



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:07 AM GMT

PDB ID : 3KR5
Title : Structure of a protease 4
Authors : McGowan, S.; Whisstock, J.C.
Deposited on : 2009-11-17
Resolution : 2.56 Å(reported)

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

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

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

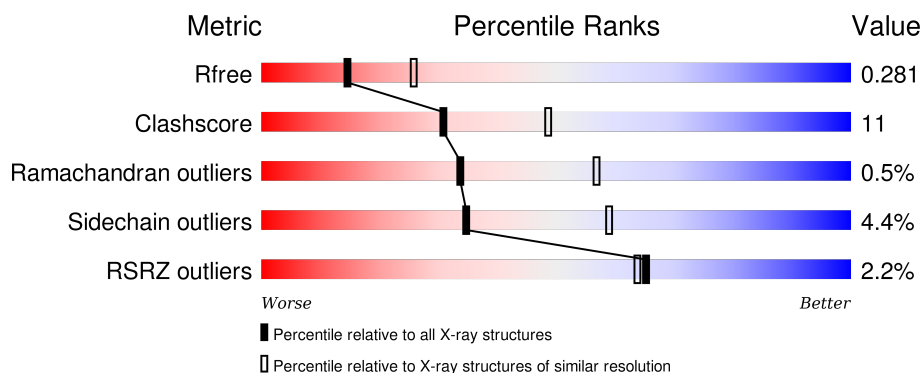
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 3324 (2.60-2.52) |
| Clashscore | 102246 | 3729 (2.60-2.52) |
| Ramachandran outliers | 100387 | 3673 (2.60-2.52) |
| Sidechain outliers | 100360 | 3673 (2.60-2.52) |
| RSRZ outliers | 91569 | 3333 (2.60-2.52) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 | 528 | <div> <div>2%</div> <div>75%</div> <div>21%</div> <div>• •</div> </div> |
| 1 | B | 528 | <div> <div>2%</div> <div>75%</div> <div>22%</div> <div>• •</div> </div> |
| 1 | C | 528 | <div> <div>76%</div> <div>21%</div> <div>• •</div> </div> |
| 1 | D | 528 | <div> <div>%</div> <div>74%</div> <div>20%</div> <div>• •</div> </div> |
| 1 | E | 528 | <div> <div>%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | F | 528 | |
| 1 | G | 528 | |
| 1 | H | 528 | |
| 1 | I | 528 | |
| 1 | J | 528 | |
| 1 | K | 528 | |
| 1 | L | 528 | |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2 | CO3 | D | 1002 | - | - | X | - |
| 2 | CO3 | J | 1002 | - | - | - | X |
| 2 | CO3 | K | 1002 | - | - | X | - |
| 5 | SO4 | E | 7 | - | - | X | - |
| 5 | SO4 | G | 26 | - | - | - | X |
| 6 | 1PE | A | 20 | - | - | - | X |
| 6 | 1PE | B | 60 | - | - | - | X |
| 6 | 1PE | D | 44 | - | - | - | X |
| 6 | 1PE | D | 67 | - | - | - | X |
| 6 | 1PE | F | 31 | - | - | - | X |
| 6 | 1PE | F | 33 | - | - | - | X |
| 6 | 1PE | G | 58 | - | - | - | X |
| 6 | 1PE | H | 64 | - | - | - | X |
| 6 | 1PE | K | 50 | - | - | - | X |
| 6 | 1PE | L | 612 | - | - | - | X |

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 50444 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 M17 leucyl aminopeptidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 518 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3980 | 2556 | 639 | 765 | 20 | | | |
| 1 | B | 518 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3929 | 2527 | 635 | 747 | 20 | | | |
| 1 | C | 518 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3953 | 2544 | 637 | 752 | 20 | | | |
| 1 | D | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3928 | 2531 | 633 | 744 | 20 | | | |
| 1 | E | 510 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3897 | 2509 | 626 | 743 | 19 | | | |
| 1 | F | 510 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3873 | 2492 | 624 | 738 | 19 | | | |
| 1 | G | 516 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3989 | 2560 | 650 | 760 | 19 | | | |
| 1 | H | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3938 | 2531 | 640 | 748 | 19 | | | |
| 1 | I | 518 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4006 | 2569 | 651 | 766 | 20 | | | |
| 1 | J | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3954 | 2539 | 639 | 756 | 20 | | | |
| 1 | K | 509 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3930 | 2525 | 637 | 749 | 19 | | | |
| 1 | L | 513 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3932 | 2526 | 634 | 753 | 19 | | | |

There are 108 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| A | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| A | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| A | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| A | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| A | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| A | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| A | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| B | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| B | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| B | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| B | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| C | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| C | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| C | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| C | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| D | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| D | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| D | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| D | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| E | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| E | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| E | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| E | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| F | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |

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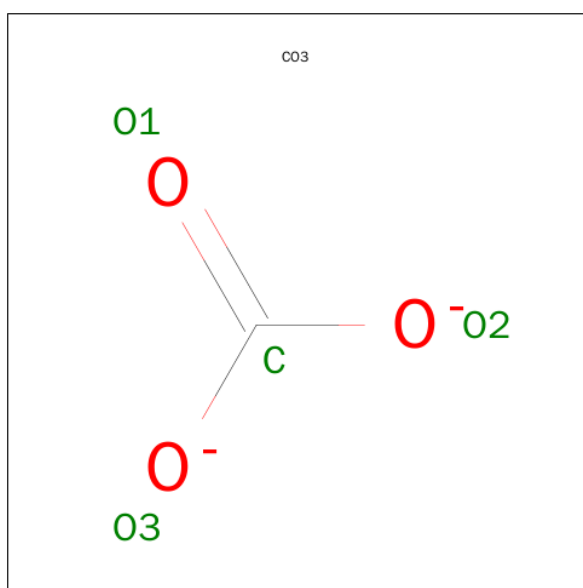
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| F | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| F | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| F | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| G | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| G | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| G | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| G | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| H | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| H | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| H | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| H | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| I | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| I | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| I | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| I | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| J | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| J | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| J | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| J | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| J | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| J | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| J | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| J | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| J | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| K | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| K | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| K | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| K | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 152 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| L | 515 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| L | 546 | GLN | ASN | ENGINEERED | UNP Q8IL11 |
| L | 606 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 607 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 608 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 609 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 610 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |
| L | 611 | HIS | - | EXPRESSION TAG | UNP Q8IL11 |

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 2 | C | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | D | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | E | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | F | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | G | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | H | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | I | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | J | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | K | 1 | Total C O 4 1 3 | 0 | 0 |
| 2 | L | 1 | Total C O 4 1 3 | 0 | 0 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

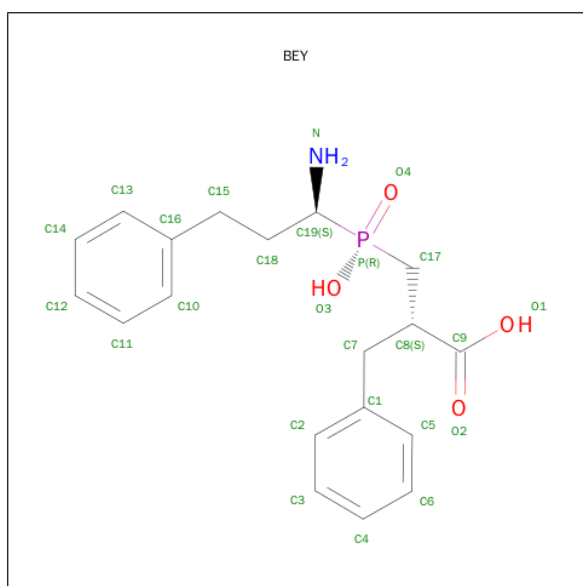
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3 | G | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | J | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | D | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | K | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | E | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | H | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | B | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | I | 2 | Total Zn 2 2 | 0 | 0 |
| 3 | C | 2 | Total Zn 2 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | A | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | L | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | F | 2 | Total | Zn | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 4 is (2S)-3-[(R)-[(1S)-1-AMINO-3-PHENYLPROPYL](HYDROXY)PHOSPHORYL]-2-BENZYLPROPANOIC ACID (three-letter code: BEY) (formula: C₁₉H₂₄NO₄P).



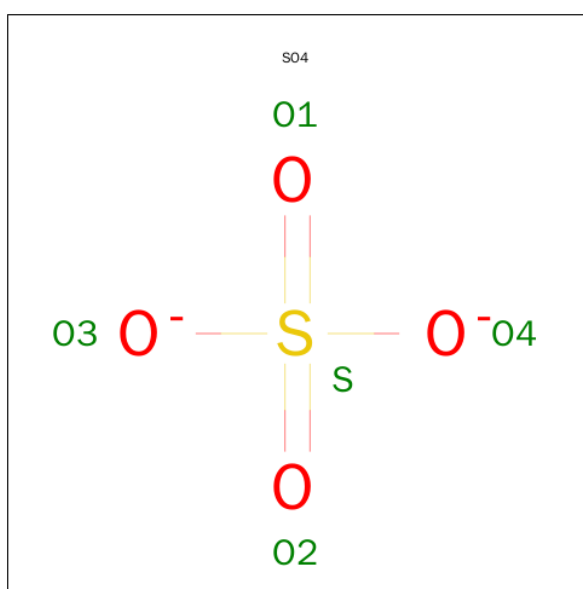
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | E | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | F | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | G | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | H | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 4 | I | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | J | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | K | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |
| 4 | L | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 25 | 19 | 1 | 4 | 1 | | |

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



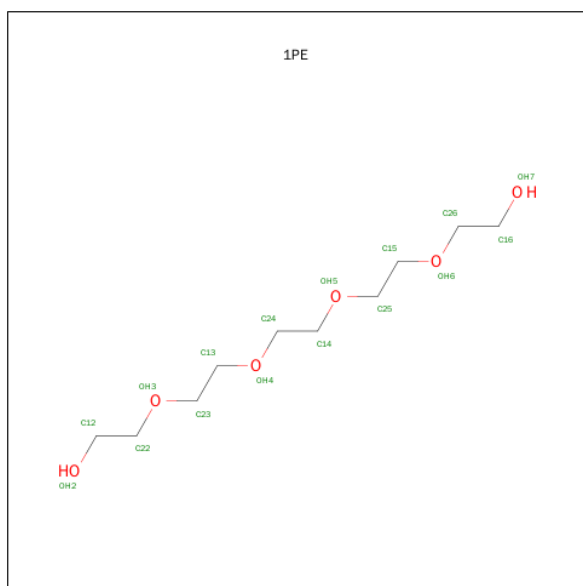
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | C | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | D | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | E | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 5 | F | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | G | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | I | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | J | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | K | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 5 | L | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 6 | A | 1 | Total | C | O | 0 | 0 |
| | | | 9 | 6 | 3 | | |
| 6 | A | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | B | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6 | B | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | B | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | C | 1 | Total | C | O | 0 | 0 |
| | | | 13 | 9 | 4 | | |
| 6 | C | 1 | Total | C | O | 0 | 0 |
| | | | 9 | 6 | 3 | | |
| 6 | D | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | D | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 8 | 3 | | |
| 6 | D | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | D | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 5 | 2 | | |
| 6 | E | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | E | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | E | 1 | Total | C | O | 0 | 0 |
| | | | 8 | 5 | 3 | | |
| 6 | F | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 6 | F | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 6 | F | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 6 | G | 1 | Total | C | O | 0 | 0 |
| | | | 9 | 6 | 3 | | |
| 6 | G | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 4 | 3 | | |
| 6 | G | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 6 | G | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 6 | G | 1 | Total | C | O | 0 | 0 |
| | | | 15 | 10 | 5 | | |
| 6 | H | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | H | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |

Continued on next page...

