 |
| 1:F:434:THR:O | 1:F:434:THR:CG2 | 2.69 | 0.40 |
| 1:F:795:ILE:HD11 | 1:F:901:MET:HE2 | 2.03 | 0.40 |
| 1:G:786:THR:HG21 | 1:G:849:SER:OG | 2.22 | 0.40 |
| 1:B:616:THR:HB | 1:B:661:TRP:CG | 2.57 | 0.40 |
| 1:B:943:TYR:O | 1:B:1011:PRO:HB3 | 2.22 | 0.40 |
| 1:E:805:VAL:CG1 | 1:E:806:LEU:N | 2.85 | 0.40 |
| 1:F:703:ALA:O | 1:F:707:VAL:HG23 | 2.21 | 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 | 790/795 (99%) | 761 (96%) | 24 (3%) | 5 (1%) | 25 | 36 |
| 1 | B | 791/795 (100%) | 756 (96%) | 32 (4%) | 3 (0%) | 34 | 48 |
| 1 | C | 791/795 (100%) | 756 (96%) | 33 (4%) | 2 (0%) | 41 | 55 |
| 1 | D | 791/795 (100%) | 761 (96%) | 28 (4%) | 2 (0%) | 41 | 55 |
| 1 | E | 791/795 (100%) | 755 (95%) | 33 (4%) | 3 (0%) | 34 | 48 |
| 1 | F | 791/795 (100%) | 750 (95%) | 36 (5%) | 5 (1%) | 25 | 36 |
| 1 | G | 791/795 (100%) | 760 (96%) | 28 (4%) | 3 (0%) | 34 | 48 |
| 1 | H | 793/795 (100%) | 765 (96%) | 26 (3%) | 2 (0%) | 41 | 55 |
| All | All | 6329/6360 (100%) | 6064 (96%) | 240 (4%) | 25 (0%) | 34 | 48 |

All (25) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 772 | VAL |
| 1 | F | 1112 | CYS |
| 1 | G | 982 | ILE |
| 1 | H | 772 | VAL |
| 1 | A | 435 | ARG |
| 1 | A | 982 | ILE |
| 1 | B | 973 | SER |
| 1 | B | 982 | ILE |
| 1 | C | 982 | ILE |
| 1 | D | 982 | ILE |
| 1 | E | 973 | SER |
| 1 | E | 982 | ILE |
| 1 | F | 982 | ILE |
| 1 | F | 1006 | SER |
| 1 | H | 982 | ILE |
| 1 | A | 772 | VAL |
| 1 | A | 973 | SER |
| 1 | G | 973 | SER |
| 1 | G | 1112 | CYS |
| 1 | F | 973 | SER |
| 1 | B | 772 | VAL |
| 1 | E | 772 | VAL |
| 1 | A | 1101 | VAL |
| 1 | F | 772 | VAL |
| 1 | C | 772 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 668/671 (100%) | 631 (94%) | 37 (6%) | 21 | 35 |
| 1 | B | 669/671 (100%) | 632 (94%) | 37 (6%) | 21 | 35 |
| 1 | C | 669/671 (100%) | 633 (95%) | 36 (5%) | 22 | 36 |
| 1 | D | 669/671 (100%) | 633 (95%) | 36 (5%) | 22 | 36 |
| 1 | E | 669/671 (100%) | 619 (92%) | 50 (8%) | 13 | 21 |
| 1 | F | 669/671 (100%) | 632 (94%) | 37 (6%) | 21 | 35 |
| 1 | G | 669/671 (100%) | 641 (96%) | 28 (4%) | 30 | 47 |
| 1 | H | 671/671 (100%) | 627 (93%) | 44 (7%) | 16 | 26 |
| All | All | 5353/5368 (100%) | 5048 (94%) | 305 (6%) | 20 | 33 |

All (305) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 395 | ILE |
| 1 | A | 434 | THR |
| 1 | A | 488 | LEU |
| 1 | A | 505 | VAL |
| 1 | A | 527 | SER |
| 1 | A | 529 | GLU |
| 1 | A | 532 | GLU |
| 1 | A | 546 | THR |
| 1 | A | 555 | ARG |
| 1 | A | 618 | LEU |
| 1 | A | 707 | VAL |
