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

Feb 28, 2014 – 03:47 PM GMT

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|---|---|---|
| PDB ID | : | 1F9W |
| Title | : | CRYSTAL STRUCTURES OF MUTANTS REVEAL A SIGNALLING PATHWAY FOR ACTIVATION OF THE KINESIN MOTOR ATPASE |
| Authors | : | Yun, M.; Zhang, X.; Park, C.G.; Park, H.W.; Endow, S.A. |
| Deposited on | : | 2000-07-11 |
| Resolution | : | 2.50 Å(reported) |

This is a full wwPDB 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/ValidationPDFNotes.html

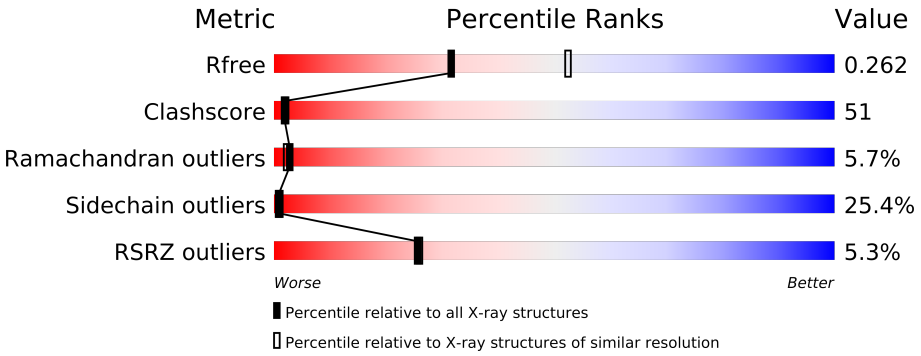
The following versions of software and data (see references) were used in the production of this report:

| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.15 2013 |
| Xtriage (Phenix) | : | dev-1323 |
| EDS | : | stable22639 |
| Percentile statistics | : | 21963 |
| Refmac | : | 5.8.0049 |
| CCP4 | : | 6.3.0 (Settle) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et. al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | stable22683 |

# 1 Overall quality at a glance

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)) |
|---|---|---|
| $R_{free}$ | 66092 | 2784 (2.50-2.50) |
| Clashscore | 79885 | 3562 (2.50-2.50) |
| Ramachandran outliers | 78287 | 3480 (2.50-2.50) |
| Sidechain outliers | 78261 | 3482 (2.50-2.50) |
| RSRZ outliers | 66119 | 2785 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 347 | |
| 1 | B | 347 | |

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4935 atoms, of which 0 are hydrogen and 0 are deuterium.

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 KINESIN-LIKE PROTEIN KAR3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2372 | 1487 | 415 | 461 | 9 | | | |
| 1 | B | 300 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2372 | 1487 | 415 | 461 | 9 | | | |

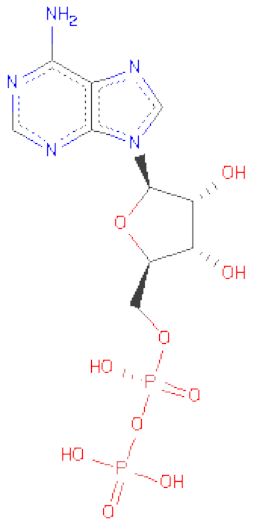
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 383 | MET | LYS | ENGINEERED | UNP P17119 |
| A | 631 | ALA | GLU | ENGINEERED | UNP P17119 |
| B | 383 | MET | LYS | ENGINEERED | UNP P17119 |
| B | 631 | ALA | GLU | ENGINEERED | UNP P17119 |

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 3 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

- Molecule 4 is water.

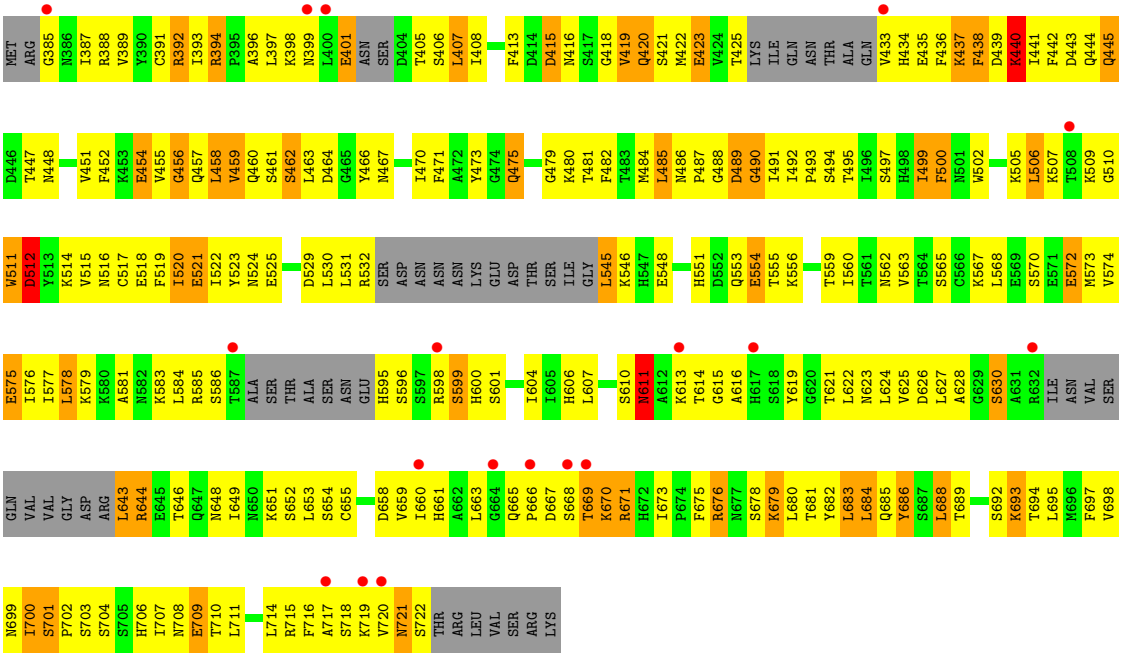
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 4 | A | 63 | Total | O | 0 | 0 |
| | | | 63 | 63 | | |
| 4 | B | 72 | Total | O | 0 | 0 |
| | | | 72 | 72 | | |

# 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.

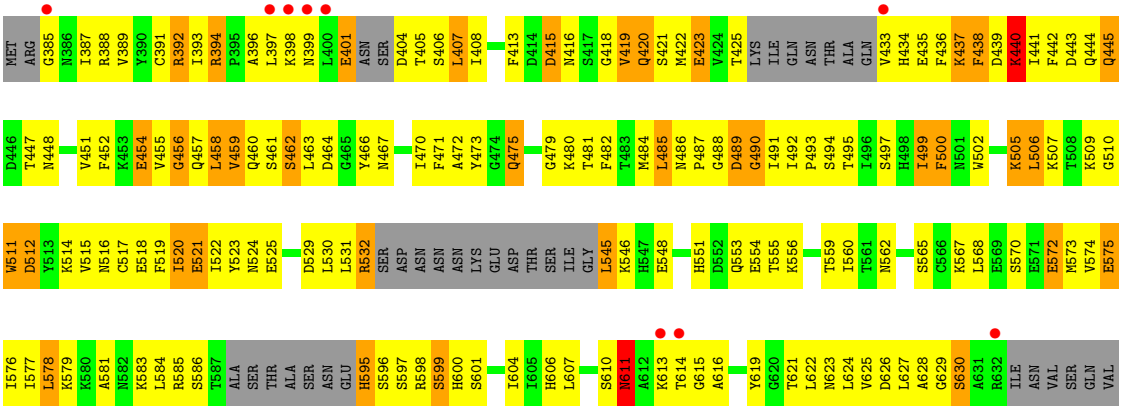
• Molecule 1: KINESIN-LIKE PROTEIN KAR3

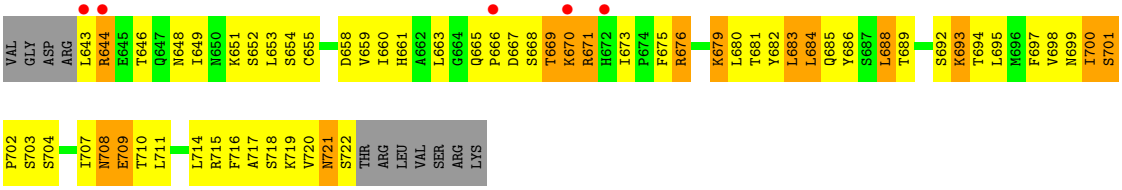
Chain A:



• Molecule 1: KINESIN-LIKE PROTEIN KAR3

Chain B:




VAL GLY ASP ARG L643 R644 E645 T646 Q647 N648 I649 N650 K651 S652 L653 S654 C655 D658 V659 I660 H661 A662 L663 G664 Q665 P666 D667 S668 T669 K670 R671 H672 I673 P674 F675 R676 K679 L680 T681 Y682 L683 L684 Q685 Y686 S687 L688 T689 S692 K693 T694 L695 H696 F697 V698 N699 I700 S701
P702 S703 S704 I707 N708 E709 T710 L711 L714 R715 F716 A717 S718 K719 V720 N721 S722 THR ARG LEU VAL SER ARG LYS

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 43 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 62.89Å 62.89Å 153.56Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 20.00 – 2.50<br>19.24 – 2.50 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 89.6 (20.00-2.50)<br>89.6 (19.24-2.50) | Depositor<br>EDS |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.80 (at 2.49Å) | Xtriage |
| Refinement program | X-PLOR | Depositor |
| R, $R_{free}$ | 0.230 , 0.276<br>0.225 , 0.262 | Depositor<br>DCC |
| $R_{free}$ test set | 1802 reflections (9.78%) | DCC |
| Wilson B-factor (Å$^2$) | 39.3 | Xtriage |
| Anisotropy | 0.446 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 55.2 | EDS |
| Estimated twinning fraction | 0.458 for h,-k,-l | Xtriage |
| L-test for twinning | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Outliers | 2 of 18420 reflections (0.011%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 4935 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 43.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.48 | 0/2408 | 0.69 | 0/3245 |
| 1 | B | 0.48 | 0/2408 | 0.69 | 0/3245 |
| All | All | 0.48 | 0/4816 | 0.69 | 0/6490 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 2372 | 0 | 2358 | 243 | 0 |
| 1 | B | 2372 | 0 | 2358 | 247 | 0 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 27 | 0 | 12 | 3 | 0 |
| 3 | B | 27 | 0 | 12 | 3 | 0 |
| 4 | A | 63 | 0 | 0 | 1 | 0 |
| 4 | B | 72 | 0 | 0 | 4 | 0 |
| All | All | 4935 | 0 | 4740 | 488 | 0 |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 51.