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| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 6 | I | 1 | Total | C | O | 0 | 0 |
| | | | 15 | 10 | 5 | | |
| 6 | I | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 8 | 3 | | |
| 6 | I | 1 | Total | C | O | 0 | 0 |
| | | | 7 | 5 | 2 | | |
| 6 | J | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 7 | 4 | | |
| 6 | J | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 6 | J | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 6 | K | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | K | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | K | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 7 | 4 | | |
| 6 | K | 1 | Total | C | O | 0 | 0 |
| | | | 6 | 4 | 2 | | |
| 6 | L | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 6 | 4 | | |
| 6 | L | 1 | Total | C | O | 0 | 0 |
| | | | 12 | 8 | 4 | | |
| 6 | L | 1 | Total | C | O | 0 | 0 |
| | | | 11 | 7 | 4 | | |

- Molecule 7 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 7 | A | 217 | Total | O | 0 | 0 |
| | | | 217 | 217 | | |
| 7 | B | 158 | Total | O | 0 | 0 |
| | | | 158 | 158 | | |
| 7 | C | 188 | Total | O | 0 | 0 |
| | | | 188 | 188 | | |
| 7 | D | 182 | Total | O | 0 | 0 |
| | | | 182 | 182 | | |
| 7 | E | 203 | Total | O | 0 | 0 |
| | | | 203 | 203 | | |
| 7 | F | 165 | Total | O | 0 | 0 |
| | | | 165 | 165 | | |

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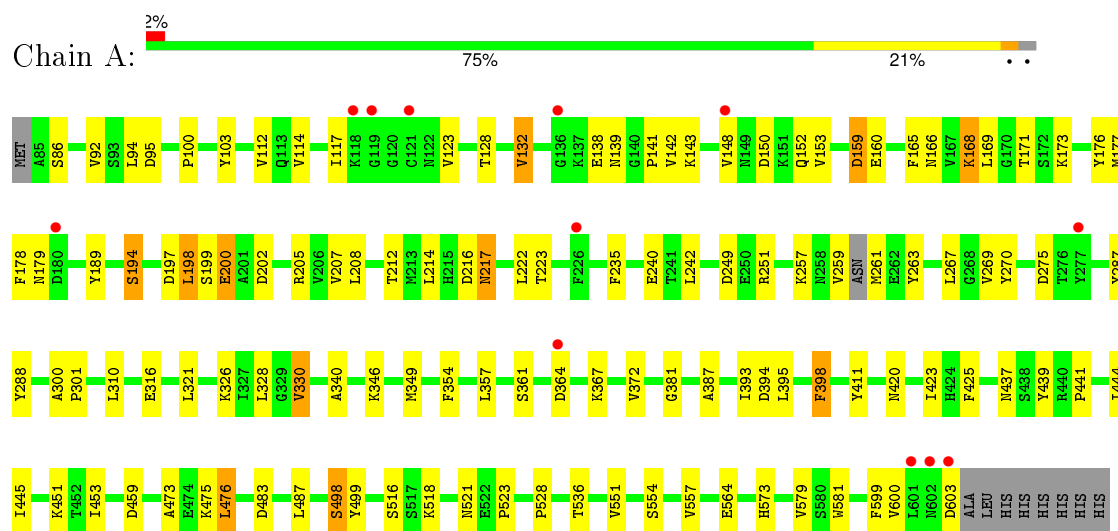
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 7 | G | 204 | Total 204 | O 204 | 0 | 0 |
| 7 | H | 203 | Total 203 | O 203 | 0 | 0 |
| 7 | I | 207 | Total 207 | O 207 | 0 | 0 |
| 7 | J | 207 | Total 207 | O 207 | 0 | 0 |
| 7 | K | 222 | Total 222 | O 222 | 0 | 0 |
| 7 | L | 158 | Total 158 | O 158 | 0 | 0 |

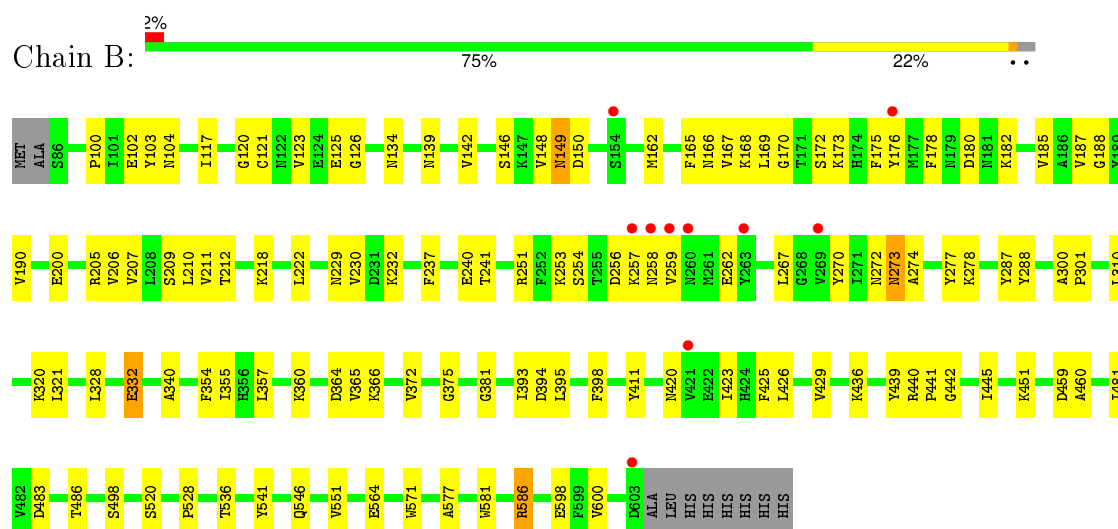
3 Residue-property plots [i](#)

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

• Molecule 1: M17 leucyl aminopeptidase

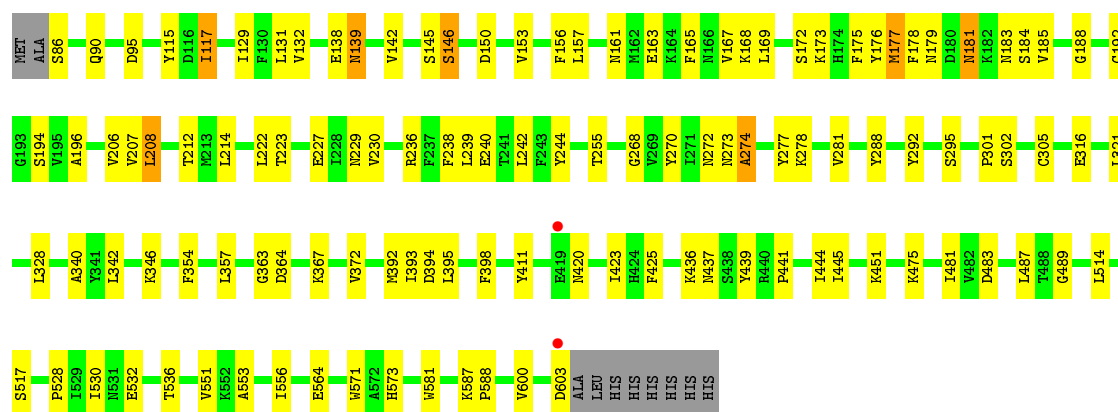


• Molecule 1: M17 leucyl aminopeptidase

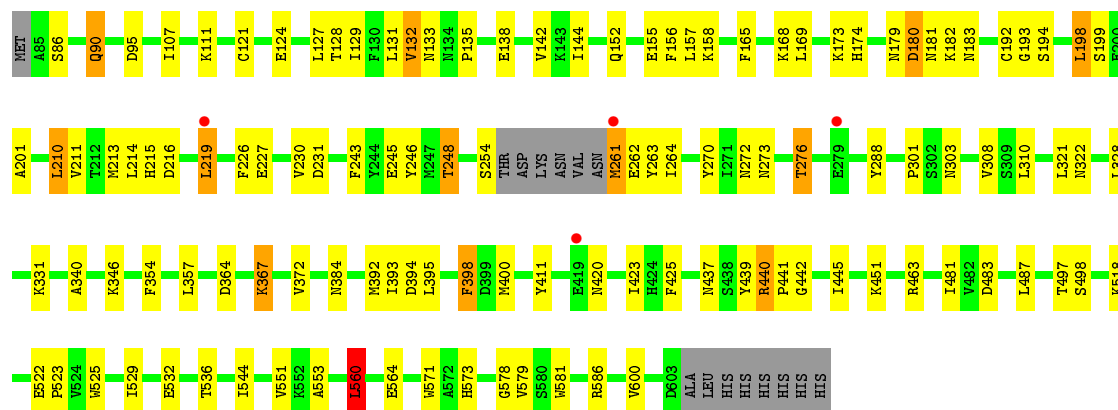
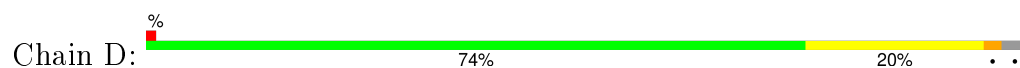


• Molecule 1: M17 leucyl aminopeptidase

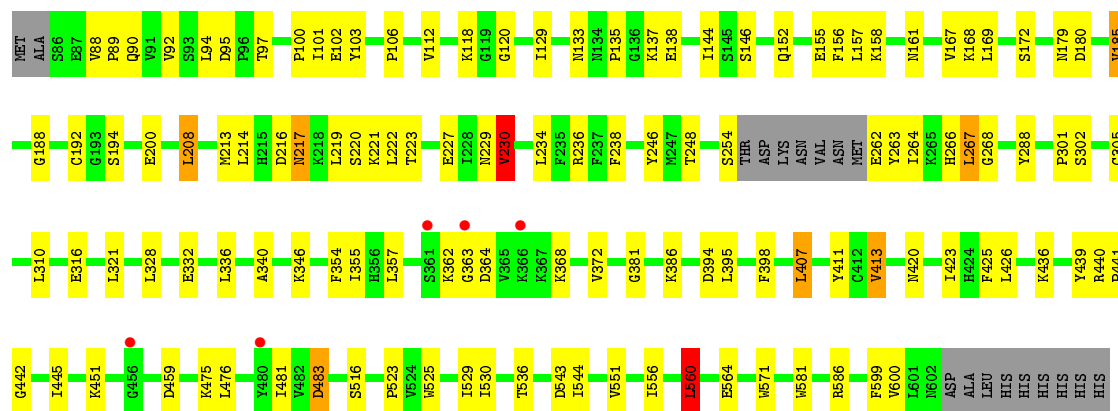
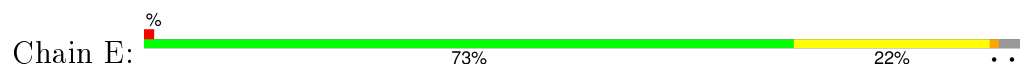