| 1 | A | 710 | TYR |
| 1 | A | 776 | LYS |
| 1 | A | 790 | GLN |
| 1 | A | 801 | ARG |
| 1 | A | 813 | LEU |
| 1 | A | 819 | ARG |
| 1 | A | 852 | VAL |
| 1 | A | 856 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 866 | VAL |
| 1 | A | 875 | ASP |
| 1 | A | 905 | ARG |
| 1 | A | 906 | LYS |
| 1 | A | 971 | LEU |
| 1 | A | 974 | THR |
| 1 | A | 977 | HIS |
| 1 | A | 980 | LEU |
| 1 | A | 995 | THR |
| 1 | A | 1007 | ASP |
| 1 | A | 1033 | GLU |
| 1 | A | 1041 | HIS |
| 1 | A | 1047 | LYS |
| 1 | A | 1073 | GLN |
| 1 | A | 1090 | GLU |
| 1 | A | 1092 | GLU |
| 1 | A | 1111 | LEU |
| 1 | A | 1116 | GLN |
| 1 | B | 348 | ARG |
| 1 | B | 434 | THR |
| 1 | B | 505 | VAL |
| 1 | B | 529 | GLU |
| 1 | B | 557 | ILE |
| 1 | B | 567 | LYS |
| 1 | B | 572 | GLN |
| 1 | B | 593 | LYS |
| 1 | B | 618 | LEU |
| 1 | B | 625 | GLN |
| 1 | B | 630 | MET |
| 1 | B | 699 | LEU |
| 1 | B | 704 | VAL |
| 1 | B | 710 | TYR |
| 1 | B | 815 | THR |
| 1 | B | 823 | THR |
| 1 | B | 856 | VAL |
| 1 | B | 875 | ASP |
| 1 | B | 901 | MET |
| 1 | B | 904 | ILE |
| 1 | B | 926 | ASN |
| 1 | B | 928 | GLU |
| 1 | B | 971 | LEU |
| 1 | B | 974 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 977 | HIS |
| 1 | B | 979 | THR |
| 1 | B | 980 | LEU |
| 1 | B | 1000 | LEU |
| 1 | B | 1003 | MET |
| 1 | B | 1017 | LYS |
| 1 | B | 1026 | SER |
| 1 | B | 1029 | LYS |
| 1 | B | 1041 | HIS |
| 1 | B | 1092 | GLU |
| 1 | B | 1095 | ARG |
| 1 | B | 1126 | GLU |
| 1 | B | 1127 | LYS |
| 1 | C | 340 | LEU |
| 1 | C | 354 | VAL |
| 1 | C | 423 | ARG |
| 1 | C | 434 | THR |
| 1 | C | 453 | GLU |
| 1 | C | 455 | VAL |
| 1 | C | 476 | VAL |
| 1 | C | 505 | VAL |
| 1 | C | 509 | THR |
| 1 | C | 569 | GLN |
| 1 | C | 618 | LEU |
| 1 | C | 623 | VAL |
| 1 | C | 639 | ARG |
| 1 | C | 707 | VAL |
| 1 | C | 752 | MET |
| 1 | C | 805 | VAL |
| 1 | C | 819 | ARG |
| 1 | C | 875 | ASP |
| 1 | C | 910 | GLU |
| 1 | C | 912 | LYS |
| 1 | C | 920 | ARG |
| 1 | C | 926 | ASN |
| 1 | C | 957 | ILE |
| 1 | C | 963 | LYS |
| 1 | C | 977 | HIS |
| 1 | C | 980 | LEU |
| 1 | C | 1007 | ASP |
| 1 | C | 1029 | LYS |
| 1 | C | 1041 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 1047 | LYS |
| 1 | C | 1064 | ARG |
| 1 | C | 1079 | VAL |
| 1 | C | 1092 | GLU |
| 1 | C | 1095 | ARG |
| 1 | C | 1124 | VAL |
| 1 | C | 1127 | LYS |
| 1 | D | 378 | THR |
| 1 | D | 455 | VAL |
| 1 | D | 485 | VAL |
| 1 | D | 505 | VAL |
| 1 | D | 555 | ARG |
| 1 | D | 567 | LYS |
| 1 | D | 635 | ILE |
| 1 | D | 648 | LEU |