All (488) close contacts within the same asymmetric unit are listed below.

| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:462:SER:HB2 | 1:B:607:LEU:HD12 | 1.31 | 1.10 |
| 1:A:668:SER:HA | 1:A:671:ARG:HB3 | 1.32 | 1.08 |
| 1:B:394:ARG:HE | 1:B:701:SER:HB2 | 1.15 | 1.07 |
| 1:A:462:SER:HB2 | 1:A:607:LEU:HD12 | 1.34 | 1.07 |
| 1:B:668:SER:HA | 1:B:671:ARG:HB3 | 1.30 | 1.05 |
| 1:A:394:ARG:HE | 1:A:701:SER:HB2 | 1.17 | 1.04 |
| 1:A:394:ARG:HG3 | 1:A:394:ARG:HH11 | 1.35 | 0.92 |
| 1:B:560:ILE:HD11 | 1:B:683:LEU:HD21 | 1.52 | 0.91 |
| 1:B:394:ARG:HG3 | 1:B:394:ARG:HH11 | 1.36 | 0.91 |
| 1:A:560:ILE:HD11 | 1:A:683:LEU:HD21 | 1.53 | 0.90 |
| 1:A:700:ILE:HG21 | 1:A:714:LEU:HD21 | 1.58 | 0.86 |
| 1:A:448:ASN:HD22 | 1:A:489:ASP:HB3 | 1.41 | 0.85 |
| 1:B:462:SER:HB2 | 1:B:607:LEU:CD1 | 2.05 | 0.85 |
| 1:B:698:VAL:HG21 | 1:B:717:ALA:HB2 | 1.59 | 0.85 |
| 1:A:462:SER:HB2 | 1:A:607:LEU:CD1 | 2.06 | 0.84 |
| 1:A:698:VAL:HG21 | 1:A:717:ALA:HB2 | 1.59 | 0.84 |
| 1:B:448:ASN:HD22 | 1:B:489:ASP:HB3 | 1.40 | 0.84 |
| 1:B:700:ILE:HG21 | 1:B:714:LEU:HD21 | 1.59 | 0.84 |
| 1:A:570:SER:OG | 1:A:572:GLU:HG2 | 1.77 | 0.84 |
| 1:B:570:SER:OG | 1:B:572:GLU:HG2 | 1.79 | 0.83 |
| 1:A:440:LYS:HD3 | 1:A:454:GLU:HG3 | 1.61 | 0.83 |
| 1:B:572:GLU:O | 1:B:576:ILE:HD12 | 1.79 | 0.82 |
| 1:B:440:LYS:HD3 | 1:B:454:GLU:HG3 | 1.62 | 0.82 |
| 1:A:572:GLU:O | 1:A:576:ILE:HD12 | 1.80 | 0.81 |
| 1:B:394:ARG:NE | 1:B:701:SER:HB2 | 1.96 | 0.80 |
| 1:A:394:ARG:HE | 1:A:701:SER:CB | 1.94 | 0.80 |
| 1:B:521:GLU:HB3 | 1:B:530:LEU:HD11 | 1.64 | 0.79 |
| 1:B:521:GLU:OE1 | 1:B:599:SER:HB2 | 1.82 | 0.79 |
| 1:B:394:ARG:HE | 1:B:701:SER:CB | 1.92 | 0.79 |
| 1:B:419:VAL:HG23 | 1:B:420:GLN:N | 1.98 | 0.79 |
| 1:B:458:LEU:HD23 | 1:B:459:VAL:N | 1.98 | 0.79 |
| 1:A:524:ASN:HA | 1:A:648:ASN:HD22 | 1.48 | 0.78 |
| 1:A:521:GLU:HB3 | 1:A:530:LEU:HD11 | 1.64 | 0.78 |
| 1:A:458:LEU:HD23 | 1:A:459:VAL:N | 1.98 | 0.78 |
| 1:A:521:GLU:OE1 | 1:A:599:SER:HB2 | 1.84 | 0.78 |
| 1:B:394:ARG:CG | 1:B:394:ARG:HH11 | 1.96 | 0.77 |
| 1:A:394:ARG:HH11 | 1:A:394:ARG:CG | 1.96 | 0.77 |
| 1:B:425:THR:OG1 | 1:B:433:VAL:HG22 | 1.86 | 0.76 |
| 1:B:574:VAL:HG12 | 1:B:578:LEU:HD23 | 1.67 | 0.76 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:A:574:VAL:HG12 | 1:A:578:LEU:HD23 | 1.67 | 0.76 |
| 1:A:419:VAL:HG23 | 1:A:420:GLN:N | 2.00 | 0.76 |
| 1:A:394:ARG:NE | 1:A:701:SER:HB2 | 1.98 | 0.76 |
| 1:B:524:ASN:HA | 1:B:648:ASN:HD22 | 1.49 | 0.75 |
| 1:A:459:VAL:HG12 | 1:A:622:LEU:CD2 | 2.18 | 0.74 |
| 1:A:559:THR:HG22 | 1:A:560:ILE:H | 1.53 | 0.73 |
| 1:A:425:THR:OG1 | 1:A:433:VAL:HG22 | 1.88 | 0.73 |
| 1:B:459:VAL:HG12 | 1:B:622:LEU:CD2 | 2.19 | 0.72 |
| 1:A:669:THR:HG23 | 1:A:670:LYS:HG2 | 1.72 | 0.72 |
| 1:A:481:THR:HG21 | 1:A:585:ARG:O | 1.90 | 0.72 |
| 1:B:669:THR:HG23 | 1:B:670:LYS:HG2 | 1.72 | 0.72 |
| 1:B:553:GLN:HA | 1:B:686:TYR:OH | 1.89 | 0.72 |
| 1:B:448:ASN:ND2 | 1:B:489:ASP:HB3 | 2.04 | 0.72 |
| 1:B:510:GLY:HA2 | 1:B:613:LYS:NZ | 2.05 | 0.72 |
| 1:B:707:ILE:O | 1:B:711:LEU:HG | 1.89 | 0.72 |
| 1:A:448:ASN:ND2 | 1:A:489:ASP:HB3 | 2.04 | 0.71 |
| 1:A:553:GLN:HA | 1:A:686:TYR:OH | 1.88 | 0.71 |
| 1:A:510:GLY:HA2 | 1:A:613:LYS:NZ | 2.06 | 0.71 |
| 1:A:715:ARG:O | 1:A:719:LYS:HG2 | 1.91 | 0.70 |
| 1:B:481:THR:HG21 | 1:B:585:ARG:O | 1.91 | 0.70 |
| 1:A:458:LEU:HD22 | 1:A:695:LEU:HD11 | 1.73 | 0.70 |
| 1:B:559:THR:HG22 | 1:B:560:ILE:H | 1.55 | 0.70 |
| 1:A:524:ASN:HA | 1:A:648:ASN:ND2 | 2.07 | 0.70 |
| 1:B:502:TRP:O | 1:B:506:LEU:HD12 | 1.92 | 0.70 |
| 1:B:387:ILE:O | 1:B:388:ARG:HD2 | 1.92 | 0.70 |
| 1:B:385:GLY:HA2 | 1:B:692:SER:O | 1.91 | 0.69 |
| 1:A:707:ILE:O | 1:A:711:LEU:HG | 1.92 | 0.69 |
| 1:B:458:LEU:HD22 | 1:B:695:LEU:HD11 | 1.75 | 0.69 |
| 1:B:604:ILE:HG23 | 1:B:623:ASN:ND2 | 2.08 | 0.69 |
| 1:A:604:ILE:HG23 | 1:A:623:ASN:ND2 | 2.08 | 0.69 |
| 1:A:475:GLN:HB2 | 1:A:709:GLU:HG3 | 1.75 | 0.69 |
| 1:B:524:ASN:HA | 1:B:648:ASN:ND2 | 2.07 | 0.69 |
| 1:A:442:PHE:CD2 | 1:A:451:VAL:HG22 | 2.29 | 0.68 |
| 1:A:502:TRP:O | 1:A:506:LEU:HD12 | 1.93 | 0.68 |
| 1:B:510:GLY:HA2 | 1:B:613:LYS:HZ2 | 1.57 | 0.68 |
| 1:B:413:PHE:HE1 | 1:B:415:ASP:HB3 | 1.59 | 0.68 |
| 1:B:475:GLN:HB2 | 1:B:709:GLU:HG3 | 1.76 | 0.68 |
| 1:A:387:ILE:O | 1:A:388:ARG:HD2 | 1.93 | 0.68 |
| 1:B:397:LEU:H | 1:B:401:GLU:CG | 2.07 | 0.68 |
| 1:A:385:GLY:HA2 | 1:A:692:SER:O | 1.93 | 0.68 |
| 1:A:600:HIS:CD2 | 1:A:680:LEU:HD22 | 2.29 | 0.68 |
| 1:A:519:PHE:HB3 | 1:A:531:LEU:HG | 1.75 | 0.67 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:401:GLU:HA | 1:B:703:SER:OG | 1.95 | 0.67 |
| 1:A:458:LEU:HD13 | 1:A:695:LEU:HD21 | 1.77 | 0.67 |
| 1:A:401:GLU:HA | 1:A:703:SER:OG | 1.94 | 0.67 |
| 1:A:600:HIS:HD2 | 1:A:680:LEU:HD22 | 1.58 | 0.67 |
| 1:A:397:LEU:H | 1:A:401:GLU:CG | 2.07 | 0.67 |
| 1:B:715:ARG:O | 1:B:719:LYS:HG2 | 1.95 | 0.67 |
| 1:B:442:PHE:CD2 | 1:B:451:VAL:HG22 | 2.31 | 0.66 |
| 1:A:413:PHE:HE1 | 1:A:415:ASP:HB3 | 1.59 | 0.66 |
| 1:B:600:HIS:CD2 | 1:B:680:LEU:HD22 | 2.30 | 0.66 |
| 1:B:600:HIS:HD2 | 1:B:680:LEU:HD22 | 1.60 | 0.66 |
| 1:A:423:GLU:HG2 | 4:A:1127:HOH:O | 1.95 | 0.66 |
| 1:B:458:LEU:HD13 | 1:B:695:LEU:HD21 | 1.78 | 0.66 |
| 1:A:407:LEU:HD11 | 1:A:704:SER:HB3 | 1.78 | 0.65 |
| 1:A:515:VAL:HG12 | 1:A:568:LEU:HB2 | 1.79 | 0.65 |
| 1:B:545:LEU:HD23 | 4:B:1161:HOH:O | 1.96 | 0.65 |
| 1:B:519:PHE:HB3 | 1:B:531:LEU:HG | 1.77 | 0.65 |
| 1:A:495:THR:HG22 | 1:A:499:ILE:HD12 | 1.78 | 0.65 |
| 1:B:473:TYR:HB2 | 1:B:627:LEU:HD12 | 1.78 | 0.65 |
| 1:A:684:LEU:HB2 | 1:A:688:LEU:HD12 | 1.80 | 0.64 |
| 1:A:408:ILE:H | 1:A:408:ILE:HD12 | 1.62 | 0.64 |
| 1:A:473:TYR:HB2 | 1:A:627:LEU:HD12 | 1.78 | 0.64 |
| 1:B:392:ARG:NH2 | 3:B:999:ADP:HN62 | 1.96 | 0.64 |
| 1:B:408:ILE:HD12 | 1:B:408:ILE:H | 1.63 | 0.64 |
| 1:A:574:VAL:CG1 | 1:A:578:LEU:HD23 | 2.27 | 0.63 |
| 1:A:522:ILE:HB | 1:A:600:HIS:HB2 | 1.80 | 0.63 |
| 1:A:518:GLU:HG3 | 1:A:565:SER:HA | 1.81 | 0.63 |
| 1:B:407:LEU:HD11 | 1:B:704:SER:HB3 | 1.80 | 0.63 |
| 1:B:684:LEU:HB2 | 1:B:688:LEU:HD12 | 1.81 | 0.63 |
| 1:B:515:VAL:HG12 | 1:B:568:LEU:HB2 | 1.81 | 0.63 |
| 1:B:455:VAL:O | 1:B:457:GLN:N | 2.32 | 0.63 |
| 1:B:574:VAL:CG1 | 1:B:578:LEU:HD23 | 2.28 | 0.62 |
| 1:B:574:VAL:O | 1:B:578:LEU:HB2 | 1.99 | 0.62 |
| 1:A:698:VAL:HG21 | 1:A:717:ALA:CB | 2.29 | 0.62 |
| 1:B:495:THR:HG22 | 1:B:499:ILE:HD12 | 1.79 | 0.62 |
| 1:B:389:VAL:O | 1:B:438:PHE:HB3 | 1.99 | 0.62 |
| 1:B:522:ILE:HB | 1:B:600:HIS:HB2 | 1.81 | 0.62 |
| 1:B:518:GLU:HG3 | 1:B:565:SER:HA | 1.81 | 0.62 |
| 1:A:574:VAL:O | 1:A:578:LEU:HB2 | 1.99 | 0.62 |
| 1:A:392:ARG:NH2 | 3:A:998:ADP:HN62 | 1.96 | 0.62 |
| 1:B:461:SER:O | 1:B:464:ASP:HB2 | 2.00 | 0.62 |
| 1:A:457:GLN:NE2 | 1:A:460:GLN:HE21 | 1.96 | 0.62 |
| 1:A:715:ARG:HA | 1:A:718:SER:HG | 1.63 | 0.62 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:A:461:SER:O | 1:A:464:ASP:HB2 | 1.99 | 0.62 |
| 1:A:556:LYS:HG3 | 1:A:686:TYR:CE1 | 2.34 | 0.61 |
| 1:B:659:VAL:HG21 | 1:B:681:THR:HG21 | 1.82 | 0.61 |
| 1:A:458:LEU:HD12 | 1:A:693:LYS:HB3 | 1.83 | 0.61 |
| 1:A:458:LEU:HD23 | 1:A:459:VAL:HG22 | 1.81 | 0.61 |
| 1:B:676:ARG:HA | 1:B:682:TYR:HB2 | 1.82 | 0.61 |
| 1:B:515:VAL:HG22 | 1:B:607:LEU:HD23 | 1.83 | 0.61 |
| 1:B:458:LEU:HD12 | 1:B:693:LYS:HB3 | 1.83 | 0.61 |
| 1:B:604:ILE:HG23 | 1:B:623:ASN:HD22 | 1.64 | 0.61 |
| 1:B:698:VAL:HG21 | 1:B:717:ALA:CB | 2.29 | 0.61 |
| 1:A:458:LEU:HD23 | 1:A:459:VAL:H | 1.66 | 0.61 |
| 1:B:473:TYR:CE1 | 1:B:630:SER:HB2 | 2.36 | 0.61 |
| 1:B:598:ARG:NH1 | 1:B:649:ILE:HD13 | 2.16 | 0.60 |
| 1:B:490:GLY:O | 1:B:493:PRO:HD2 | 2.02 | 0.60 |
| 1:A:455:VAL:O | 1:A:457:GLN:N | 2.33 | 0.60 |
| 1:A:676:ARG:HA | 1:A:682:TYR:HB2 | 1.83 | 0.60 |
| 1:A:667:ASP:CG | 1:A:670:LYS:HG3 | 2.22 | 0.60 |
| 1:A:389:VAL:HG11 | 1:A:717:ALA:HB1 | 1.83 | 0.60 |
| 1:B:457:GLN:NE2 | 1:B:460:GLN:HE21 | 1.98 | 0.60 |
| 1:B:667:ASP:CG | 1:B:670:LYS:HG3 | 2.22 | 0.60 |
| 1:B:556:LYS:HG3 | 1:B:686:TYR:CE1 | 2.37 | 0.60 |
| 1:A:473:TYR:CE1 | 1:A:630:SER:HB2 | 2.37 | 0.60 |
| 1:A:700:ILE:HD12 | 1:A:701:SER:O | 2.02 | 0.60 |
| 1:B:545:LEU:HD22 | 1:B:546:LYS:H | 1.66 | 0.60 |
| 1:A:545:LEU:HD22 | 1:A:546:LYS:H | 1.66 | 0.59 |
| 1:A:471:PHE:O | 1:A:697:PHE:HB2 | 2.01 | 0.59 |
| 1:B:458:LEU:HD23 | 1:B:459:VAL:HG22 | 1.84 | 0.59 |