• Molecule 1: M17 leucyl aminopeptidase

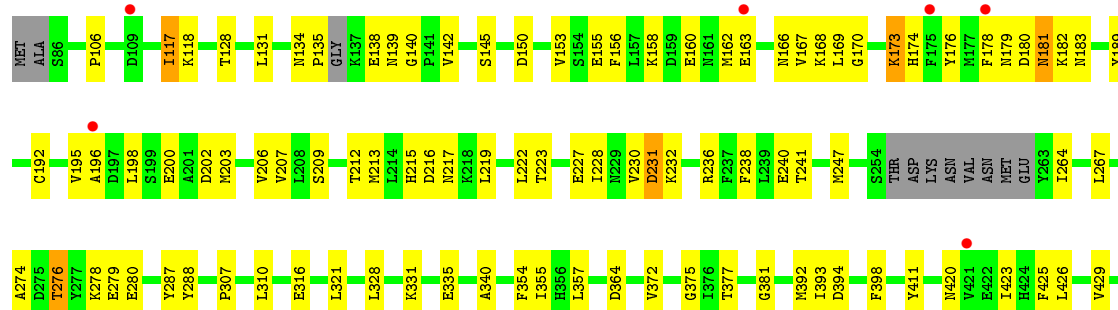


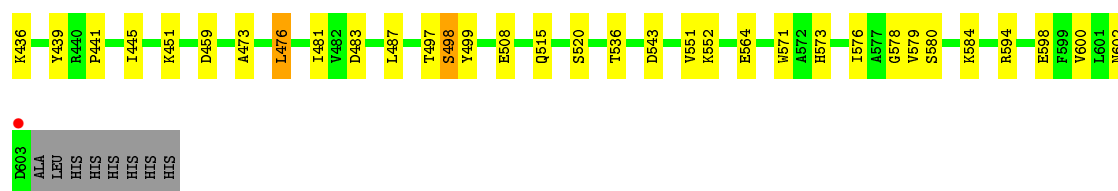
• Molecule 1: M17 leucyl aminopeptidase



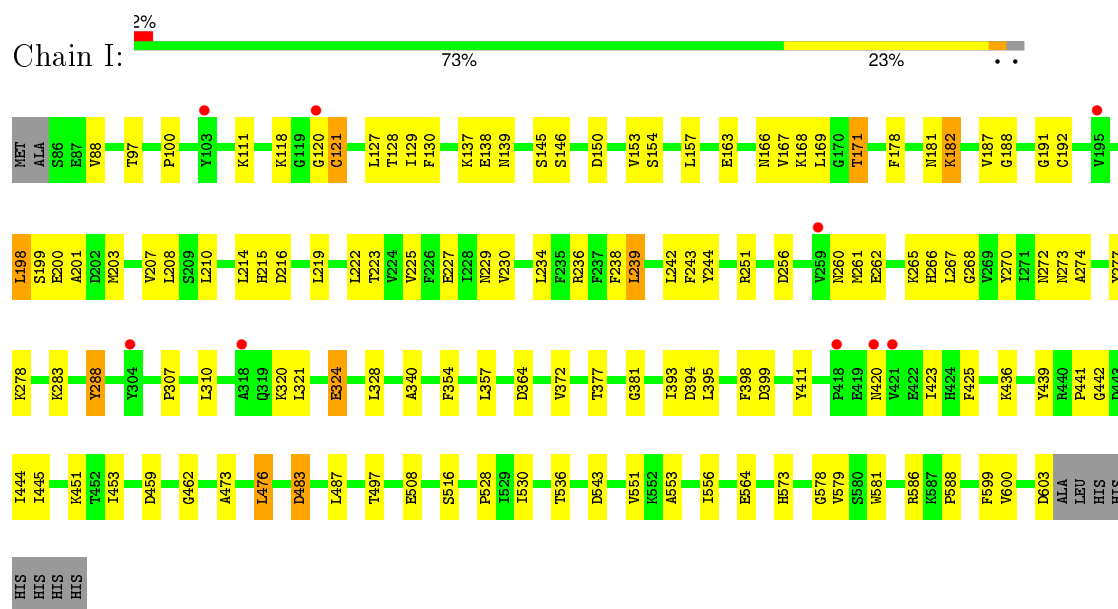
• Molecule 1: M17 leucyl aminopeptidase



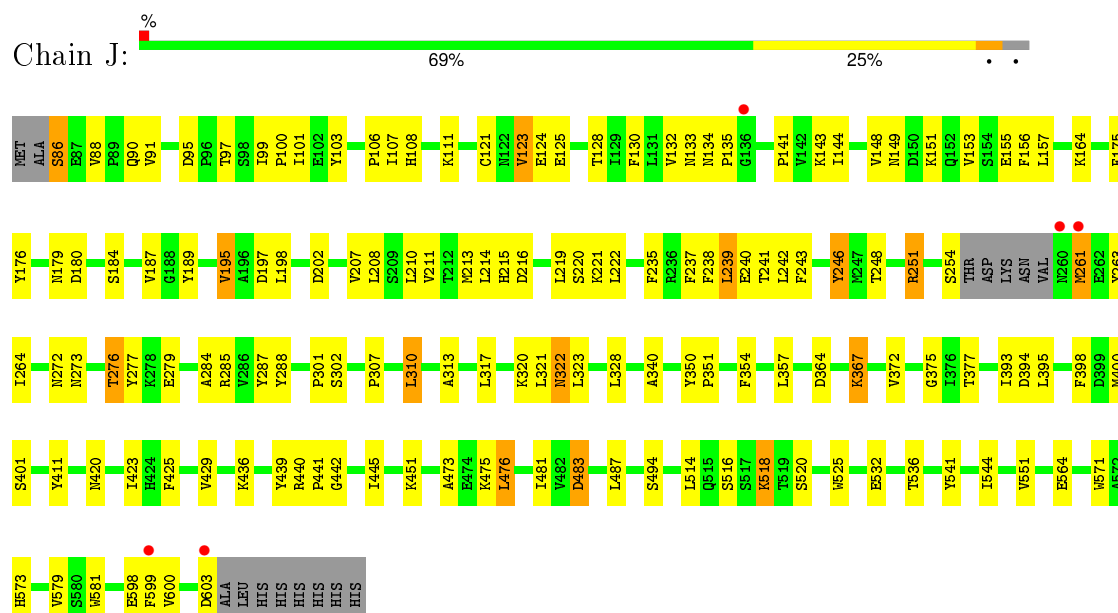




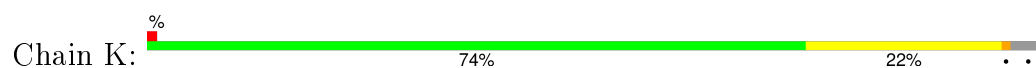
• Molecule 1: M17 leucyl aminopeptidase

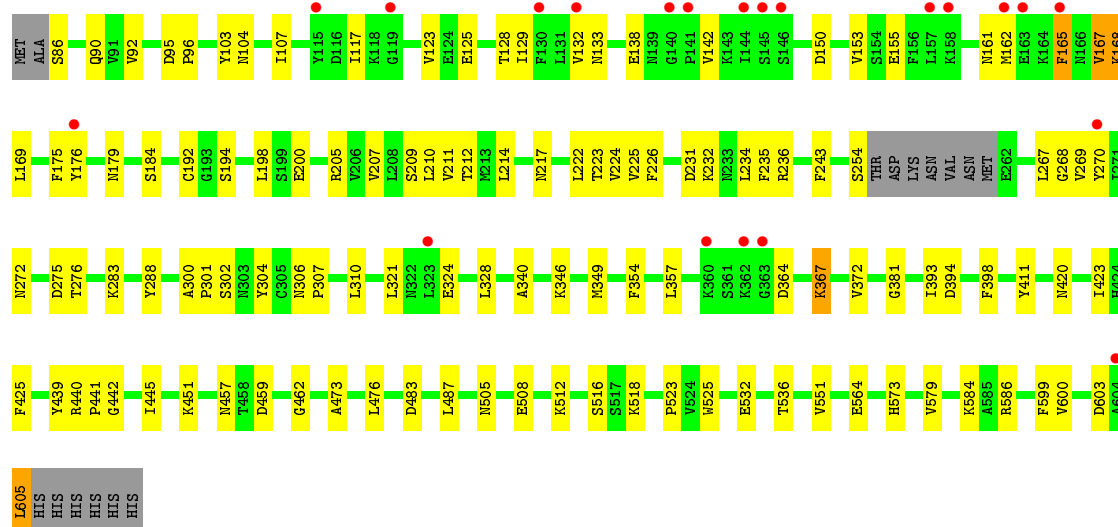


• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 172.08Å 174.16Å 227.71Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 77.70 – 2.56 77.70 – 2.56 | Depositor EDS |
| % Data completeness (in resolution range) | 98.8 (77.70-2.56) 98.8 (77.70-2.56) | Depositor EDS |
| R_{merge} | 0.55 | Depositor |
| R_{sym} | 0.16 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.02 (at 2.55Å) | Xtriage |
| Refinement program | REFMAC 5.5.0102 | Depositor |
| R, R_{free} | 0.220 , 0.278 0.224 , 0.281 | Depositor DCC |
| R_{free} test set | 10903 reflections (5.27%) | DCC |
| Wilson B-factor (Å ²) | 25.1 | Xtriage |
| Anisotropy | 0.511 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 49.0 | EDS |
| Estimated twinning fraction | 0.000 for k,h,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$ | Xtriage |
| Outliers | 4 of 217775 reflections (0.002%) | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 50444 | wwPDB-VP |
| Average B, all atoms (Å ²) | 29.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.88 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.3151e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CO3, BEY, ZN, 1PE

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 | 0.67 | 0/4057 | 0.71 | 1/5500 (0.0%) |
| 1 | B | 0.63 | 0/4007 | 0.69 | 2/5442 (0.0%) |
| 1 | C | 0.67 | 1/4031 (0.0%) | 0.71 | 0/5469 |
| 1 | D | 0.69 | 0/4005 | 0.74 | 6/5429 (0.1%) |
| 1 | E | 0.71 | 1/3974 (0.0%) | 0.76 | 6/5393 (0.1%) |
| 1 | F | 0.64 | 1/3949 (0.0%) | 0.76 | 3/5364 (0.1%) |
| 1 | G | 0.69 | 0/4066 | 0.71 | 1/5505 (0.0%) |
| 1 | H | 0.66 | 0/4014 | 0.68 | 0/5434 |
| 1 | I | 0.68 | 0/4084 | 0.79 | 3/5531 (0.1%) |
| 1 | J | 0.70 | 0/4031 | 0.72 | 0/5461 |
| 1 | K | 0.72 | 0/4006 | 0.75 | 1/5427 (0.0%) |
| 1 | L | 0.66 | 0/4009 | 0.69 | 1/5440 (0.0%) |
| All | All | 0.68 | 3/48233 (0.0%) | 0.72 | 24/65395 (0.0%) |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | E | 305 | CYS | CB-SG | -5.60 | 1.72 | 1.81 |
| 1 | C | 305 | CYS | CB-SG | -5.25 | 1.73 | 1.81 |
| 1 | F | 430 | CYS | CB-SG | -5.20 | 1.73 | 1.81 |