| 1 | D | 704 | VAL |
| 1 | D | 707 | VAL |
| 1 | D | 709 | VAL |
| 1 | D | 710 | TYR |
| 1 | D | 751 | LYS |
| 1 | D | 776 | LYS |
| 1 | D | 790 | GLN |
| 1 | D | 803 | ARG |
| 1 | D | 875 | ASP |
| 1 | D | 904 | ILE |
| 1 | D | 905 | ARG |
| 1 | D | 912 | LYS |
| 1 | D | 924 | LEU |
| 1 | D | 926 | ASN |
| 1 | D | 928 | GLU |
| 1 | D | 931 | GLU |
| 1 | D | 957 | ILE |
| 1 | D | 963 | LYS |
| 1 | D | 971 | LEU |
| 1 | D | 980 | LEU |
| 1 | D | 986 | THR |
| 1 | D | 1009 | ILE |
| 1 | D | 1041 | HIS |
| 1 | D | 1064 | ARG |
| 1 | D | 1092 | GLU |
| 1 | D | 1095 | ARG |
| 1 | D | 1114 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 1127 | LYS |
| 1 | E | 340 | LEU |
| 1 | E | 353 | THR |
| 1 | E | 354 | VAL |
| 1 | E | 368 | GLU |
| 1 | E | 399 | ASP |
| 1 | E | 448 | LYS |
| 1 | E | 482 | GLU |
| 1 | E | 505 | VAL |
| 1 | E | 529 | GLU |
| 1 | E | 569 | GLN |
| 1 | E | 570 | ASN |
| 1 | E | 572 | GLN |
| 1 | E | 574 | ARG |
| 1 | E | 623 | VAL |
| 1 | E | 625 | GLN |
| 1 | E | 639 | ARG |
| 1 | E | 642 | HIS |
| 1 | E | 644 | THR |
| 1 | E | 649 | LEU |
| 1 | E | 653 | ILE |
| 1 | E | 686 | LYS |
| 1 | E | 704 | VAL |
| 1 | E | 710 | TYR |
| 1 | E | 790 | GLN |
| 1 | E | 813 | LEU |
| 1 | E | 815 | THR |
| 1 | E | 823 | THR |
| 1 | E | 852 | VAL |
| 1 | E | 856 | VAL |
| 1 | E | 875 | ASP |
| 1 | E | 905 | ARG |
| 1 | E | 910 | GLU |
| 1 | E | 911 | GLU |
| 1 | E | 919 | ILE |
| 1 | E | 926 | ASN |
| 1 | E | 942 | LYS |
| 1 | E | 957 | ILE |
| 1 | E | 969 | LYS |
| 1 | E | 974 | THR |
| 1 | E | 977 | HIS |
| 1 | E | 980 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 984 | ASN |
| 1 | E | 999 | ARG |
| 1 | E | 1007 | ASP |
| 1 | E | 1010 | SER |
| 1 | E | 1026 | SER |
| 1 | E | 1077 | SER |
| 1 | E | 1081 | ASN |
| 1 | E | 1095 | ARG |
| 1 | E | 1127 | LYS |
| 1 | F | 345 | GLN |
| 1 | F | 353 | THR |
| 1 | F | 371 | LYS |
| 1 | F | 448 | LYS |
| 1 | F | 449 | THR |
| 1 | F | 492 | GLN |
| 1 | F | 632 | GLU |
| 1 | F | 687 | ARG |
| 1 | F | 699 | LEU |
| 1 | F | 704 | VAL |
| 1 | F | 710 | TYR |
| 1 | F | 776 | LYS |
| 1 | F | 793 | ILE |
| 1 | F | 813 | LEU |
| 1 | F | 815 | THR |
| 1 | F | 856 | VAL |
| 1 | F | 875 | ASP |
| 1 | F | 898 | VAL |
| 1 | F | 904 | ILE |
| 1 | F | 905 | ARG |
| 1 | F | 919 | ILE |
| 1 | F | 974 | THR |
| 1 | F | 977 | HIS |
| 1 | F | 979 | THR |
| 1 | F | 980 | LEU |
| 1 | F | 982 | ILE |
| 1 | F | 984 | ASN |
| 1 | F | 999 | ARG |
| 1 | F | 1000 | LEU |
| 1 | F | 1003 | MET |
| 1 | F | 1007 | ASP |
| 1 | F | 1009 | ILE |