| 1:A:694:THR:O | 1:A:695:LEU:HD23 | 2.03 | 0.59 |
| 1:B:598:ARG:HD3 | 1:B:649:ILE:CD1 | 2.32 | 0.59 |
| 1:B:389:VAL:HG11 | 1:B:717:ALA:HB1 | 1.83 | 0.59 |
| 1:A:397:LEU:H | 1:A:401:GLU:HG3 | 1.67 | 0.59 |
| 1:A:684:LEU:O | 1:A:688:LEU:HD12 | 2.02 | 0.59 |
| 1:A:515:VAL:HG22 | 1:A:607:LEU:HD23 | 1.85 | 0.59 |
| 1:B:457:GLN:O | 1:B:460:GLN:HG2 | 2.02 | 0.59 |
| 1:B:585:ARG:CZ | 1:B:601:SER:HB3 | 2.33 | 0.59 |
| 1:A:457:GLN:O | 1:A:460:GLN:HG2 | 2.02 | 0.59 |
| 1:A:604:ILE:HG23 | 1:A:623:ASN:HD22 | 1.66 | 0.59 |
| 1:B:490:GLY:C | 1:B:493:PRO:HD2 | 2.24 | 0.58 |
| 1:A:585:ARG:CZ | 1:A:601:SER:HB3 | 2.32 | 0.58 |
| 1:B:458:LEU:HD23 | 1:B:459:VAL:H | 1.66 | 0.58 |
| 1:A:700:ILE:HG21 | 1:A:714:LEU:CD2 | 2.30 | 0.58 |
| 1:A:389:VAL:O | 1:A:438:PHE:HB3 | 2.04 | 0.58 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:A:601:SER:OG | 1:A:626:ASP:HB3 | 2.02 | 0.58 |
| 1:B:700:ILE:HG21 | 1:B:714:LEU:CD2 | 2.32 | 0.58 |
| 1:A:521:GLU:OE1 | 1:A:599:SER:CB | 2.51 | 0.58 |
| 1:B:471:PHE:O | 1:B:697:PHE:HB2 | 2.03 | 0.58 |
| 1:A:598:ARG:HD3 | 1:A:649:ILE:CD1 | 2.33 | 0.58 |
| 1:A:698:VAL:CG2 | 1:A:717:ALA:HB2 | 2.32 | 0.57 |
| 1:B:598:ARG:HD3 | 1:B:649:ILE:HD11 | 1.85 | 0.57 |
| 1:B:673:ILE:HB | 1:B:675:PHE:CE2 | 2.39 | 0.57 |
| 1:A:490:GLY:C | 1:A:493:PRO:HD2 | 2.25 | 0.57 |
| 1:A:545:LEU:HD21 | 1:B:572:GLU:HB2 | 1.87 | 0.57 |
| 1:B:521:GLU:OE1 | 1:B:599:SER:CB | 2.50 | 0.57 |
| 1:B:694:THR:O | 1:B:695:LEU:HD23 | 2.04 | 0.57 |
| 1:B:684:LEU:O | 1:B:688:LEU:HD12 | 2.04 | 0.57 |
| 1:A:598:ARG:NH1 | 1:A:649:ILE:HD13 | 2.20 | 0.57 |
| 1:A:485:LEU:O | 1:A:486:ASN:C | 2.43 | 0.57 |
| 1:A:490:GLY:O | 1:A:493:PRO:HD2 | 2.04 | 0.57 |
| 1:A:413:PHE:CE1 | 1:A:415:ASP:HB3 | 2.40 | 0.56 |
| 1:B:668:SER:CA | 1:B:671:ARG:HB3 | 2.21 | 0.56 |
| 1:B:481:THR:CG2 | 1:B:585:ARG:HB2 | 2.35 | 0.56 |
| 1:A:387:ILE:C | 1:A:388:ARG:HD2 | 2.26 | 0.56 |
| 1:B:397:LEU:H | 1:B:401:GLU:HG3 | 1.68 | 0.56 |
| 1:B:700:ILE:HD12 | 1:B:701:SER:O | 2.05 | 0.56 |
| 1:B:585:ARG:NH1 | 1:B:601:SER:HB3 | 2.21 | 0.56 |
| 1:B:719:LYS:HG3 | 1:B:720:VAL:N | 2.21 | 0.56 |
| 1:A:585:ARG:NH1 | 1:A:601:SER:HB3 | 2.20 | 0.56 |
| 1:B:601:SER:OG | 1:B:626:ASP:HB3 | 2.04 | 0.56 |
| 1:B:392:ARG:NH2 | 3:B:999:ADP:N6 | 2.54 | 0.56 |
| 1:A:523:TYR:HB2 | 1:A:599:SER:HB3 | 1.86 | 0.56 |
| 1:A:572:GLU:HB2 | 1:B:545:LEU:HD21 | 1.88 | 0.56 |
| 1:A:704:SER:HA | 1:A:707:ILE:HG12 | 1.88 | 0.56 |
| 1:B:485:LEU:O | 1:B:486:ASN:C | 2.43 | 0.56 |
| 1:A:392:ARG:NH2 | 3:A:998:ADP:N6 | 2.54 | 0.55 |
| 1:A:407:LEU:H | 1:A:407:LEU:HD12 | 1.72 | 0.55 |
| 1:B:387:ILE:C | 1:B:388:ARG:HD2 | 2.26 | 0.55 |
| 1:A:659:VAL:HG21 | 1:A:681:THR:HG21 | 1.88 | 0.55 |
| 1:B:407:LEU:HD12 | 1:B:407:LEU:H | 1.71 | 0.55 |
| 1:A:480:LYS:HA | 1:A:699:ASN:ND2 | 2.22 | 0.55 |
| 1:A:719:LYS:HG3 | 1:A:720:VAL:N | 2.22 | 0.55 |
| 1:A:599:SER:O | 1:A:628:ALA:HB2 | 2.07 | 0.55 |
| 1:B:393:ILE:HD12 | 1:B:393:ILE:H | 1.72 | 0.55 |
| 1:B:704:SER:HA | 1:B:707:ILE:HG12 | 1.88 | 0.55 |
| 1:A:511:TRP:HA | 1:A:611:ASN:HB2 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:A:715:ARG:HA | 1:A:718:SER:OG | 2.06 | 0.55 |
| 1:B:480:LYS:HA | 1:B:699:ASN:ND2 | 2.22 | 0.55 |
| 1:B:391:CYS:HB3 | 1:B:441:ILE:HG23 | 1.86 | 0.55 |
| 1:B:523:TYR:HB2 | 1:B:599:SER:HB3 | 1.88 | 0.54 |
| 1:B:437:LYS:O | 1:B:437:LYS:HG3 | 2.07 | 0.54 |
| 1:A:481:THR:CG2 | 1:A:585:ARG:HB2 | 2.37 | 0.54 |
| 1:A:704:SER:HA | 1:A:707:ILE:HD11 | 1.89 | 0.54 |
| 1:A:393:ILE:H | 1:A:393:ILE:HD12 | 1.73 | 0.54 |
| 1:B:698:VAL:CG2 | 1:B:717:ALA:HB2 | 2.33 | 0.54 |
| 1:B:599:SER:O | 1:B:628:ALA:HB2 | 2.08 | 0.54 |
| 1:B:667:ASP:OD2 | 1:B:670:LYS:HG3 | 2.08 | 0.54 |
| 1:A:704:SER:HA | 1:A:707:ILE:CG1 | 2.38 | 0.54 |
| 1:A:598:ARG:HD3 | 1:A:649:ILE:HD11 | 1.88 | 0.54 |
| 1:B:679:LYS:O | 1:B:683:LEU:HB2 | 2.08 | 0.54 |
| 1:B:394:ARG:NH1 | 1:B:394:ARG:HG3 | 2.13 | 0.54 |
| 1:B:704:SER:HA | 1:B:707:ILE:CG1 | 2.38 | 0.54 |
| 1:A:673:ILE:HB | 1:A:675:PHE:CE2 | 2.41 | 0.54 |
| 1:B:397:LEU:H | 1:B:401:GLU:HG2 | 1.72 | 0.54 |
| 1:B:461:SER:O | 1:B:464:ASP:N | 2.40 | 0.54 |
| 1:A:397:LEU:H | 1:A:401:GLU:HG2 | 1.73 | 0.53 |
| 1:A:667:ASP:OD2 | 1:A:670:LYS:HG3 | 2.09 | 0.53 |
| 1:B:715:ARG:HA | 1:B:718:SER:OG | 2.07 | 0.53 |
| 1:A:394:ARG:HH12 | 1:A:397:LEU:HD11 | 1.73 | 0.53 |
| 1:B:413:PHE:CE1 | 1:B:415:ASP:HB3 | 2.40 | 0.53 |
| 1:A:559:THR:HG22 | 1:A:560:ILE:N | 2.23 | 0.53 |
| 1:A:679:LYS:O | 1:A:683:LEU:HB2 | 2.08 | 0.53 |
| 1:B:572:GLU:O | 1:B:576:ILE:CD1 | 2.56 | 0.53 |
| 1:A:648:ASN:O | 1:A:651:LYS:HB3 | 2.09 | 0.53 |
| 1:A:510:GLY:HA2 | 1:A:613:LYS:HZ3 | 1.73 | 0.53 |
| 1:B:422:MET:HB3 | 1:B:441:ILE:CD1 | 2.39 | 0.53 |
| 1:A:500:PHE:CE1 | 1:A:574:VAL:HG21 | 2.44 | 0.52 |
| 1:A:401:GLU:HA | 1:A:703:SER:CB | 2.39 | 0.52 |
| 1:A:559:THR:O | 1:A:560:ILE:HG13 | 2.10 | 0.52 |
| 1:B:521:GLU:HB3 | 1:B:530:LEU:CD1 | 2.38 | 0.52 |
| 1:B:704:SER:HA | 1:B:707:ILE:HD11 | 1.90 | 0.52 |
| 1:B:606:HIS:ND1 | 1:B:619:TYR:OH | 2.37 | 0.52 |
| 1:B:394:ARG:HH12 | 1:B:397:LEU:HD11 | 1.74 | 0.52 |
| 1:A:391:CYS:HB3 | 1:A:441:ILE:HG23 | 1.90 | 0.52 |
| 1:A:521:GLU:HB3 | 1:A:530:LEU:CD1 | 2.37 | 0.52 |
| 1:B:443:ASP:HB3 | 1:B:445:GLN:NE2 | 2.25 | 0.52 |
| 1:A:422:MET:HB3 | 1:A:441:ILE:CD1 | 2.39 | 0.52 |
| 1:B:500:PHE:CE1 | 1:B:574:VAL:HG21 | 2.43 | 0.52 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:A:684:LEU:C | 1:A:688:LEU:HD12 | 2.30 | 0.52 |
| 1:A:518:GLU:OE1 | 1:A:606:HIS:NE2 | 2.38 | 0.52 |
| 1:A:492:ILE:HB | 1:A:493:PRO:HD3 | 1.92 | 0.52 |
| 1:A:437:LYS:O | 1:A:437:LYS:HG3 | 2.10 | 0.52 |
| 1:B:416:ASN:C | 1:B:418:GLY:N | 2.63 | 0.52 |
| 1:A:416:ASN:C | 1:A:418:GLY:H | 2.14 | 0.51 |
| 1:B:644:ARG:C | 1:B:646:THR:N | 2.64 | 0.51 |
| 1:B:559:THR:HG22 | 1:B:560:ILE:N | 2.24 | 0.51 |
| 1:B:511:TRP:HA | 1:B:611:ASN:HB2 | 1.90 | 0.51 |
| 1:B:559:THR:O | 1:B:560:ILE:HG13 | 2.10 | 0.51 |
| 1:A:610:SER:OG | 1:A:611:ASN:N | 2.42 | 0.51 |
| 1:B:481:THR:HG21 | 1:B:585:ARG:HB2 | 1.92 | 0.51 |
| 1:A:443:ASP:HB3 | 1:A:445:GLN:NE2 | 2.26 | 0.51 |
| 1:A:458:LEU:CD1 | 1:A:693:LYS:HB3 | 2.41 | 0.51 |
| 1:B:663:LEU:HD21 | 1:B:689:THR:HG22 | 1.93 | 0.51 |
| 1:A:517:CYS:HA | 1:A:604:ILE:O | 2.11 | 0.51 |
| 1:B:458:LEU:CD1 | 1:B:693:LYS:HB3 | 2.41 | 0.51 |
| 1:B:610:SER:OG | 1:B:611:ASN:N | 2.42 | 0.51 |
| 1:A:644:ARG:C | 1:A:646:THR:N | 2.63 | 0.51 |
| 1:A:668:SER:CA | 1:A:671:ARG:HB3 | 2.23 | 0.51 |
| 1:B:487:PRO:O | 1:B:489:ASP:N | 2.39 | 0.51 |
| 1:A:545:LEU:HD13 | 1:A:562:ASN:HB3 | 1.93 | 0.50 |
| 1:B:648:ASN:O | 1:B:651:LYS:HB3 | 2.11 | 0.50 |
| 1:B:715:ARG:HA | 1:B:718:SER:HG | 1.76 | 0.50 |
| 1:A:457:GLN:HE21 | 1:A:460:GLN:HE21 | 1.57 | 0.50 |
| 1:B:684:LEU:C | 1:B:688:LEU:HD12 | 2.31 | 0.50 |
| 1:A:495:THR:O | 1:A:499:ILE:HB | 2.11 | 0.50 |
| 1:B:545:LEU:HD13 | 1:B:562:ASN:HB3 | 1.93 | 0.50 |
| 1:B:416:ASN:C | 1:B:418:GLY:H | 2.14 | 0.50 |
| 1:A:704:SER:O | 1:A:707:ILE:HG12 | 2.12 | 0.49 |
| 1:B:401:GLU:HA | 1:B:703:SER:CB | 2.41 | 0.49 |
| 1:A:573:MET:HE2 | 1:A:577:ILE:HG13 | 1.94 | 0.49 |
| 1:B:467:ASN:HA | 1:B:621:THR:O | 2.12 | 0.49 |
| 1:A:423:GLU:HA | 1:A:434:HIS:O | 2.12 | 0.49 |
| 1:B:520:ILE:HG22 | 1:B:529:ASP:HA | 1.94 | 0.49 |
| 1:A:459:VAL:HG12 | 1:A:622:LEU:HD23 | 1.94 | 0.49 |
| 1:A:510:GLY:HA2 | 1:A:613:LYS:HZ2 | 1.76 | 0.49 |
| 1:B:704:SER:O | 1:B:707:ILE:HG12 | 2.13 | 0.49 |
| 1:B:649:ILE:HG22 | 1:B:653:LEU:HD12 | 1.94 | 0.49 |
| 1:B:423:GLU:HA | 1:B:434:HIS:O | 2.13 | 0.49 |
| 1:A:419:VAL:HG11 | 1:A:437:LYS:HE3 | 1.95 | 0.49 |
| 1:A:479:GLY:HA2 | 3:A:998:ADP:H8 | 1.78 | 0.49 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:394:ARG:CD | 1:B:701:SER:HA | 2.42 | 0.49 |
| 1:A:416:ASN:C | 1:A:418:GLY:N | 2.63 | 0.49 |
| 1:A:663:LEU:HD21 | 1:A:689:THR:HG22 | 1.95 | 0.49 |
| 1:A:438:PHE:N | 1:A:438:PHE:CD2 | 2.80 | 0.49 |
| 1:B:517:CYS:HA | 1:B:604:ILE:O | 2.13 | 0.49 |
| 1:B:655:CYS:O | 1:B:659:VAL:HG23 | 2.13 | 0.49 |
| 1:A:704:SER:HA | 1:A:707:ILE:CD1 | 2.43 | 0.48 |
| 1:B:495:THR:O | 1:B:499:ILE:HB | 2.12 | 0.48 |
| 1:B:458:LEU:HD12 | 1:B:693:LYS:CG | 2.44 | 0.48 |
| 1:B:704:SER:HA | 1:B:707:ILE:CD1 | 2.44 | 0.48 |
| 1:A:649:ILE:HG22 | 1:A:653:LEU:HD12 | 1.96 | 0.48 |
| 1:B:505:LYS:HZ1 | 1:B:509:LYS:HD3 | 1.77 | 0.48 |
| 1:B:487:PRO:C | 1:B:489:ASP:H | 2.15 | 0.48 |