All (24) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | I | 586 | ARG | NE-CZ-NH2 | 17.78 | 129.19 | 120.30 |
| 1 | I | 586 | ARG | NE-CZ-NH1 | -17.07 | 111.76 | 120.30 |
| 1 | F | 586 | ARG | NE-CZ-NH2 | 16.73 | 128.66 | 120.30 |
| 1 | F | 586 | ARG | NE-CZ-NH1 | -16.10 | 112.25 | 120.30 |
| 1 | F | 586 | ARG | CD-NE-CZ | 8.03 | 134.84 | 123.60 |
| 1 | I | 586 | ARG | CD-NE-CZ | 7.90 | 134.65 | 123.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | D | 560 | LEU | CB-CG-CD1 | 6.85 | 122.64 | 111.00 |
| 1 | K | 586 | ARG | NE-CZ-NH1 | 6.31 | 123.46 | 120.30 |
| 1 | D | 210 | LEU | CA-CB-CG | 5.94 | 128.96 | 115.30 |
| 1 | E | 560 | LEU | CA-CB-CG | 5.93 | 128.95 | 115.30 |
| 1 | E | 407 | LEU | CB-CG-CD1 | 5.88 | 120.99 | 111.00 |
| 1 | D | 586 | ARG | NE-CZ-NH2 | -5.77 | 117.42 | 120.30 |
| 1 | E | 407 | LEU | CB-CG-CD2 | 5.75 | 120.78 | 111.00 |
| 1 | E | 560 | LEU | CB-CG-CD1 | 5.65 | 120.61 | 111.00 |
| 1 | E | 586 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | D | 560 | LEU | CA-CB-CG | 5.54 | 128.03 | 115.30 |
| 1 | E | 413 | VAL | CG1-CB-CG2 | 5.49 | 119.69 | 110.90 |
| 1 | G | 586 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 1 | A | 330 | VAL | CG1-CB-CG2 | 5.38 | 119.51 | 110.90 |
| 1 | D | 463 | ARG | NE-CZ-NH2 | -5.37 | 117.61 | 120.30 |
| 1 | B | 586 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 1 | L | 586 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | D | 440 | ARG | NE-CZ-NH2 | -5.10 | 117.75 | 120.30 |
| 1 | B | 586 | ARG | NE-CZ-NH1 | 5.03 | 122.82 | 120.30 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3980 | 0 | 3912 | 93 | 0 |
| 1 | B | 3929 | 0 | 3828 | 87 | 1 |
| 1 | C | 3953 | 0 | 3882 | 89 | 0 |
| 1 | D | 3928 | 0 | 3876 | 102 | 0 |
| 1 | E | 3897 | 0 | 3822 | 92 | 0 |
| 1 | F | 3873 | 0 | 3772 | 98 | 0 |
| 1 | G | 3989 | 0 | 3976 | 95 | 0 |
| 1 | H | 3938 | 0 | 3931 | 84 | 0 |
| 1 | I | 4006 | 0 | 3986 | 93 | 0 |
| 1 | J | 3954 | 0 | 3923 | 120 | 0 |
| 1 | K | 3930 | 0 | 3901 | 84 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | L | 3932 | 0 | 3862 | 86 | 0 |
| 2 | A | 4 | 0 | 0 | 0 | 0 |
| 2 | B | 4 | 0 | 0 | 0 | 0 |
| 2 | C | 4 | 0 | 0 | 0 | 0 |
| 2 | D | 4 | 0 | 0 | 2 | 0 |
| 2 | E | 4 | 0 | 0 | 0 | 0 |
| 2 | F | 4 | 0 | 0 | 0 | 0 |
| 2 | G | 4 | 0 | 0 | 0 | 0 |
| 2 | H | 4 | 0 | 0 | 1 | 0 |
| 2 | I | 4 | 0 | 0 | 1 | 0 |
| 2 | J | 4 | 0 | 0 | 1 | 0 |
| 2 | K | 4 | 0 | 0 | 2 | 0 |
| 2 | L | 4 | 0 | 0 | 1 | 0 |
| 3 | A | 2 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| 3 | E | 2 | 0 | 0 | 0 | 0 |
| 3 | F | 2 | 0 | 0 | 0 | 0 |
| 3 | G | 2 | 0 | 0 | 0 | 0 |
| 3 | H | 2 | 0 | 0 | 0 | 0 |
| 3 | I | 2 | 0 | 0 | 0 | 0 |
| 3 | J | 2 | 0 | 0 | 0 | 0 |
| 3 | K | 2 | 0 | 0 | 0 | 0 |
| 3 | L | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 25 | 0 | 21 | 4 | 0 |
| 4 | B | 25 | 0 | 22 | 2 | 0 |
| 4 | C | 25 | 0 | 21 | 5 | 0 |
| 4 | D | 25 | 0 | 22 | 6 | 0 |
| 4 | E | 25 | 0 | 22 | 2 | 0 |
| 4 | F | 25 | 0 | 21 | 2 | 0 |
| 4 | G | 25 | 0 | 21 | 2 | 0 |
| 4 | H | 25 | 0 | 22 | 7 | 0 |
| 4 | I | 25 | 0 | 22 | 2 | 0 |
| 4 | J | 25 | 0 | 22 | 3 | 0 |
| 4 | K | 25 | 0 | 22 | 4 | 0 |
| 4 | L | 25 | 0 | 22 | 2 | 0 |
| 5 | A | 15 | 0 | 0 | 0 | 0 |
| 5 | C | 5 | 0 | 0 | 1 | 0 |
| 5 | D | 5 | 0 | 0 | 0 | 0 |
| 5 | E | 10 | 0 | 0 | 3 | 0 |
| 5 | F | 5 | 0 | 0 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | G | 10 | 0 | 0 | 0 | 0 |
| 5 | I | 5 | 0 | 0 | 1 | 0 |
| 5 | J | 10 | 0 | 0 | 2 | 0 |
| 5 | K | 5 | 0 | 0 | 0 | 0 |
| 5 | L | 5 | 0 | 0 | 0 | 0 |
| 6 | A | 21 | 0 | 22 | 2 | 0 |
| 6 | B | 30 | 0 | 30 | 3 | 0 |
| 6 | C | 22 | 0 | 24 | 1 | 0 |
| 6 | D | 38 | 0 | 38 | 5 | 0 |
| 6 | E | 32 | 0 | 36 | 3 | 0 |
| 6 | F | 30 | 0 | 39 | 1 | 0 |
| 6 | G | 43 | 0 | 47 | 4 | 0 |
| 6 | H | 20 | 0 | 20 | 1 | 0 |
| 6 | I | 33 | 0 | 37 | 5 | 0 |
| 6 | J | 31 | 0 | 36 | 9 | 0 |
| 6 | K | 41 | 0 | 44 | 8 | 0 |
| 6 | L | 33 | 0 | 40 | 5 | 0 |
| 7 | A | 217 | 0 | 0 | 12 | 0 |
| 7 | B | 158 | 0 | 0 | 7 | 0 |
| 7 | C | 188 | 0 | 0 | 6 | 0 |
| 7 | D | 182 | 0 | 0 | 5 | 1 |
| 7 | E | 203 | 0 | 0 | 15 | 0 |
| 7 | F | 165 | 0 | 0 | 14 | 0 |
| 7 | G | 204 | 0 | 0 | 11 | 0 |
| 7 | H | 203 | 0 | 0 | 6 | 0 |
| 7 | I | 207 | 0 | 0 | 6 | 0 |
| 7 | J | 207 | 0 | 0 | 18 | 0 |
| 7 | K | 222 | 0 | 0 | 7 | 0 |
| 7 | L | 158 | 0 | 0 | 11 | 0 |
| All | All | 50444 | 0 | 47344 | 1043 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1043) 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:H:436:LYS:HE2 | 7:I:3958:HOH:O | 1.43 | 1.15 |
| 1:B:257:LYS:HA | 1:B:258:ASN:HB3 | 1.34 | 1.09 |
| 1:J:518:LYS:HE2 | 7:J:2650:HOH:O | 1.52 | 1.08 |
| 1:I:214:LEU:HD21 | 1:I:222:LEU:HD22 | 1.39 | 1.03 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:320:LYS:NZ | 6:J:3:1PE:H142 | 1.74 | 1.02 |
| 1:G:136:GLY:HA3 | 1:G:137:LYS:CB | 1.86 | 1.02 |
| 1:B:436:LYS:HE2 | 7:C:3093:HOH:O | 1.59 | 0.99 |
| 1:J:254:SER:HB2 | 7:L:2793:HOH:O | 1.61 | 0.99 |
| 1:B:586:ARG:HA | 7:B:1076:HOH:O | 1.62 | 0.98 |
| 1:A:361:SER:HB3 | 7:A:755:HOH:O | 1.63 | 0.98 |
| 1:E:230:VAL:HG22 | 1:E:234:LEU:HB3 | 1.47 | 0.96 |
| 1:A:259:VAL:O | 1:A:261:MET:N | 2.00 | 0.94 |
| 1:K:133:ASN:HA | 1:K:167:VAL:HG11 | 1.48 | 0.94 |
| 1:C:230:VAL:O | 1:C:277:TYR:OH | 1.86 | 0.93 |
| 1:A:173:LYS:NZ | 1:D:216:ASP:OD2 | 2.01 | 0.92 |
| 1:I:230:VAL:O | 1:I:277:TYR:OH | 1.89 | 0.89 |
| 1:K:96:PRO:HA | 6:K:50:1PE:H142 | 1.58 | 0.86 |
| 1:B:274:ALA:O | 1:B:278:LYS:HG3 | 1.76 | 0.86 |
| 1:D:254:SER:HB2 | 7:F:1110:HOH:O | 1.75 | 0.86 |
| 1:J:320:LYS:HZ3 | 6:J:3:1PE:H142 | 1.40 | 0.86 |
| 1:B:178:PHE:HZ | 1:F:155:GLU:HG2 | 1.42 | 0.83 |
| 1:J:411:TYR:HE1 | 6:J:2:1PE:H151 | 1.44 | 0.82 |