| 1 | F | 1041 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 1044 | LYS |
| 1 | F | 1073 | GLN |
| 1 | F | 1093 | LYS |
| 1 | F | 1095 | ARG |
| 1 | G | 378 | THR |
| 1 | G | 516 | LYS |
| 1 | G | 555 | ARG |
| 1 | G | 569 | GLN |
| 1 | G | 593 | LYS |
| 1 | G | 687 | ARG |
| 1 | G | 699 | LEU |
| 1 | G | 704 | VAL |
| 1 | G | 710 | TYR |
| 1 | G | 751 | LYS |
| 1 | G | 801 | ARG |
| 1 | G | 815 | THR |
| 1 | G | 852 | VAL |
| 1 | G | 854 | ARG |
| 1 | G | 866 | VAL |
| 1 | G | 875 | ASP |
| 1 | G | 905 | ARG |
| 1 | G | 920 | ARG |
| 1 | G | 957 | ILE |
| 1 | G | 958 | THR |
| 1 | G | 980 | LEU |
| 1 | G | 999 | ARG |
| 1 | G | 1029 | LYS |
| 1 | G | 1033 | GLU |
| 1 | G | 1047 | LYS |
| 1 | G | 1073 | GLN |
| 1 | G | 1093 | LYS |
| 1 | G | 1095 | ARG |
| 1 | H | 359 | SER |
| 1 | H | 403 | ILE |
| 1 | H | 453 | GLU |
| 1 | H | 476 | VAL |
| 1 | H | 509 | THR |
| 1 | H | 529 | GLU |
| 1 | H | 532 | GLU |
| 1 | H | 557 | ILE |
| 1 | H | 572 | GLN |
| 1 | H | 574 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 593 | LYS |
| 1 | H | 623 | VAL |
| 1 | H | 666 | LEU |
| 1 | H | 709 | VAL |
| 1 | H | 710 | TYR |
| 1 | H | 711 | GLN |
| 1 | H | 776 | LYS |
| 1 | H | 801 | ARG |
| 1 | H | 856 | VAL |
| 1 | H | 874 | LYS |
| 1 | H | 875 | ASP |
| 1 | H | 905 | ARG |
| 1 | H | 920 | ARG |
| 1 | H | 926 | ASN |
| 1 | H | 935 | ARG |
| 1 | H | 950 | VAL |
| 1 | H | 957 | ILE |
| 1 | H | 958 | THR |
| 1 | H | 963 | LYS |
| 1 | H | 979 | THR |
| 1 | H | 980 | LEU |
| 1 | H | 984 | ASN |
| 1 | H | 1000 | LEU |
| 1 | H | 1003 | MET |
| 1 | H | 1013 | GLN |
| 1 | H | 1025 | LYS |
| 1 | H | 1073 | GLN |
| 1 | H | 1081 | ASN |
| 1 | H | 1089 | GLN |
| 1 | H | 1092 | GLU |
| 1 | H | 1095 | ARG |
| 1 | H | 1114 | GLU |
| 1 | H | 1124 | VAL |
| 1 | H | 1127 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 406 | HIS |
| 1 | A | 470 | GLN |
| 1 | A | 492 | GLN |
| 1 | A | 494 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 615 | GLN |
| 1 | A | 642 | HIS |
| 1 | A | 719 | HIS |
| 1 | A | 724 | GLN |
| 1 | A | 744 | HIS |
| 1 | A | 749 | HIS |
| 1 | A | 775 | GLN |
| 1 | A | 790 | GLN |
| 1 | A | 853 | HIS |
| 1 | A | 952 | GLN |
| 1 | A | 977 | HIS |
| 1 | A | 993 | ASN |
| 1 | A | 1041 | HIS |
| 1 | A | 1073 | GLN |
| 1 | A | 1075 | GLN |
| 1 | A | 1081 | ASN |
| 1 | B | 350 | HIS |
| 1 | B | 406 | HIS |
| 1 | B | 470 | GLN |
| 1 | B | 522 | HIS |
| 1 | B | 552 | ASN |
| 1 | B | 586 | ASN |
| 1 | B | 615 | GLN |
| 1 | B | 719 | HIS |