| 1:B:439:ASP:O | 1:B:440:LYS:CB | 2.61 | 0.48 |
| 1:B:419:VAL:HG11 | 1:B:437:LYS:HE3 | 1.94 | 0.48 |
| 1:A:520:ILE:HG22 | 1:A:529:ASP:HA | 1.94 | 0.48 |
| 1:B:611:ASN:OD1 | 1:B:613:LYS:HB2 | 2.13 | 0.48 |
| 1:A:467:ASN:HA | 1:A:621:THR:O | 2.13 | 0.48 |
| 1:B:560:ILE:HD12 | 4:B:1210:HOH:O | 2.12 | 0.48 |
| 1:B:492:ILE:HB | 1:B:493:PRO:HD3 | 1.95 | 0.48 |
| 1:B:573:MET:HE2 | 1:B:577:ILE:HG13 | 1.94 | 0.48 |
| 1:B:568:LEU:HD22 | 1:B:574:VAL:HG22 | 1.96 | 0.48 |
| 1:B:440:LYS:HG2 | 1:B:442:PHE:CE1 | 2.49 | 0.48 |
| 1:B:457:GLN:HE21 | 1:B:460:GLN:HE21 | 1.60 | 0.48 |
| 1:A:458:LEU:HD12 | 1:A:693:LYS:CG | 2.43 | 0.48 |
| 1:A:482:PHE:O | 1:A:486:ASN:HB2 | 2.14 | 0.48 |
| 1:A:573:MET:CE | 1:A:577:ILE:HG13 | 2.43 | 0.48 |
| 1:A:448:ASN:HB2 | 1:A:489:ASP:CG | 2.33 | 0.47 |
| 1:B:448:ASN:HB2 | 1:B:489:ASP:CG | 2.34 | 0.47 |
| 1:B:492:ILE:HG12 | 1:B:624:LEU:CD1 | 2.44 | 0.47 |
| 1:B:479:GLY:HA2 | 3:B:999:ADP:H8 | 1.79 | 0.47 |
| 1:B:644:ARG:HA | 1:B:644:ARG:HD3 | 1.55 | 0.47 |
| 1:A:481:THR:HG21 | 1:A:585:ARG:HB2 | 1.96 | 0.47 |
| 1:A:461:SER:O | 1:A:464:ASP:N | 2.44 | 0.47 |
| 1:A:470:ILE:HG13 | 1:A:624:LEU:CD2 | 2.44 | 0.47 |
| 1:B:389:VAL:HG21 | 1:B:721:ASN:HB2 | 1.95 | 0.47 |
| 1:A:655:CYS:O | 1:A:659:VAL:HG23 | 2.14 | 0.47 |
| 1:A:394:ARG:CD | 1:A:701:SER:HA | 2.43 | 0.47 |
| 1:A:439:ASP:O | 1:A:440:LYS:CB | 2.62 | 0.47 |
| 1:A:606:HIS:ND1 | 1:A:619:TYR:OH | 2.40 | 0.47 |
| 1:A:644:ARG:HD3 | 1:A:644:ARG:HA | 1.55 | 0.47 |
| 1:A:611:ASN:OD1 | 1:A:613:LYS:HB2 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:598:ARG:HH11 | 1:B:649:ILE:CD1 | 2.28 | 0.47 |
| 1:A:644:ARG:C | 1:A:646:THR:H | 2.16 | 0.47 |
| 1:A:568:LEU:HD22 | 1:A:574:VAL:HG22 | 1.96 | 0.47 |
| 1:A:572:GLU:CD | 1:A:572:GLU:H | 2.16 | 0.47 |
| 1:B:644:ARG:C | 1:B:646:THR:H | 2.17 | 0.47 |
| 1:A:394:ARG:HD3 | 1:A:702:PRO:HD3 | 1.97 | 0.47 |
| 1:B:518:GLU:OE1 | 1:B:606:HIS:NE2 | 2.39 | 0.47 |
| 1:B:545:LEU:CD2 | 1:B:546:LYS:H | 2.28 | 0.46 |
| 1:B:599:SER:C | 1:B:628:ALA:HB2 | 2.35 | 0.46 |
| 1:B:711:LEU:O | 1:B:715:ARG:HB2 | 2.16 | 0.46 |
| 1:A:421:SER:HA | 1:A:436:PHE:O | 2.15 | 0.46 |
| 1:B:421:SER:HA | 1:B:436:PHE:O | 2.14 | 0.46 |
| 1:B:611:ASN:O | 1:B:615:GLY:N | 2.47 | 0.46 |
| 1:B:510:GLY:HA3 | 1:B:613:LYS:HD3 | 1.97 | 0.46 |
| 1:A:719:LYS:HG3 | 1:A:720:VAL:H | 1.81 | 0.46 |
| 1:A:492:ILE:HG12 | 1:A:624:LEU:CD1 | 2.45 | 0.46 |
| 1:A:389:VAL:HG21 | 1:A:721:ASN:HB2 | 1.96 | 0.46 |
| 1:A:394:ARG:NH1 | 1:A:394:ARG:HG3 | 2.12 | 0.46 |
| 1:B:572:GLU:H | 1:B:572:GLU:CD | 2.18 | 0.46 |
| 1:B:517:CYS:HB2 | 1:B:604:ILE:O | 2.15 | 0.46 |
| 1:B:500:PHE:HE1 | 1:B:574:VAL:HG21 | 1.81 | 0.46 |
| 1:A:611:ASN:O | 1:A:615:GLY:N | 2.49 | 0.46 |
| 1:A:684:LEU:HB2 | 1:A:688:LEU:CD1 | 2.45 | 0.46 |
| 1:B:394:ARG:HD3 | 1:B:702:PRO:HD3 | 1.97 | 0.46 |
| 1:A:572:GLU:O | 1:A:576:ILE:CD1 | 2.57 | 0.46 |
| 1:B:455:VAL:O | 1:B:456:GLY:C | 2.54 | 0.46 |
| 1:A:455:VAL:O | 1:A:456:GLY:C | 2.54 | 0.46 |
| 1:A:555:THR:O | 1:A:556:LYS:HB2 | 2.16 | 0.46 |
| 1:B:482:PHE:O | 1:B:486:ASN:HB2 | 2.16 | 0.46 |
| 1:A:545:LEU:CD2 | 1:A:546:LYS:H | 2.29 | 0.46 |
| 1:A:711:LEU:O | 1:A:715:ARG:HB2 | 2.16 | 0.46 |
| 1:B:438:PHE:CD2 | 1:B:438:PHE:N | 2.81 | 0.46 |
| 1:A:440:LYS:HG2 | 1:A:442:PHE:CE1 | 2.51 | 0.46 |
| 1:A:715:ARG:CA | 1:A:718:SER:HG | 2.28 | 0.46 |
| 1:B:472:ALA:O | 1:B:480:LYS:HD2 | 2.16 | 0.46 |
| 1:A:573:MET:HG3 | 1:A:577:ILE:HD12 | 1.97 | 0.45 |
| 1:A:452:PHE:CD1 | 1:A:494:SER:HB2 | 2.51 | 0.45 |
| 1:A:422:MET:HB3 | 1:A:441:ILE:HD12 | 1.98 | 0.45 |
| 1:A:625:VAL:HG12 | 1:A:627:LEU:HD23 | 1.99 | 0.45 |
| 1:B:401:GLU:OE2 | 1:B:401:GLU:N | 2.49 | 0.45 |
| 1:A:599:SER:C | 1:A:628:ALA:HB2 | 2.36 | 0.45 |
| 1:B:445:GLN:HG3 | 1:B:445:GLN:H | 1.42 | 0.45 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:452:PHE:CD1 | 1:B:494:SER:HB2 | 2.52 | 0.45 |
| 1:A:413:PHE:HE1 | 1:A:415:ASP:CB | 2.29 | 0.45 |
| 1:A:487:PRO:C | 1:A:489:ASP:H | 2.18 | 0.45 |
| 1:A:401:GLU:N | 1:A:401:GLU:OE2 | 2.50 | 0.45 |
| 1:A:654:SER:O | 1:A:658:ASP:OD2 | 2.35 | 0.45 |
| 1:B:510:GLY:CA | 1:B:613:LYS:HD3 | 2.46 | 0.44 |
| 1:B:719:LYS:HG3 | 1:B:720:VAL:H | 1.81 | 0.44 |
| 1:A:480:LYS:N | 1:A:699:ASN:HD22 | 2.14 | 0.44 |
| 1:B:459:VAL:HG12 | 1:B:622:LEU:HD23 | 1.95 | 0.44 |
| 1:A:510:GLY:HA3 | 1:A:613:LYS:HD3 | 2.00 | 0.44 |
| 1:A:598:ARG:HH11 | 1:A:649:ILE:CD1 | 2.31 | 0.44 |
| 1:B:573:MET:CE | 1:B:577:ILE:HG13 | 2.47 | 0.44 |
| 1:A:510:GLY:CA | 1:A:613:LYS:HD3 | 2.48 | 0.44 |
| 1:B:470:ILE:HG13 | 1:B:624:LEU:CD2 | 2.47 | 0.44 |
| 1:A:445:GLN:HG3 | 1:A:445:GLN:H | 1.41 | 0.44 |
| 1:A:570:SER:HB2 | 1:A:572:GLU:OE2 | 2.18 | 0.44 |
| 1:A:394:ARG:NH1 | 1:A:394:ARG:CG | 2.66 | 0.44 |
| 1:A:487:PRO:O | 1:A:489:ASP:N | 2.41 | 0.44 |
| 1:B:598:ARG:HH11 | 1:B:649:ILE:HD13 | 1.82 | 0.44 |
| 1:A:509:LYS:HB3 | 1:A:509:LYS:HE3 | 1.73 | 0.44 |
| 1:A:460:GLN:OE1 | 1:A:502:TRP:NE1 | 2.50 | 0.44 |
| 1:B:578:LEU:HD13 | 1:B:578:LEU:HA | 1.79 | 0.43 |
| 1:A:438:PHE:HE1 | 1:A:717:ALA:HB3 | 1.83 | 0.43 |
| 1:B:684:LEU:HB2 | 1:B:688:LEU:CD1 | 2.46 | 0.43 |
| 1:A:643:LEU:HB3 | 1:A:644:ARG:H | 1.52 | 0.43 |
| 1:B:716:PHE:CD1 | 1:B:717:ALA:N | 2.86 | 0.43 |
| 1:A:716:PHE:CD1 | 1:A:717:ALA:N | 2.87 | 0.43 |
| 1:B:458:LEU:HD12 | 1:B:693:LYS:CB | 2.48 | 0.43 |
| 1:B:460:GLN:OE1 | 1:B:502:TRP:NE1 | 2.50 | 0.43 |
| 1:B:438:PHE:HE1 | 1:B:717:ALA:HB3 | 1.84 | 0.43 |
| 1:A:458:LEU:HD12 | 1:A:693:LYS:HG2 | 2.00 | 0.43 |
| 1:A:517:CYS:HB2 | 1:A:604:ILE:O | 2.18 | 0.43 |
| 1:A:710:THR:HG22 | 1:A:714:LEU:HD11 | 2.00 | 0.43 |
| 1:B:389:VAL:HG12 | 1:B:438:PHE:HD1 | 1.83 | 0.43 |
| 1:B:611:ASN:CG | 1:B:611:ASN:O | 2.57 | 0.43 |
| 1:B:479:GLY:C | 1:B:699:ASN:HD22 | 2.22 | 0.43 |
| 1:A:479:GLY:C | 1:A:699:ASN:HD22 | 2.22 | 0.43 |
| 1:A:394:ARG:HE | 1:A:701:SER:CA | 2.31 | 0.43 |
| 1:A:570:SER:CB | 1:A:572:GLU:HG2 | 2.47 | 0.43 |
| 1:B:570:SER:HB2 | 1:B:572:GLU:OE2 | 2.18 | 0.43 |
| 1:A:448:ASN:HD22 | 1:A:490:GLY:N | 2.16 | 0.43 |
| 1:B:555:THR:O | 1:B:556:LYS:HB2 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:707:ILE:O | 1:B:711:LEU:CG | 2.63 | 0.43 |
| 1:B:621:THR:CG2 | 1:B:623:ASN:HD21 | 2.31 | 0.43 |
| 1:B:625:VAL:HG12 | 1:B:627:LEU:HD23 | 2.00 | 0.43 |
| 1:B:480:LYS:N | 1:B:699:ASN:HD22 | 2.16 | 0.43 |
| 1:B:573:MET:HG3 | 1:B:577:ILE:HD12 | 2.00 | 0.43 |
| 1:B:660:ILE:O | 1:B:661:HIS:C | 2.57 | 0.43 |
| 1:A:458:LEU:HD12 | 1:A:693:LYS:CB | 2.47 | 0.43 |
| 1:A:393:ILE:HD13 | 1:A:443:ASP:HA | 2.00 | 0.43 |
| 1:B:462:SER:HA | 1:B:466:TYR:O | 2.19 | 0.43 |
| 1:A:551:HIS:CE1 | 1:A:685:GLN:HG2 | 2.54 | 0.43 |
| 1:B:708:ASN:HA | 1:B:708:ASN:HD22 | 1.58 | 0.42 |
| 1:B:393:ILE:HD13 | 1:B:443:ASP:HA | 2.01 | 0.42 |
| 1:A:457:GLN:NE2 | 1:A:460:GLN:NE2 | 2.66 | 0.42 |
| 1:A:485:LEU:HD21 | 1:A:581:ALA:HB3 | 2.01 | 0.42 |
| 1:A:572:GLU:CD | 1:A:572:GLU:N | 2.72 | 0.42 |
| 1:A:500:PHE:HE1 | 1:A:574:VAL:HG21 | 1.82 | 0.42 |
| 1:A:470:ILE:HG13 | 1:A:624:LEU:HD22 | 2.02 | 0.42 |
| 1:A:554:GLU:HB2 | 1:A:555:THR:H | 1.69 | 0.42 |
| 1:B:422:MET:HB3 | 1:B:441:ILE:HD12 | 2.02 | 0.42 |
| 1:B:509:LYS:HE3 | 1:B:509:LYS:HB3 | 1.72 | 0.42 |
| 1:B:710:THR:HG22 | 1:B:714:LEU:HD11 | 2.00 | 0.42 |
| 1:A:660:ILE:O | 1:A:661:HIS:C | 2.58 | 0.42 |
| 1:A:574:VAL:CG1 | 1:A:578:LEU:CD2 | 2.97 | 0.42 |
| 1:A:394:ARG:HD3 | 1:A:701:SER:HA | 2.01 | 0.42 |
| 1:B:570:SER:CB | 1:B:572:GLU:HG2 | 2.48 | 0.42 |
| 1:B:551:HIS:CE1 | 1:B:685:GLN:HG2 | 2.55 | 0.42 |
| 1:A:671:ARG:HE | 1:A:671:ARG:HB2 | 1.39 | 0.42 |
| 1:A:456:GLY:C | 1:A:459:VAL:HG23 | 2.40 | 0.42 |
| 1:A:611:ASN:O | 1:A:611:ASN:CG | 2.57 | 0.42 |
| 1:B:394:ARG:HE | 1:B:701:SER:CA | 2.31 | 0.42 |
| 1:A:655:CYS:SG | 1:A:678:SER:HB2 | 2.60 | 0.42 |
| 1:B:654:SER:O | 1:B:658:ASP:OD2 | 2.37 | 0.42 |
| 1:B:457:GLN:O | 1:B:460:GLN:CG | 2.67 | 0.41 |
| 1:B:437:LYS:O | 1:B:437:LYS:CG | 2.68 | 0.41 |
| 1:A:560:ILE:CG2 | 1:A:563:VAL:HG21 | 2.51 | 0.41 |
| 1:A:389:VAL:HG12 | 1:A:438:PHE:HD1 | 1.84 | 0.41 |
| 1:B:394:ARG:HD3 | 1:B:701:SER:HA | 2.01 | 0.41 |
| 1:B:458:LEU:HD12 | 1:B:693:LYS:HG2 | 2.03 | 0.41 |
| 1:B:505:LYS:HD2 | 4:B:1133:HOH:O | 2.20 | 0.41 |
| 1:A:512:ASP:OD1 | 1:A:512:ASP:C | 2.59 | 0.41 |
| 1:B:595:HIS:C | 1:B:597:SER:N | 2.74 | 0.41 |
| 1:A:683:LEU:HD22 | 1:A:683:LEU:O | 2.21 | 0.41 |