| 1:I:328:LEU:HB2 | 1:I:354:PHE:HB3 | 1.61 | 0.82 |
| 1:I:121:CYS:SG | 1:I:225:VAL:HG21 | 2.19 | 0.82 |
| 1:F:231:ASP:HB2 | 7:F:3092:HOH:O | 1.79 | 0.82 |
| 1:D:127:LEU:HD11 | 1:D:129:ILE:HD11 | 1.60 | 0.82 |
| 1:E:229:ASN:O | 1:E:230:VAL:HB | 1.79 | 0.81 |
| 1:L:90:GLN:NE2 | 1:L:95:ASP:O | 2.13 | 0.81 |
| 1:F:117:ILE:HG13 | 1:F:270:TYR:HB3 | 1.60 | 0.81 |
| 1:G:178:PHE:HZ | 1:J:155:GLU:HG2 | 1.45 | 0.81 |
| 1:J:401:SER:HB3 | 7:J:748:HOH:O | 1.81 | 0.80 |
| 1:B:175:PHE:CD2 | 1:B:188:GLY:HA2 | 2.17 | 0.80 |
| 1:L:328:LEU:HB2 | 1:L:354:PHE:HB3 | 1.62 | 0.79 |
| 1:G:367:LYS:HG2 | 1:G:603:ASP:OD1 | 1.83 | 0.79 |
| 1:G:328:LEU:HB2 | 1:G:354:PHE:HB3 | 1.64 | 0.79 |
| 1:F:114:VAL:HG21 | 1:F:278:LYS:HG2 | 1.63 | 0.79 |
| 1:C:532:GLU:OE1 | 1:D:498:SER:OG | 1.99 | 0.79 |
| 1:C:328:LEU:HB2 | 1:C:354:PHE:HB3 | 1.66 | 0.77 |
| 1:A:216:ASP:O | 1:D:173:LYS:HE3 | 1.85 | 0.77 |
| 1:K:328:LEU:HB2 | 1:K:354:PHE:HB3 | 1.65 | 0.77 |
| 1:K:538:ASN:HB2 | 7:K:5283:HOH:O | 1.83 | 0.77 |
| 1:L:349:MET:HB2 | 7:L:2456:HOH:O | 1.84 | 0.77 |
| 1:K:173:LYS:HA | 7:K:1921:HOH:O | 1.84 | 0.77 |
| 1:J:328:LEU:HB2 | 1:J:354:PHE:HB3 | 1.65 | 0.76 |
| 1:B:175:PHE:HD2 | 1:B:188:GLY:HA2 | 1.50 | 0.76 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:340:ALA:HA | 1:I:445:ILE:HD12 | 1.68 | 0.76 |
| 1:J:394:ASP:HA | 1:L:441:PRO:HB2 | 1.68 | 0.75 |
| 1:B:328:LEU:HB2 | 1:B:354:PHE:HB3 | 1.66 | 0.75 |
| 1:H:328:LEU:HB2 | 1:H:354:PHE:HB3 | 1.66 | 0.75 |
| 1:E:144:ILE:HG13 | 1:E:157:LEU:HD22 | 1.68 | 0.75 |
| 1:E:230:VAL:HG23 | 1:E:234:LEU:HD23 | 1.67 | 0.74 |
| 1:D:90:GLN:HB3 | 1:D:95:ASP:HB2 | 1.66 | 0.74 |
| 1:J:164:LYS:HE2 | 7:J:944:HOH:O | 1.86 | 0.74 |
| 1:E:103:TYR:HB2 | 5:E:22:SO4:O3 | 1.88 | 0.74 |
| 1:K:441:PRO:HB2 | 1:L:394:ASP:HA | 1.68 | 0.74 |
| 1:G:441:PRO:HB2 | 1:H:394:ASP:HA | 1.70 | 0.74 |
| 1:E:441:PRO:HB2 | 1:F:394:ASP:HA | 1.69 | 0.74 |
| 6:J:45:1PE:H242 | 7:J:3061:HOH:O | 1.88 | 0.74 |
| 1:G:168:LYS:O | 1:G:171:THR:HG22 | 1.87 | 0.74 |
| 1:A:340:ALA:HA | 1:A:445:ILE:HD12 | 1.71 | 0.73 |
| 1:J:207:VAL:HG11 | 1:J:241:THR:HG22 | 1.71 | 0.72 |
| 1:H:192:CYS:HB3 | 1:H:198:LEU:HD11 | 1.71 | 0.72 |
| 1:A:178:PHE:CZ | 1:D:155:GLU:HG2 | 2.23 | 0.72 |
| 1:D:328:LEU:HB2 | 1:D:354:PHE:HB3 | 1.71 | 0.72 |
| 1:A:178:PHE:HZ | 1:D:155:GLU:CG | 2.02 | 0.72 |
| 1:C:363:GLY:HA3 | 7:C:4562:HOH:O | 1.90 | 0.72 |
| 1:D:219:LEU:H | 1:D:219:LEU:HD13 | 1.54 | 0.72 |
| 1:E:328:LEU:HB2 | 1:E:354:PHE:HB3 | 1.71 | 0.72 |
| 1:F:328:LEU:HB2 | 1:F:354:PHE:HB3 | 1.69 | 0.72 |
| 1:G:321:LEU:HD11 | 1:G:411:TYR:HA | 1.71 | 0.72 |
| 1:L:340:ALA:HA | 1:L:445:ILE:HD12 | 1.72 | 0.72 |
| 1:C:172:SER:O | 1:C:173:LYS:HD2 | 1.90 | 0.72 |
| 1:C:274:ALA:O | 1:C:278:LYS:HG3 | 1.89 | 0.71 |
| 1:D:394:ASP:HA | 1:F:441:PRO:HB2 | 1.72 | 0.71 |
| 1:E:475:LYS:HD3 | 7:E:4546:HOH:O | 1.89 | 0.71 |
| 1:E:321:LEU:HD11 | 1:E:411:TYR:HA | 1.72 | 0.71 |
| 1:I:215:HIS:O | 1:I:216:ASP:HB2 | 1.88 | 0.71 |
| 1:L:132:VAL:HG21 | 1:L:142:VAL:HG13 | 1.72 | 0.71 |
| 1:J:237:PHE:HA | 1:J:240:GLU:OE1 | 1.91 | 0.71 |
| 1:L:176:TYR:OH | 1:L:217:ASN:OD1 | 2.04 | 0.71 |
| 1:F:117:ILE:HD11 | 1:F:225:VAL:HG13 | 1.72 | 0.71 |
| 1:I:178:PHE:HZ | 1:K:155:GLU:HG2 | 1.56 | 0.71 |
| 1:K:451:LYS:HD3 | 6:K:42:1PE:H231 | 1.73 | 0.71 |
| 1:B:253:LYS:HD2 | 1:B:256:ASP:HB3 | 1.73 | 0.71 |
| 1:K:144:ILE:HG13 | 1:K:157:LEU:HD22 | 1.73 | 0.71 |
| 1:A:321:LEU:HD11 | 1:A:411:TYR:HA | 1.71 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:132:VAL:HG21 | 1:C:142:VAL:HG13 | 1.73 | 0.70 |
| 1:J:321:LEU:O | 1:J:322:ASN:HB2 | 1.90 | 0.70 |
| 1:D:179:ASN:OD1 | 1:D:183:ASN:HB2 | 1.92 | 0.70 |
| 1:I:128:THR:HB | 1:I:187:VAL:HG13 | 1.73 | 0.70 |
| 1:K:340:ALA:HA | 1:K:445:ILE:HD12 | 1.71 | 0.70 |
| 1:C:321:LEU:HD11 | 1:C:411:TYR:HA | 1.74 | 0.70 |
| 1:H:392:MET:CE | 4:H:1003:BEY:H12 | 2.22 | 0.70 |
| 1:A:173:LYS:CE | 1:D:216:ASP:OD2 | 2.40 | 0.70 |
| 1:F:340:ALA:HA | 1:F:445:ILE:HD12 | 1.72 | 0.70 |
| 1:K:321:LEU:HD11 | 1:K:411:TYR:HA | 1.74 | 0.70 |
| 1:D:340:ALA:HA | 1:D:445:ILE:HD12 | 1.74 | 0.70 |
| 1:K:386:LYS:NZ | 4:K:1003:BEY:O3 | 2.23 | 0.69 |
| 1:D:321:LEU:HD11 | 1:D:411:TYR:HA | 1.73 | 0.69 |
| 1:C:173:LYS:NZ | 1:E:217:ASN:OD1 | 2.25 | 0.69 |
| 1:L:104:ASN:OD1 | 6:L:1:1PE:H141 | 1.92 | 0.69 |
| 1:J:151:LYS:N | 1:J:180:ASP:OD2 | 2.24 | 0.69 |
| 1:H:321:LEU:HD11 | 1:H:411:TYR:HA | 1.73 | 0.69 |
| 1:A:441:PRO:HB2 | 1:B:394:ASP:HA | 1.74 | 0.69 |
| 1:G:340:ALA:HA | 1:G:445:ILE:HD12 | 1.75 | 0.69 |
| 1:D:441:PRO:HB2 | 1:E:394:ASP:HA | 1.74 | 0.69 |
| 1:B:257:LYS:HA | 1:B:258:ASN:CB | 2.18 | 0.69 |
| 1:J:320:LYS:HZ1 | 6:J:3:1PE:H142 | 1.58 | 0.69 |
| 1:H:240:GLU:OE2 | 1:H:287:TYR:HD2 | 1.75 | 0.69 |
| 1:E:100:PRO:O | 1:E:101:ILE:HD13 | 1.92 | 0.69 |
| 1:F:321:LEU:HD11 | 1:F:411:TYR:HA | 1.76 | 0.68 |
| 1:G:207:VAL:HG11 | 1:G:241:THR:HG22 | 1.75 | 0.68 |
| 1:I:244:TYR:OH | 1:I:588:PRO:O | 2.12 | 0.68 |
| 1:H:232:LYS:HE3 | 1:H:276:THR:HB | 1.74 | 0.68 |
| 1:H:441:PRO:HB2 | 1:I:394:ASP:HA | 1.75 | 0.68 |
| 1:D:174:HIS:CE1 | 1:D:213:MET:HG2 | 2.29 | 0.68 |
| 1:K:133:ASN:HB2 | 1:K:193:GLY:O | 1.94 | 0.68 |
| 1:I:321:LEU:HD11 | 1:I:411:TYR:HA | 1.76 | 0.68 |
| 1:K:133:ASN:CA | 1:K:167:VAL:HG11 | 2.23 | 0.68 |
| 1:L:321:LEU:HD11 | 1:L:411:TYR:HA | 1.76 | 0.68 |
| 1:H:392:MET:HE1 | 4:H:1003:BEY:H12 | 1.75 | 0.68 |
| 1:H:340:ALA:HA | 1:H:445:ILE:HD12 | 1.75 | 0.67 |
| 6:D:63:1PE:C25 | 7:D:3204:HOH:O | 2.42 | 0.67 |
| 1:A:178:PHE:HZ | 1:D:155:GLU:HG2 | 1.58 | 0.67 |
| 1:J:219:LEU:HD11 | 7:J:3193:HOH:O | 1.94 | 0.67 |
| 1:G:117:ILE:HD11 | 1:G:226:PHE:O | 1.95 | 0.67 |
| 1:F:107:ILE:HG21 | 1:F:243:PHE:HB3 | 1.77 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:332:GLU:HB3 | 7:B:675:HOH:O | 1.93 | 0.67 |