| 1 | B | 744 | HIS |
| 1 | B | 749 | HIS |
| 1 | B | 775 | GLN |
| 1 | B | 782 | GLN |
| 1 | B | 790 | GLN |
| 1 | B | 833 | GLN |
| 1 | B | 853 | HIS |
| 1 | B | 918 | GLN |
| 1 | B | 926 | ASN |
| 1 | B | 948 | ASN |
| 1 | B | 952 | GLN |
| 1 | B | 977 | HIS |
| 1 | C | 406 | HIS |
| 1 | C | 494 | ASN |
| 1 | C | 513 | ASN |
| 1 | C | 522 | HIS |
| 1 | C | 552 | ASN |
| 1 | C | 570 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 586 | ASN |
| 1 | C | 596 | GLN |
| 1 | C | 614 | ASN |
| 1 | C | 615 | GLN |
| 1 | C | 711 | GLN |
| 1 | C | 719 | HIS |
| 1 | C | 744 | HIS |
| 1 | C | 749 | HIS |
| 1 | C | 775 | GLN |
| 1 | C | 850 | GLN |
| 1 | C | 853 | HIS |
| 1 | C | 926 | ASN |
| 1 | C | 977 | HIS |
| 1 | C | 1018 | GLN |
| 1 | C | 1041 | HIS |
| 1 | C | 1075 | GLN |
| 1 | C | 1089 | GLN |
| 1 | D | 345 | GLN |
| 1 | D | 406 | HIS |
| 1 | D | 437 | GLN |
| 1 | D | 470 | GLN |
| 1 | D | 492 | GLN |
| 1 | D | 494 | ASN |
| 1 | D | 552 | ASN |
| 1 | D | 625 | GLN |
| 1 | D | 642 | HIS |
| 1 | D | 711 | GLN |
| 1 | D | 719 | HIS |
| 1 | D | 724 | GLN |
| 1 | D | 744 | HIS |
| 1 | D | 749 | HIS |
| 1 | D | 775 | GLN |
| 1 | D | 782 | GLN |
| 1 | D | 790 | GLN |
| 1 | D | 834 | GLN |
| 1 | D | 853 | HIS |
| 1 | D | 926 | ASN |
| 1 | D | 952 | GLN |
| 1 | D | 977 | HIS |
| 1 | D | 1041 | HIS |
| 1 | D | 1075 | GLN |
| 1 | E | 349 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | E | 406 | HIS |
| 1 | E | 470 | GLN |
| 1 | E | 494 | ASN |
| 1 | E | 522 | HIS |
| 1 | E | 552 | ASN |
| 1 | E | 570 | ASN |
| 1 | E | 572 | GLN |
| 1 | E | 586 | ASN |
| 1 | E | 600 | GLN |
| 1 | E | 625 | GLN |
| 1 | E | 642 | HIS |
| 1 | E | 719 | HIS |
| 1 | E | 744 | HIS |
| 1 | E | 749 | HIS |
| 1 | E | 775 | GLN |
| 1 | E | 790 | GLN |
| 1 | E | 837 | HIS |
| 1 | E | 853 | HIS |
| 1 | E | 926 | ASN |
| 1 | E | 952 | GLN |
| 1 | E | 977 | HIS |
| 1 | E | 984 | ASN |
| 1 | E | 1075 | GLN |
| 1 | E | 1081 | ASN |
| 1 | F | 406 | HIS |
| 1 | F | 552 | ASN |
| 1 | F | 560 | HIS |
| 1 | F | 586 | ASN |
| 1 | F | 600 | GLN |
| 1 | F | 615 | GLN |
| 1 | F | 642 | HIS |
| 1 | F | 719 | HIS |
| 1 | F | 720 | ASN |
| 1 | F | 744 | HIS |
| 1 | F | 749 | HIS |
| 1 | F | 790 | GLN |
| 1 | F | 853 | HIS |
| 1 | F | 926 | ASN |
| 1 | F | 977 | HIS |
| 1 | F | 993 | ASN |
| 1 | F | 1041 | HIS |
| 1 | F | 1073 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | F | 1075 | GLN |
| 1 | F | 1089 | GLN |
| 1 | G | 406 | HIS |
| 1 | G | 437 | GLN |
| 1 | G | 492 | GLN |
| 1 | G | 494 | ASN |