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| Atom-1 | Atom-2 | Distance(Å) | Clash(Å) |
|---|---|---|---|
| 1:B:448:ASN:HD22 | 1:B:490:GLY:N | 2.18 | 0.41 |
| 1:B:532:ARG:O | 1:B:532:ARG:HG3 | 2.19 | 0.41 |
| 1:B:404:ASP:N | 4:B:1138:HOH:O | 2.53 | 0.41 |
| 1:A:575:GLU:O | 1:A:579:LYS:HB2 | 2.20 | 0.41 |
| 1:A:462:SER:HA | 1:A:466:TYR:O | 2.20 | 0.41 |
| 1:B:667:ASP:OD1 | 1:B:670:LYS:HG3 | 2.21 | 0.41 |
| 1:B:407:LEU:HD13 | 1:B:707:ILE:HG13 | 2.02 | 0.41 |
| 1:B:456:GLY:C | 1:B:459:VAL:HG23 | 2.40 | 0.41 |
| 1:B:581:ALA:HA | 1:B:584:LEU:HD12 | 2.03 | 0.41 |
| 1:B:572:GLU:N | 1:B:572:GLU:CD | 2.74 | 0.41 |
| 1:A:457:GLN:O | 1:A:460:GLN:CG | 2.68 | 0.41 |
| 1:A:610:SER:O | 1:A:611:ASN:CB | 2.68 | 0.41 |
| 1:A:407:LEU:HD13 | 1:A:707:ILE:HG13 | 2.03 | 0.41 |
| 1:B:663:LEU:HD13 | 1:B:688:LEU:O | 2.21 | 0.41 |
| 1:B:575:GLU:O | 1:B:579:LYS:HB2 | 2.20 | 0.41 |
| 1:B:708:ASN:HA | 1:B:711:LEU:HD12 | 2.03 | 0.40 |
| 1:B:574:VAL:CG1 | 1:B:578:LEU:CD2 | 2.97 | 0.40 |
| 1:B:439:ASP:O | 1:B:440:LYS:HB2 | 2.22 | 0.40 |
| 1:A:425:THR:OG1 | 1:A:433:VAL:CG2 | 2.65 | 0.40 |
| 1:A:581:ALA:HA | 1:A:584:LEU:HD12 | 2.02 | 0.40 |
| 1:A:614:THR:HG22 | 1:A:614:THR:O | 2.22 | 0.40 |
| 1:B:614:THR:O | 1:B:614:THR:HG22 | 2.21 | 0.40 |
| 1:B:470:ILE:HG13 | 1:B:624:LEU:HD22 | 2.04 | 0.40 |
| 1:B:455:VAL:C | 1:B:457:GLN:N | 2.74 | 0.40 |
| 1:B:683:LEU:O | 1:B:683:LEU:HD22 | 2.21 | 0.40 |
| 1:A:475:GLN:HE22 | 1:A:706:HIS:HB3 | 1.87 | 0.40 |
| 1:B:709:GLU:O | 1:B:709:GLU:CD | 2.60 | 0.40 |
| 1:B:663:LEU:HG | 1:B:673:ILE:HD13 | 2.03 | 0.40 |
| 1:A:598:ARG:HH11 | 1:A:649:ILE:HD13 | 1.85 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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 | 288/347 (83%) | 233 (81%) | 39 (14%) | 16 (6%) | 3 2 |
| 1 | B | 288/347 (83%) | 233 (81%) | 38 (13%) | 17 (6%) | 2 2 |
| All | All | 576/694 (83%) | 466 (81%) | 77 (13%) | 33 (6%) | 3 2 |