| 1:J:441:PRO:HB2 | 1:K:394:ASP:HA | 1.75 | 0.67 |
| 1:A:208:LEU:O | 1:A:212:THR:HG23 | 1.94 | 0.67 |
| 1:E:340:ALA:HA | 1:E:445:ILE:HD12 | 1.75 | 0.67 |
| 1:B:441:PRO:HB2 | 1:C:394:ASP:HA | 1.76 | 0.67 |
| 1:A:328:LEU:HB2 | 1:A:354:PHE:HB3 | 1.76 | 0.66 |
| 1:C:340:ALA:HA | 1:C:445:ILE:HD12 | 1.76 | 0.66 |
| 1:I:169:LEU:HA | 1:I:191:GLY:O | 1.94 | 0.66 |
| 1:F:156:PHE:O | 1:F:162:MET:HE3 | 1.95 | 0.66 |
| 1:I:274:ALA:O | 1:I:278:LYS:HG3 | 1.95 | 0.66 |
| 1:G:173:LYS:HD2 | 1:J:176:TYR:HE1 | 1.61 | 0.66 |
| 1:C:274:ALA:HB1 | 1:C:278:LYS:HE3 | 1.78 | 0.65 |
| 1:L:462:GLY:N | 2:L:1002:CO3:O2 | 2.27 | 0.65 |
| 1:J:215:HIS:O | 1:J:261:MET:HB3 | 1.96 | 0.65 |
| 1:B:230:VAL:O | 1:B:277:TYR:OH | 2.09 | 0.65 |
| 1:L:107:ILE:HG21 | 1:L:243:PHE:HB3 | 1.78 | 0.65 |
| 1:C:173:LYS:HE3 | 1:E:217:ASN:OD1 | 1.97 | 0.65 |
| 1:B:102:GLU:CG | 7:B:4121:HOH:O | 2.45 | 0.65 |
| 1:B:139:ASN:O | 1:B:166:ASN:HB2 | 1.97 | 0.65 |
| 1:B:321:LEU:HD11 | 1:B:411:TYR:HA | 1.77 | 0.65 |
| 2:D:1002:CO3:O2 | 4:D:1003:BEY:H7A | 1.97 | 0.64 |
| 1:B:218:LYS:HG2 | 1:B:262:GLU:CD | 2.18 | 0.64 |
| 1:G:394:ASP:HA | 1:I:441:PRO:HB2 | 1.78 | 0.64 |
| 1:C:153:VAL:HG12 | 1:C:157:LEU:CD1 | 2.27 | 0.64 |
| 1:I:129:ILE:HA | 1:I:188:GLY:O | 1.97 | 0.64 |
| 1:I:230:VAL:HG22 | 1:I:234:LEU:HB3 | 1.79 | 0.64 |
| 1:B:232:LYS:HB2 | 7:B:4536:HOH:O | 1.96 | 0.64 |
| 1:A:132:VAL:HG21 | 1:A:142:VAL:HG13 | 1.80 | 0.64 |
| 1:H:274:ALA:O | 1:H:278:LYS:HG3 | 1.97 | 0.64 |
| 1:H:240:GLU:OE2 | 1:H:287:TYR:CD2 | 2.51 | 0.64 |
| 1:G:136:GLY:CA | 1:G:137:LYS:CB | 2.72 | 0.63 |
| 1:H:150:ASP:OD2 | 1:H:153:VAL:HG23 | 1.98 | 0.63 |
| 1:B:142:VAL:HG23 | 1:B:162:MET:HB3 | 1.80 | 0.63 |
| 1:D:451:LYS:HE2 | 6:D:44:1PE:H151 | 1.79 | 0.63 |
| 1:J:123:VAL:O | 1:J:123:VAL:HG23 | 1.96 | 0.63 |
| 1:K:176:TYR:OH | 1:K:217:ASN:OD1 | 2.14 | 0.63 |
| 1:D:423:ILE:HD11 | 1:D:600:VAL:HG13 | 1.80 | 0.63 |
| 1:J:321:LEU:O | 1:J:322:ASN:CB | 2.43 | 0.63 |
| 1:J:88:VAL:HG11 | 1:J:97:THR:O | 1.98 | 0.63 |
| 1:D:331:LYS:CD | 1:D:331:LYS:H | 2.09 | 0.63 |
| 1:A:372:VAL:O | 1:A:483:ASP:HA | 1.99 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:118:LYS:HE3 | 7:I:4080:HOH:O | 1.98 | 0.63 |
| 1:J:340:ALA:HA | 1:J:445:ILE:HD12 | 1.81 | 0.63 |
| 1:D:192:CYS:HB3 | 1:D:198:LEU:HD21 | 1.79 | 0.63 |
| 1:H:173:LYS:HB2 | 1:H:189:TYR:CE1 | 2.33 | 0.63 |
| 1:C:178:PHE:HZ | 1:E:155:GLU:HG2 | 1.64 | 0.63 |
| 1:L:231:ASP:HB3 | 1:L:234:LEU:H | 1.64 | 0.62 |
| 1:D:124:GLU:HA | 1:D:179:ASN:ND2 | 2.14 | 0.62 |
| 1:I:238:PHE:HD2 | 1:I:239:LEU:HD13 | 1.63 | 0.62 |
| 1:A:498:SER:OG | 1:F:532:GLU:OE1 | 2.17 | 0.62 |
| 1:D:273:ASN:O | 1:D:276:THR:HG23 | 2.00 | 0.62 |
| 1:K:236:ARG:NE | 1:K:240:GLU:OE2 | 2.27 | 0.62 |
| 1:C:146:SER:OG | 1:C:227:GLU:OE2 | 2.16 | 0.62 |
| 1:J:144:ILE:HG13 | 1:J:157:LEU:HD22 | 1.81 | 0.62 |
| 1:H:167:VAL:O | 1:H:168:LYS:C | 2.36 | 0.62 |
| 1:J:198:LEU:HD22 | 1:J:202:ASP:HB3 | 1.82 | 0.62 |
| 1:A:523:PRO:HA | 7:A:1372:HOH:O | 1.98 | 0.62 |
| 1:L:451:LYS:HE2 | 6:L:612:1PE:H241 | 1.82 | 0.62 |
| 1:L:367:LYS:HG2 | 1:L:603:ASP:OD2 | 1.99 | 0.62 |
| 1:A:499:TYR:CZ | 1:A:523:PRO:HB3 | 2.35 | 0.62 |
| 1:L:138:GLU:HA | 1:L:194:SER:OG | 1.99 | 0.62 |
| 1:B:148:VAL:O | 1:B:150:ASP:N | 2.28 | 0.62 |
| 1:C:153:VAL:HG12 | 1:C:157:LEU:HD11 | 1.80 | 0.62 |
| 1:A:499:TYR:CD2 | 1:A:523:PRO:HB2 | 2.34 | 0.62 |
| 1:L:523:PRO:HD3 | 7:L:644:HOH:O | 1.99 | 0.62 |
| 1:H:192:CYS:O | 1:H:198:LEU:HD21 | 1.99 | 0.61 |
| 1:K:554:SER:HB3 | 7:K:3921:HOH:O | 1.99 | 0.61 |
| 1:C:173:LYS:CE | 1:E:217:ASN:OD1 | 2.49 | 0.61 |
| 1:H:174:HIS:HB3 | 1:L:175:PHE:CD1 | 2.35 | 0.61 |
| 1:A:518:LYS:HB2 | 7:A:3052:HOH:O | 2.00 | 0.61 |
| 1:F:213:MET:O | 1:F:217:ASN:HB2 | 1.99 | 0.61 |
| 1:K:451:LYS:HE3 | 1:K:564:GLU:O | 2.00 | 0.61 |
| 1:D:124:GLU:HA | 1:D:179:ASN:HD22 | 1.66 | 0.61 |
| 1:J:423:ILE:HD11 | 1:J:600:VAL:HG13 | 1.81 | 0.61 |
| 1:J:123:VAL:HG21 | 1:J:153:VAL:HG21 | 1.83 | 0.61 |
| 1:G:372:VAL:O | 1:G:483:ASP:HA | 2.01 | 0.61 |
| 1:B:320:LYS:NZ | 6:B:61:1PE:H241 | 2.15 | 0.61 |
| 1:G:132:VAL:HG21 | 1:G:142:VAL:HG13 | 1.83 | 0.60 |
| 1:E:436:LYS:HG2 | 5:E:7:SO4:O4 | 2.00 | 0.60 |
| 1:A:394:ASP:HA | 1:C:441:PRO:HB2 | 1.82 | 0.60 |
| 1:C:223:THR:HA | 1:C:268:GLY:O | 2.01 | 0.60 |
| 1:D:529:ILE:CG2 | 1:D:560:LEU:HD13 | 2.31 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:214:LEU:HD21 | 1:C:222:LEU:HD22 | 1.82 | 0.60 |
| 1:I:230:VAL:HG23 | 1:I:234:LEU:HD23 | 1.83 | 0.60 |
| 1:H:174:HIS:HB3 | 1:L:175:PHE:CE1 | 2.36 | 0.60 |
| 1:G:201:ALA:HB1 | 1:L:532:GLU:OE1 | 2.01 | 0.60 |
| 1:H:106:PRO:HD2 | 1:H:247:MET:SD | 2.42 | 0.60 |
| 1:D:301:PRO:HB3 | 1:F:442:GLY:O | 2.01 | 0.60 |
| 1:B:176:TYR:OH | 1:F:155:GLU:HG3 | 2.02 | 0.60 |
| 2:K:1002:CO3:O2 | 4:K:1003:BEY:H17A | 2.02 | 0.60 |
| 1:D:132:VAL:HG21 | 1:D:142:VAL:HG13 | 1.83 | 0.60 |
| 1:F:237:PHE:HA | 1:F:240:GLU:OE1 | 2.01 | 0.60 |
| 1:A:387:ALA:HB1 | 7:A:5072:HOH:O | 2.01 | 0.60 |
| 1:L:209:SER:O | 1:L:212:THR:HB | 2.01 | 0.60 |
| 1:J:321:LEU:HD11 | 1:J:411:TYR:HA | 1.82 | 0.60 |
| 1:D:155:GLU:O | 1:D:158:LYS:HG2 | 2.02 | 0.60 |
| 1:E:451:LYS:HE3 | 1:E:564:GLU:O | 2.02 | 0.59 |
| 1:L:451:LYS:HG3 | 6:L:612:1PE:H131 | 1.85 | 0.59 |
| 1:J:123:VAL:CG2 | 1:J:153:VAL:HG21 | 2.32 | 0.59 |
| 1:G:473:ALA:O | 1:G:476:LEU:HB2 | 2.03 | 0.59 |
| 1:A:398:PHE:HZ | 4:A:1003:BEY:H13 | 1.67 | 0.59 |
| 1:D:219:LEU:HD23 | 1:D:264:ILE:HG22 | 1.83 | 0.59 |
| 1:E:152:GLN:HG2 | 1:E:180:ASP:OD1 | 2.03 | 0.59 |
| 1:K:122:ASN:OD1 | 1:K:149:ASN:HB2 | 2.02 | 0.59 |
| 1:L:605:LEU:HD21 | 7:L:5436:HOH:O | 2.01 | 0.59 |
| 1:C:138:GLU:O | 1:C:139:ASN:HB2 | 2.03 | 0.59 |
| 1:B:451:LYS:HE3 | 1:B:564:GLU:O | 2.03 | 0.58 |