| 1 | G | 552 | ASN |
| 1 | G | 600 | GLN |
| 1 | G | 615 | GLN |
| 1 | G | 625 | GLN |
| 1 | G | 720 | ASN |
| 1 | G | 724 | GLN |
| 1 | G | 744 | HIS |
| 1 | G | 749 | HIS |
| 1 | G | 775 | GLN |
| 1 | G | 782 | GLN |
| 1 | G | 790 | GLN |
| 1 | G | 853 | HIS |
| 1 | G | 939 | ASN |
| 1 | G | 952 | GLN |
| 1 | G | 977 | HIS |
| 1 | G | 1031 | ASN |
| 1 | G | 1081 | ASN |
| 1 | H | 350 | HIS |
| 1 | H | 398 | GLN |
| 1 | H | 406 | HIS |
| 1 | H | 600 | GLN |
| 1 | H | 615 | GLN |
| 1 | H | 711 | GLN |
| 1 | H | 724 | GLN |
| 1 | H | 744 | HIS |
| 1 | H | 749 | HIS |
| 1 | H | 775 | GLN |
| 1 | H | 782 | GLN |
| 1 | H | 853 | HIS |
| 1 | H | 926 | ASN |
| 1 | H | 948 | ASN |
| 1 | H | 977 | HIS |
| 1 | H | 984 | ASN |
| 1 | H | 1013 | GLN |
| 1 | H | 1071 | ASN |
| 1 | H | 1073 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 1075 | GLN |
| 1 | H | 1081 | ASN |
| 1 | H | 1116 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | CHT | E | 2000 | - | 6,6,6 | 0.74 | 0 | 8,8,8 | 0.48 | 0 |
| 2 | CHT | B | 2000 | - | 6,6,6 | 0.74 | 0 | 8,8,8 | 0.47 | 0 |
| 2 | CHT | A | 2000 | - | 6,6,6 | 0.57 | 0 | 8,8,8 | 0.55 | 0 |
| 2 | CHT | D | 2000 | - | 6,6,6 | 1.20 | 0 | 8,8,8 | 1.04 | 0 |
| 2 | CHT | F | 2000 | - | 6,6,6 | 0.65 | 0 | 8,8,8 | 0.81 | 0 |
| 2 | CHT | C | 2000 | - | 6,6,6 | 0.75 | 0 | 8,8,8 | 0.57 | 0 |
| 2 | CHT | H | 2000 | - | 6,6,6 | 0.62 | 0 | 8,8,8 | 0.68 | 0 |
| 2 | CHT | G | 2000 | - | 6,6,6 | 0.68 | 0 | 8,8,8 | 0.78 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | CHT | E | 2000 | - | - | 0/4/4/4 | - |
| 2 | CHT | B | 2000 | - | - | 3/4/4/4 | - |
| 2 | CHT | A | 2000 | - | - | 0/4/4/4 | - |
| 2 | CHT | D | 2000 | - | - | 1/4/4/4 | - |
| 2 | CHT | F | 2000 | - | - | 4/4/4/4 | - |
| 2 | CHT | C | 2000 | - | - | 0/4/4/4 | - |
| 2 | CHT | H | 2000 | - | - | 3/4/4/4 | - |
| 2 | CHT | G | 2000 | - | - | 4/4/4/4 | - |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | D | 2000 | CHT | O6-C4-C5-N1 |
| 2 | F | 2000 | CHT | O6-C4-C5-N1 |
| 2 | H | 2000 | CHT | C4-C5-N1-C6 |
| 2 | H | 2000 | CHT | C4-C5-N1-C7 |
| 2 | H | 2000 | CHT | C4-C5-N1-C8 |
| 2 | G | 2000 | CHT | C4-C5-N1-C6 |
| 2 | G | 2000 | CHT | C4-C5-N1-C8 |
| 2 | F | 2000 | CHT | C4-C5-N1-C8 |
| 2 | F | 2000 | CHT | C4-C5-N1-C6 |
| 2 | F | 2000 | CHT | C4-C5-N1-C7 |
| 2 | G | 2000 | CHT | C4-C5-N1-C7 |
| 2 | G | 2000 | CHT | O6-C4-C5-N1 |
| 2 | B | 2000 | CHT | C4-C5-N1-C6 |
| 2 | B | 2000 | CHT | C4-C5-N1-C8 |
| 2 | B | 2000 | CHT | C4-C5-N1-C7 |

There are no ring outliers.