All (33) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 405 | THR |
| 1 | A | 415 | ASP |
| 1 | A | 420 | GLN |
| 1 | A | 440 | LYS |
| 1 | A | 511 | TRP |
| 1 | A | 611 | ASN |
| 1 | B | 405 | THR |
| 1 | B | 415 | ASP |
| 1 | B | 420 | GLN |
| 1 | B | 440 | LYS |
| 1 | B | 511 | TRP |
| 1 | B | 611 | ASN |
| 1 | A | 396 | ALA |
| 1 | A | 419 | VAL |
| 1 | A | 438 | PHE |
| 1 | A | 456 | GLY |
| 1 | A | 490 | GLY |
| 1 | A | 512 | ASP |
| 1 | A | 525 | GLU |
| 1 | A | 666 | PRO |
| 1 | B | 396 | ALA |
| 1 | B | 419 | VAL |
| 1 | B | 438 | PHE |
| 1 | B | 456 | GLY |
| 1 | B | 490 | GLY |
| 1 | B | 512 | ASP |
| 1 | B | 525 | GLU |
| 1 | B | 666 | PRO |
| 1 | A | 616 | ALA |
| 1 | B | 488 | GLY |
| 1 | B | 616 | ALA |
| 1 | A | 488 | GLY |
| 1 | B | 629 | 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 | 274/316 (87%) | 204 (74%) | 70 (26%) | 1 1 |
| 1 | B | 274/316 (87%) | 205 (75%) | 69 (25%) | 1 1 |
| All | All | 548/632 (87%) | 409 (75%) | 139 (25%) | 1 1 |