| 1:L:169:LEU:HD23 | 1:L:205:ARG:HH21 | 1.69 | 0.58 |
| 1:B:340:ALA:HA | 1:B:445:ILE:HD12 | 1.85 | 0.58 |
| 1:E:230:VAL:CG2 | 1:E:234:LEU:HB3 | 2.27 | 0.58 |
| 1:J:240:GLU:OE2 | 1:J:287:TYR:HD2 | 1.86 | 0.58 |
| 1:H:117:ILE:HG23 | 1:H:118:LYS:N | 2.18 | 0.58 |
| 1:D:423:ILE:HD11 | 1:D:600:VAL:CG1 | 2.34 | 0.58 |
| 1:F:372:VAL:O | 1:F:483:ASP:HA | 2.03 | 0.58 |
| 1:H:170:GLY:O | 1:H:209:SER:OG | 2.21 | 0.58 |
| 1:E:372:VAL:O | 1:E:483:ASP:HA | 2.03 | 0.58 |
| 1:G:208:LEU:O | 1:G:212:THR:HG23 | 2.03 | 0.58 |
| 1:L:423:ILE:HD11 | 1:L:600:VAL:HG13 | 1.85 | 0.58 |
| 1:A:441:PRO:HG2 | 1:B:393:ILE:HG12 | 1.84 | 0.58 |
| 1:D:107:ILE:HG21 | 1:D:243:PHE:HB3 | 1.85 | 0.58 |
| 1:B:486:THR:O | 4:B:1003:BEY:N | 2.37 | 0.58 |
| 1:K:473:ALA:O | 1:K:476:LEU:HB2 | 2.04 | 0.57 |
| 1:I:138:GLU:O | 1:I:139:ASN:HB2 | 2.04 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:E:386:LYS:NZ | 4:E:1003:BEY:O3 | 2.34 | 0.57 |
| 1:A:554:SER:HB3 | 7:A:2697:HOH:O | 2.04 | 0.57 |
| 1:F:179:ASN:OD1 | 1:F:183:ASN:HB2 | 2.04 | 0.57 |
| 1:A:117:ILE:HG13 | 1:A:270:TYR:HB3 | 1.85 | 0.57 |
| 1:K:125:GLU:HG3 | 1:K:221:LYS:HD2 | 1.85 | 0.57 |
| 1:B:218:LYS:HG2 | 1:B:262:GLU:OE2 | 2.04 | 0.57 |
| 1:F:249:ASP:OD2 | 1:F:251:ARG:NH2 | 2.29 | 0.57 |
| 1:B:207:VAL:HG11 | 1:B:241:THR:HG22 | 1.85 | 0.57 |
| 1:B:123:VAL:HG12 | 1:B:185:VAL:HG21 | 1.86 | 0.57 |
| 1:F:489:GLY:N | 4:F:1003:BEY:O1 | 2.33 | 0.57 |
| 1:G:324:GLU:HG3 | 7:G:3727:HOH:O | 2.05 | 0.57 |
| 1:J:440:ARG:NH2 | 7:J:635:HOH:O | 2.37 | 0.57 |
| 1:G:136:GLY:N | 7:G:3954:HOH:O | 2.38 | 0.57 |
| 1:J:411:TYR:CE1 | 6:J:2:1PE:H151 | 2.33 | 0.57 |
| 1:A:321:LEU:CD1 | 1:A:411:TYR:HA | 2.35 | 0.57 |
| 1:D:138:GLU:HA | 1:D:194:SER:OG | 2.05 | 0.57 |
| 1:I:320:LYS:NZ | 6:I:21:1PE:OH7 | 2.37 | 0.57 |
| 1:C:475:LYS:HD3 | 7:C:3447:HOH:O | 2.04 | 0.57 |
| 1:A:487:LEU:O | 4:A:1003:BEY:H17A | 2.05 | 0.57 |
| 1:J:301:PRO:HB3 | 1:L:442:GLY:O | 2.04 | 0.57 |
| 1:D:215:HIS:C | 1:D:261:MET:HB3 | 2.26 | 0.56 |
| 1:D:215:HIS:O | 1:D:261:MET:HB3 | 2.05 | 0.56 |
| 1:C:244:TYR:OH | 1:C:588:PRO:O | 2.23 | 0.56 |
| 1:E:213:MET:HG3 | 7:E:1714:HOH:O | 2.04 | 0.56 |
| 1:L:473:ALA:O | 1:L:476:LEU:HB2 | 2.05 | 0.56 |
| 1:D:248:THR:HG23 | 1:D:263:TYR:OH | 2.06 | 0.56 |
| 1:F:347:GLY:N | 7:F:618:HOH:O | 2.38 | 0.56 |
| 1:L:381:GLY:HA2 | 1:L:459:ASP:OD1 | 2.05 | 0.56 |
| 1:A:381:GLY:HA2 | 1:A:459:ASP:OD1 | 2.05 | 0.56 |
| 1:F:179:ASN:CG | 1:F:183:ASN:HB2 | 2.26 | 0.56 |
| 1:A:103:TYR:CD1 | 6:A:20:1PE:H251 | 2.41 | 0.56 |
| 1:F:381:GLY:HA2 | 1:F:459:ASP:OD1 | 2.05 | 0.56 |
| 1:J:254:SER:CB | 7:L:2793:HOH:O | 2.35 | 0.56 |
| 1:K:133:ASN:HA | 1:K:167:VAL:CG1 | 2.29 | 0.56 |
| 1:E:332:GLU:HG3 | 7:E:4802:HOH:O | 2.04 | 0.56 |
| 1:F:423:ILE:HD11 | 1:F:600:VAL:HG13 | 1.87 | 0.56 |
| 1:J:322:ASN:HA | 7:J:3618:HOH:O | 2.06 | 0.56 |
| 1:B:240:GLU:OE2 | 1:B:287:TYR:HD2 | 1.88 | 0.56 |
| 1:E:423:ILE:HD11 | 1:E:600:VAL:HG13 | 1.88 | 0.56 |
| 1:D:372:VAL:O | 1:D:483:ASP:HA | 2.05 | 0.56 |
| 1:I:436:LYS:HG2 | 5:I:17:SO4:O3 | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:L:222:LEU:O | 1:L:267:LEU:HA | 2.06 | 0.56 |
| 1:J:211:VAL:HG12 | 7:J:5351:HOH:O | 2.04 | 0.56 |
| 1:L:372:VAL:O | 1:L:483:ASP:HA | 2.06 | 0.56 |
| 1:F:320:LYS:HD3 | 6:F:31:1PE:H141 | 1.88 | 0.56 |
| 1:J:123:VAL:CG2 | 1:J:123:VAL:O | 2.53 | 0.55 |
| 1:K:463:ARG:NE | 2:K:1002:CO3:O1 | 2.27 | 0.55 |
| 1:D:451:LYS:HE3 | 1:D:564:GLU:O | 2.06 | 0.55 |
| 1:K:372:VAL:O | 1:K:483:ASP:HA | 2.06 | 0.55 |
| 1:G:451:LYS:HE3 | 1:G:564:GLU:O | 2.05 | 0.55 |
| 1:C:117:ILE:HG22 | 1:C:272:ASN:HA | 1.89 | 0.55 |
| 1:H:145:SER:N | 1:H:227:GLU:OE1 | 2.38 | 0.55 |
| 1:I:127:LEU:HB2 | 1:I:219:LEU:HD22 | 1.87 | 0.55 |
| 1:G:236:ARG:HD3 | 1:G:283:LYS:HD3 | 1.88 | 0.55 |
| 2:J:1002:CO3:O1 | 4:J:1003:BEY:H7A | 2.06 | 0.55 |
| 1:G:357:LEU:HB2 | 1:G:425:PHE:HB2 | 1.88 | 0.55 |
| 1:H:179:ASN:OD1 | 1:H:183:ASN:HB2 | 2.06 | 0.55 |
| 1:G:487:LEU:O | 4:G:1003:BEY:H17A | 2.06 | 0.55 |
| 1:L:133:ASN:HB3 | 1:L:192:CYS:HB2 | 1.87 | 0.55 |
| 1:F:473:ALA:O | 1:F:476:LEU:HB2 | 2.07 | 0.55 |
| 1:B:121:CYS:HA | 1:B:270:TYR:CE2 | 2.41 | 0.55 |
| 1:F:117:ILE:HD11 | 1:F:225:VAL:CG1 | 2.37 | 0.55 |
| 1:A:216:ASP:O | 1:A:217:ASN:HB2 | 2.06 | 0.55 |
| 1:J:215:HIS:C | 1:J:261:MET:HB3 | 2.26 | 0.55 |
| 1:I:178:PHE:CZ | 1:K:155:GLU:HG2 | 2.41 | 0.55 |
| 1:C:146:SER:N | 1:C:227:GLU:OE2 | 2.21 | 0.55 |
| 1:F:214:LEU:HB3 | 1:F:246:TYR:CE1 | 2.41 | 0.55 |
| 1:B:272:ASN:O | 1:B:273:ASN:C | 2.45 | 0.55 |
| 1:K:330:VAL:HG21 | 7:K:5424:HOH:O | 2.07 | 0.55 |
| 1:F:114:VAL:HG23 | 1:F:278:LYS:HE2 | 1.89 | 0.55 |
| 1:E:146:SER:OG | 1:E:227:GLU:OE2 | 2.11 | 0.55 |
| 1:E:336:LEU:HD21 | 7:E:4649:HOH:O | 2.05 | 0.55 |
| 1:E:321:LEU:CD1 | 1:E:411:TYR:HA | 2.37 | 0.55 |
| 1:G:423:ILE:HD11 | 1:G:600:VAL:HG13 | 1.88 | 0.55 |
| 1:G:168:LYS:O | 1:G:171:THR:CG2 | 2.55 | 0.55 |
| 1:H:117:ILE:HG23 | 1:H:118:LYS:H | 1.70 | 0.55 |
| 1:F:433:MET:HG3 | 7:F:615:HOH:O | 2.07 | 0.55 |
| 1:J:132:VAL:HG11 | 1:J:144:ILE:HD13 | 1.89 | 0.54 |
| 1:E:386:LYS:HA | 7:E:623:HOH:O | 2.06 | 0.54 |
| 1:B:207:VAL:HG21 | 1:B:241:THR:HB | 1.88 | 0.54 |
| 1:H:372:VAL:O | 1:H:483:ASP:HA | 2.08 | 0.54 |
| 1:D:254:SER:CB | 7:F:1110:HOH:O | 2.44 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:90:GLN:NE2 | 1:G:95:ASP:O | 2.40 | 0.54 |
| 1:B:222:LEU:HD23 | 1:B:267:LEU:CD1 | 2.38 | 0.54 |
| 1:K:423:ILE:HD11 | 1:K:600:VAL:HG13 | 1.90 | 0.54 |
| 1:G:171:THR:HG22 | 1:G:191:GLY:HA3 | 1.89 | 0.54 |
| 1:D:152:GLN:HG2 | 1:D:180:ASP:OD1 | 2.07 | 0.54 |
| 1:G:176:TYR:CE2 | 1:J:156:PHE:HB2 | 2.42 | 0.54 |
| 1:D:131:LEU:O | 1:D:227:GLU:HB2 | 2.08 | 0.54 |
| 1:J:357:LEU:HB2 | 1:J:425:PHE:HB2 | 1.90 | 0.54 |