3 monomers are involved in 4 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | A | 2000 | CHT | 1 | 0 |
| 2 | C | 2000 | CHT | 1 | 0 |
| 2 | G | 2000 | CHT | 2 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 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 | 792/795 (99%) | -0.69 | 0 100 100 | 12, 20, 34, 67 | 0 |
| 1 | B | 793/795 (99%) | -0.67 | 0 100 100 | 15, 24, 39, 59 | 0 |
| 1 | C | 793/795 (99%) | -0.59 | 1 (0%) 95 95 | 13, 24, 42, 73 | 0 |
| 1 | D | 793/795 (99%) | -0.67 | 0 100 100 | 12, 21, 34, 50 | 0 |
| 1 | E | 793/795 (99%) | -0.43 | 1 (0%) 95 95 | 18, 32, 52, 71 | 0 |
| 1 | F | 793/795 (99%) | -0.35 | 9 (1%) 80 79 | 18, 34, 55, 84 | 0 |
| 1 | G | 793/795 (99%) | -0.58 | 0 100 100 | 15, 27, 45, 65 | 0 |
| 1 | H | 795/795 (100%) | -0.56 | 2 (0%) 94 93 | 16, 28, 46, 77 | 0 |
| All | All | 6345/6360 (99%) | -0.57 | 13 (0%) 95 94 | 12, 26, 46, 84 | 0 |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | H | 819 | ARG | 3.1 |
| 1 | F | 561 | ALA | 3.0 |
| 1 | F | 572 | GLN | 2.5 |
| 1 | H | 334 | THR | 2.5 |
| 1 | F | 557 | ILE | 2.4 |
| 1 | F | 404 | VAL | 2.2 |
| 1 | F | 554 | ALA | 2.2 |
| 1 | F | 565 | ALA | 2.2 |
| 1 | F | 579 | THR | 2.2 |
| 1 | F | 558 | ALA | 2.1 |
| 1 | C | 566 | ALA | 2.1 |
| 1 | F | 935 | ARG | 2.1 |
| 1 | E | 805 | VAL | 2.1 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | CHT | F | 2000 | 7/7 | 0.92 | 0.20 | 42,45,47,48 | 0 |
| 2 | CHT | D | 2000 | 7/7 | 0.94 | 0.18 | 25,29,30,33 | 0 |
| 2 | CHT | H | 2000 | 7/7 | 0.95 | 0.14 | 27,30,30,33 | 0 |
| 2 | CHT | E | 2000 | 7/7 | 0.96 | 0.13 | 30,31,32,32 | 0 |
| 2 | CHT | G | 2000 | 7/7 | 0.97 | 0.11 | 24,24,25,27 | 0 |
| 2 | CHT | C | 2000 | 7/7 | 0.97 | 0.11 | 17,18,18,18 | 0 |
| 2 | CHT | A | 2000 | 7/7 | 0.98 | 0.12 | 14,14,15,16 | 0 |
| 2 | CHT | B | 2000 | 7/7 | 0.98 | 0.11 | 19,19,20,20 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.