All (139) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 392 | ARG |
| 1 | A | 394 | ARG |
| 1 | A | 398 | LYS |
| 1 | A | 399 | ASN |
| 1 | A | 401 | GLU |
| 1 | A | 406 | SER |
| 1 | A | 407 | LEU |
| 1 | A | 423 | GLU |
| 1 | A | 435 | GLU |
| 1 | A | 437 | LYS |
| 1 | A | 440 | LYS |
| 1 | A | 444 | GLN |
| 1 | A | 445 | GLN |
| 1 | A | 447 | THR |
| 1 | A | 454 | GLU |
| 1 | A | 458 | LEU |
| 1 | A | 459 | VAL |
| 1 | A | 462 | SER |
| 1 | A | 463 | LEU |
| 1 | A | 475 | GLN |
| 1 | A | 484 | MET |
| 1 | A | 485 | LEU |
| 1 | A | 489 | ASP |
| 1 | A | 491 | ILE |
| 1 | A | 497 | SER |
| 1 | A | 499 | ILE |
| 1 | A | 500 | PHE |
| 1 | A | 505 | LYS |
| 1 | A | 506 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 507 | LYS |
| 1 | A | 512 | ASP |
| 1 | A | 514 | LYS |
| 1 | A | 516 | ASN |
| 1 | A | 520 | ILE |
| 1 | A | 521 | GLU |
| 1 | A | 532 | ARG |
| 1 | A | 545 | LEU |
| 1 | A | 548 | GLU |
| 1 | A | 554 | GLU |
| 1 | A | 567 | LYS |
| 1 | A | 572 | GLU |
| 1 | A | 575 | GLU |
| 1 | A | 578 | LEU |
| 1 | A | 583 | LYS |
| 1 | A | 586 | SER |
| 1 | A | 595 | HIS |
| 1 | A | 596 | SER |
| 1 | A | 599 | SER |
| 1 | A | 611 | ASN |
| 1 | A | 630 | SER |
| 1 | A | 643 | LEU |
| 1 | A | 644 | ARG |
| 1 | A | 652 | SER |
| 1 | A | 665 | GLN |
| 1 | A | 669 | THR |
| 1 | A | 670 | LYS |
| 1 | A | 671 | ARG |
| 1 | A | 676 | ARG |
| 1 | A | 679 | LYS |
| 1 | A | 683 | LEU |
| 1 | A | 684 | LEU |
| 1 | A | 686 | TYR |
| 1 | A | 688 | LEU |
| 1 | A | 693 | LYS |
| 1 | A | 700 | ILE |
| 1 | A | 701 | SER |
| 1 | A | 708 | ASN |
| 1 | A | 709 | GLU |
| 1 | A | 721 | ASN |
| 1 | A | 722 | SER |
| 1 | B | 392 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 394 | ARG |
| 1 | B | 398 | LYS |
| 1 | B | 399 | ASN |
| 1 | B | 401 | GLU |
| 1 | B | 406 | SER |
| 1 | B | 407 | LEU |
| 1 | B | 423 | GLU |
| 1 | B | 435 | GLU |
| 1 | B | 437 | LYS |
| 1 | B | 440 | LYS |
| 1 | B | 444 | GLN |
| 1 | B | 445 | GLN |
| 1 | B | 447 | THR |
| 1 | B | 454 | GLU |
| 1 | B | 458 | LEU |
| 1 | B | 459 | VAL |
| 1 | B | 462 | SER |
| 1 | B | 463 | LEU |
| 1 | B | 475 | GLN |
| 1 | B | 484 | MET |
| 1 | B | 485 | LEU |
| 1 | B | 489 | ASP |
| 1 | B | 491 | ILE |
| 1 | B | 497 | SER |
| 1 | B | 499 | ILE |
| 1 | B | 500 | PHE |
| 1 | B | 505 | LYS |
| 1 | B | 506 | LEU |
| 1 | B | 507 | LYS |
| 1 | B | 512 | ASP |
| 1 | B | 514 | LYS |
| 1 | B | 516 | ASN |
| 1 | B | 520 | ILE |
| 1 | B | 521 | GLU |
| 1 | B | 532 | ARG |
| 1 | B | 545 | LEU |
| 1 | B | 548 | GLU |
| 1 | B | 554 | GLU |
| 1 | B | 567 | LYS |
| 1 | B | 572 | GLU |
| 1 | B | 575 | GLU |
| 1 | B | 578 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 583 | LYS |
| 1 | B | 586 | SER |
| 1 | B | 595 | HIS |
| 1 | B | 596 | SER |
| 1 | B | 599 | SER |
| 1 | B | 611 | ASN |
| 1 | B | 630 | SER |
| 1 | B | 643 | LEU |
| 1 | B | 644 | ARG |
| 1 | B | 652 | SER |
| 1 | B | 665 | GLN |
| 1 | B | 669 | THR |
| 1 | B | 670 | LYS |
| 1 | B | 671 | ARG |
| 1 | B | 676 | ARG |
| 1 | B | 679 | LYS |
| 1 | B | 683 | LEU |
| 1 | B | 684 | LEU |
| 1 | B | 688 | LEU |
| 1 | B | 693 | LYS |
| 1 | B | 700 | ILE |
| 1 | B | 701 | SER |
| 1 | B | 708 | ASN |
| 1 | B | 709 | GLU |
| 1 | B | 721 | ASN |
| 1 | B | 722 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 416 | ASN |
| 1 | A | 448 | ASN |
| 1 | A | 457 | GLN |
| 1 | A | 475 | GLN |
| 1 | A | 486 | ASN |
| 1 | A | 516 | ASN |
| 1 | A | 623 | ASN |
| 1 | A | 685 | GLN |
| 1 | A | 699 | ASN |
| 1 | A | 706 | HIS |
| 1 | A | 708 | ASN |
| 1 | A | 721 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 416 | ASN |
| 1 | B | 448 | ASN |
| 1 | B | 457 | GLN |
| 1 | B | 475 | GLN |
| 1 | B | 486 | ASN |
| 1 | B | 516 | ASN |
| 1 | B | 623 | ASN |
| 1 | B | 685 | GLN |
| 1 | B | 699 | ASN |
| 1 | B | 706 | HIS |
| 1 | B | 708 | ASN |
| 1 | B | 721 | ASN |

#### 5.3.3 RNA

There are no RNA chains 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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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 | ADP | A | 998 | 2 | 29,29,29 | 1.45 | 5 (17%) | 45,45,45 | 2.19 | 6 (13%) |
| 3 | ADP | B | 999 | 2 | 29,29,29 | 1.51 | 6 (20%) | 45,45,45 | 2.22 | 6 (13%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | ADP | A | 998 | 2 | - | 0/16/32/32 | 0/1/3/3 |
| 3 | ADP | B | 999 | 2 | - | 0/16/32/32 | 0/1/3/3 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | B | 999 | ADP | C4-N9 | -4.37 | 1.31 | 1.37 |
| 3 | A | 998 | ADP | C4-N9 | -4.17 | 1.31 | 1.37 |
| 3 | A | 998 | ADP | PB-O3A | -2.89 | 1.55 | 1.60 |
| 3 | B | 999 | ADP | PB-O3A | -2.83 | 1.55 | 1.60 |
| 3 | B | 999 | ADP | C5-N7 | -2.71 | 1.30 | 1.40 |
| 3 | A | 998 | ADP | C5-N7 | -2.51 | 1.30 | 1.40 |
| 3 | B | 999 | ADP | O4'-C1' | 2.48 | 1.45 | 1.41 |
| 3 | A | 998 | ADP | O4'-C1' | 2.32 | 1.44 | 1.41 |
| 3 | B | 999 | ADP | PB-O2B | 2.24 | 1.62 | 1.54 |
| 3 | B | 999 | ADP | C8-N9 | -2.22 | 1.33 | 1.36 |
| 3 | A | 998 | ADP | PB-O2B | 2.03 | 1.62 | 1.54 |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | B | 999 | ADP | N3-C2-N1 | -12.14 | 118.56 | 128.71 |
| 3 | A | 998 | ADP | N3-C2-N1 | -11.94 | 118.72 | 128.71 |
| 3 | B | 999 | ADP | N3-C4-N9 | 4.65 | 133.82 | 125.43 |
| 3 | A | 998 | ADP | N3-C4-N9 | 4.54 | 133.63 | 125.43 |
| 3 | B | 999 | ADP | C2-N3-C4 | 3.16 | 123.00 | 114.01 |
| 3 | A | 998 | ADP | C2-N3-C4 | 3.04 | 122.67 | 114.01 |
| 3 | B | 999 | ADP | C5-C4-N3 | -2.97 | 119.24 | 125.70 |
| 3 | A | 998 | ADP | C5-C4-N3 | -2.95 | 119.27 | 125.70 |
| 3 | A | 998 | ADP | C4-C5-N7 | -2.80 | 107.12 | 109.52 |
| 3 | B | 999 | ADP | C4-C5-N7 | -2.62 | 107.28 | 109.52 |
| 3 | B | 999 | ADP | O4'-C1'-N9 | 2.34 | 110.61 | 108.44 |
| 3 | A | 998 | ADP | O4'-C1'-N9 | 2.03 | 110.33 | 108.44 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 | 300/347 (86%) | 0.45 | 18 (6%) | 21 | 21 | 16, 41, 75, 86 | 0 |
| 1 | B | 300/347 (86%) | 0.40 | 14 (4%) | 30 | 31 | 14, 41, 76, 84 | 0 |
| All | All | 600/694 (86%) | 0.43 | 32 (5%) | 25 | 26 | 14, 41, 76, 86 | 0 |

All (32) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 666 | PRO | 4.8 |
| 1 | A | 587 | THR | 4.4 |
| 1 | B | 632 | ARG | 4.1 |
| 1 | B | 643 | LEU | 4.1 |
| 1 | A | 385 | GLY | 4.0 |
| 1 | A | 666 | PRO | 4.0 |
| 1 | A | 664 | GLY | 4.0 |
| 1 | A | 400 | LEU | 3.7 |
| 1 | A | 632 | ARG | 3.7 |
| 1 | A | 669 | THR | 3.6 |
| 1 | B | 399 | ASN | 3.4 |
| 1 | B | 670 | LYS | 3.1 |
| 1 | B | 644 | ARG | 3.1 |
| 1 | A | 508 | THR | 3.0 |
| 1 | B | 433 | VAL | 2.9 |
| 1 | A | 668 | SER | 2.9 |
| 1 | A | 617 | HIS | 2.9 |
| 1 | A | 433 | VAL | 2.7 |
| 1 | A | 720 | VAL | 2.6 |
| 1 | B | 613 | LYS | 2.6 |
| 1 | B | 385 | GLY | 2.5 |
| 1 | B | 397 | LEU | 2.4 |
| 1 | A | 613 | LYS | 2.4 |
| 1 | B | 614 | THR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 672 | HIS | 2.3 |
| 1 | A | 598 | ARG | 2.3 |
| 1 | B | 400 | LEU | 2.2 |
| 1 | A | 719 | LYS | 2.1 |
| 1 | B | 398 | LYS | 2.1 |
| 1 | A | 399 | ASN | 2.0 |
| 1 | A | 717 | ALA | 2.0 |
| 1 | A | 660 | ILE | 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 | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | MG | A | 996 | 1/1 | 0.20 | 0.80 | 36,36,36,36 | 0 |
| 3 | ADP | A | 998 | 27/27 | 0.17 | -0.12 | 27,42,53,57 | 0 |
| 2 | MG | B | 997 | 1/1 | 0.18 | -0.21 | 38,38,38,38 | 0 |
| 3 | ADP | B | 999 | 27/27 | 0.15 | -0.25 | 28,40,55,58 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.