| 1:H:316:GLU:HG3 | 6:H:65:1PE:H142 | 1.89 | 0.54 |
| 1:A:100:PRO:HA | 7:A:4912:HOH:O | 2.07 | 0.54 |
| 1:J:442:GLY:O | 1:K:301:PRO:HB3 | 2.08 | 0.54 |
| 1:G:178:PHE:CZ | 1:J:155:GLU:HG2 | 2.36 | 0.53 |
| 7:J:3061:HOH:O | 1:K:254:SER:C | 2.46 | 0.53 |
| 1:C:167:VAL:O | 1:C:168:LYS:C | 2.46 | 0.53 |
| 1:I:127:LEU:HB2 | 1:I:219:LEU:CD2 | 2.38 | 0.53 |
| 1:A:451:LYS:HE3 | 1:A:564:GLU:O | 2.07 | 0.53 |
| 1:C:156:PHE:O | 1:C:161:ASN:HB2 | 2.08 | 0.53 |
| 1:J:451:LYS:HG2 | 6:J:45:1PE:H241 | 1.89 | 0.53 |
| 1:K:116:ASP:HA | 1:K:271:ILE:O | 2.08 | 0.53 |
| 1:B:117:ILE:HD11 | 1:B:146:SER:OG | 2.08 | 0.53 |
| 1:I:201:ALA:HB1 | 1:J:532:GLU:OE2 | 2.07 | 0.53 |
| 1:C:169:LEU:HD11 | 1:C:206:VAL:HG23 | 1.91 | 0.53 |
| 1:L:487:LEU:O | 4:L:1003:BEY:H17A | 2.08 | 0.53 |
| 1:I:230:VAL:HG23 | 1:I:234:LEU:CG | 2.38 | 0.53 |
| 1:G:173:LYS:HE2 | 1:J:216:ASP:OD2 | 2.09 | 0.53 |
| 1:F:236:ARG:O | 1:F:240:GLU:HG3 | 2.08 | 0.53 |
| 1:E:451:LYS:HG2 | 6:E:43:1PE:H141 | 1.89 | 0.53 |
| 1:E:221:LYS:HG3 | 1:E:266:HIS:HB2 | 1.90 | 0.53 |
| 1:C:372:VAL:O | 1:C:483:ASP:HA | 2.09 | 0.53 |
| 1:C:530:ILE:HD12 | 1:C:556:ILE:HD13 | 1.89 | 0.53 |
| 1:G:381:GLY:HA2 | 1:G:459:ASP:OD1 | 2.09 | 0.53 |
| 1:I:150:ASP:OD2 | 1:I:153:VAL:HG23 | 2.09 | 0.53 |
| 1:H:222:LEU:HD23 | 1:H:267:LEU:CD1 | 2.39 | 0.53 |
| 1:A:173:LYS:HE2 | 1:D:216:ASP:OD2 | 2.08 | 0.53 |
| 1:K:108:HIS:CD2 | 6:K:5:1PE:H131 | 2.43 | 0.53 |
| 1:A:168:LYS:O | 1:A:171:THR:HG22 | 2.09 | 0.53 |
| 1:I:372:VAL:O | 1:I:483:ASP:HA | 2.09 | 0.53 |
| 1:L:457:ASN:ND2 | 4:L:1003:BEY:H3 | 2.24 | 0.53 |
| 1:A:240:GLU:OE2 | 1:A:287:TYR:HD2 | 1.92 | 0.53 |
| 1:F:360:LYS:CD | 7:F:2922:HOH:O | 2.56 | 0.53 |
| 1:E:102:GLU:HB3 | 7:E:2665:HOH:O | 2.08 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:451:LYS:HE3 | 1:C:564:GLU:O | 2.09 | 0.53 |
| 1:I:238:PHE:CD2 | 1:I:239:LEU:HD13 | 2.43 | 0.53 |
| 1:A:473:ALA:O | 1:A:476:LEU:HB2 | 2.09 | 0.53 |
| 1:D:179:ASN:O | 1:D:181:ASN:N | 2.42 | 0.53 |
| 1:F:362:LYS:CB | 1:K:163:GLU:OE1 | 2.57 | 0.53 |
| 1:L:125:GLU:N | 7:L:2009:HOH:O | 2.35 | 0.53 |
| 1:D:321:LEU:CD1 | 1:D:411:TYR:HA | 2.37 | 0.53 |
| 1:A:257:LYS:HG3 | 7:A:3234:HOH:O | 2.08 | 0.53 |
| 1:E:90:GLN:NE2 | 1:E:95:ASP:O | 2.41 | 0.53 |
| 1:C:272:ASN:O | 1:C:273:ASN:HB2 | 2.09 | 0.53 |
| 1:L:225:VAL:HG22 | 1:L:270:TYR:HB2 | 1.91 | 0.52 |
| 1:F:508:GLU:OE2 | 1:F:508:GLU:HA | 2.08 | 0.52 |
| 1:B:103:TYR:HB3 | 6:B:60:1PE:H242 | 1.91 | 0.52 |
| 1:C:165:PHE:CD2 | 1:C:173:LYS:HG2 | 2.45 | 0.52 |
| 1:L:451:LYS:HE3 | 1:L:564:GLU:O | 2.10 | 0.52 |
| 1:E:262:GLU:N | 7:E:5300:HOH:O | 2.42 | 0.52 |
| 1:B:423:ILE:HD11 | 1:B:600:VAL:HG13 | 1.91 | 0.52 |
| 1:J:130:PHE:O | 1:J:189:TYR:HA | 2.10 | 0.52 |
| 1:B:372:VAL:O | 1:B:483:ASP:HA | 2.10 | 0.52 |
| 1:C:184:SER:CB | 7:C:2540:HOH:O | 2.57 | 0.52 |
| 1:J:215:HIS:ND1 | 7:J:5351:HOH:O | 2.33 | 0.52 |
| 1:K:321:LEU:CD1 | 1:K:411:TYR:HA | 2.40 | 0.52 |
| 1:L:357:LEU:HB2 | 1:L:425:PHE:HB2 | 1.90 | 0.52 |
| 1:G:244:TYR:OH | 1:G:588:PRO:O | 2.28 | 0.52 |
| 1:I:230:VAL:CG2 | 1:I:234:LEU:HB3 | 2.38 | 0.52 |
| 1:J:121:CYS:HB2 | 1:J:148:VAL:HG12 | 1.91 | 0.52 |
| 1:G:441:PRO:HG2 | 1:H:393:ILE:HG12 | 1.91 | 0.52 |
| 1:J:451:LYS:HE3 | 1:J:564:GLU:O | 2.09 | 0.52 |
| 1:F:357:LEU:HB2 | 1:F:425:PHE:HB2 | 1.91 | 0.52 |
| 1:H:169:LEU:HD23 | 7:H:3248:HOH:O | 2.08 | 0.52 |
| 1:J:207:VAL:O | 1:J:211:VAL:HG23 | 2.09 | 0.52 |
| 1:H:576:ILE:HD12 | 1:H:580:SER:HB2 | 1.91 | 0.52 |
| 1:B:357:LEU:HB2 | 1:B:425:PHE:HB2 | 1.92 | 0.52 |
| 1:E:529:ILE:CG2 | 1:E:560:LEU:HD13 | 2.39 | 0.52 |
| 1:A:178:PHE:HZ | 1:D:155:GLU:HG3 | 1.73 | 0.52 |
| 1:I:320:LYS:CE | 6:I:21:1PE:H131 | 2.39 | 0.52 |
| 2:H:1002:CO3:O3 | 4:H:1003:BEY:H17A | 2.10 | 0.52 |
| 1:J:423:ILE:HD11 | 1:J:600:VAL:CG1 | 2.40 | 0.52 |
| 1:I:451:LYS:HE3 | 1:I:564:GLU:O | 2.10 | 0.52 |
| 1:D:214:LEU:HB3 | 1:D:246:TYR:CE1 | 2.45 | 0.52 |
| 1:D:357:LEU:HB2 | 1:D:425:PHE:HB2 | 1.91 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:120:GLY:HA3 | 1:B:149:ASN:OD1 | 2.11 | 0.51 |
| 1:D:384:ASN:HB3 | 7:D:1189:HOH:O | 2.10 | 0.51 |
| 1:J:106:PRO:HG2 | 1:J:263:TYR:CE2 | 2.45 | 0.51 |
| 1:H:176:TYR:OH | 1:L:155:GLU:HG3 | 2.10 | 0.51 |
| 1:G:231:ASP:OD1 | 1:G:234:LEU:N | 2.26 | 0.51 |
| 1:F:169:LEU:HD21 | 1:F:202:ASP:HA | 1.90 | 0.51 |
| 1:K:442:GLY:O | 1:L:301:PRO:HB3 | 2.10 | 0.51 |
| 1:L:321:LEU:CD1 | 1:L:411:TYR:HA | 2.39 | 0.51 |
| 1:A:139:ASN:HD21 | 1:A:168:LYS:HG3 | 1.75 | 0.51 |
| 1:F:169:LEU:HD23 | 1:F:205:ARG:HE | 1.75 | 0.51 |
| 1:H:487:LEU:O | 4:H:1003:BEY:C17 | 2.58 | 0.51 |
| 1:E:112:VAL:HG13 | 1:E:267:LEU:HG | 1.91 | 0.51 |
| 1:C:423:ILE:HD11 | 1:C:600:VAL:HG13 | 1.92 | 0.51 |
| 1:H:357:LEU:HB2 | 1:H:425:PHE:HB2 | 1.92 | 0.51 |
| 1:H:473:ALA:O | 1:H:476:LEU:HB2 | 2.10 | 0.51 |
| 1:B:321:LEU:CD1 | 1:B:411:TYR:HA | 2.40 | 0.51 |
| 1:D:392:MET:HE1 | 4:D:1003:BEY:H12 | 1.93 | 0.51 |
| 1:B:172:SER:O | 1:B:173:LYS:HD2 | 2.11 | 0.51 |
| 1:G:221:LYS:HG3 | 1:G:266:HIS:HB2 | 1.92 | 0.51 |
| 1:I:230:VAL:HG23 | 1:I:234:LEU:CD2 | 2.41 | 0.51 |
| 1:E:423:ILE:HD11 | 1:E:600:VAL:CG1 | 2.40 | 0.51 |
| 1:L:487:LEU:HD22 | 1:L:573:HIS:CE1 | 2.46 | 0.51 |
| 1:G:364:ASP:O | 1:G:420:ASN:HA | 2.10 | 0.51 |
| 1:D:442:GLY:O | 1:E:301:PRO:HB3 | 2.10 | 0.51 |
| 1:D:392:MET:CE | 4:D:1003:BEY:H12 | 2.40 | 0.51 |
| 1:A:150:ASP:OD1 | 1:A:179:ASN:HB2 | 2.10 | 0.51 |
| 1:C:357:LEU:HB2 | 1:C:425:PHE:HB2 | 1.92 | 0.51 |
| 1:F:179:ASN:ND2 | 1:F:183:ASN:HB2 | 2.25 | 0.51 |
| 1:I:153:VAL:O | 1:I:157:LEU:HG | 2.10 | 0.51 |
| 1:F:157:LEU:HD21 | 1:F:187:VAL:HG11 | 1.93 | 0.51 |
| 1:F:114:VAL:CG2 | 1:F:278:LYS:HG2 | 2.37 | 0.51 |
| 1:J:473:ALA:O | 1:J:476:LEU:HB2 | 2.11 | 0.51 |
| 1:I:423:ILE:HD11 | 1:I:600:VAL:HG13 | 1.93 | 0.51 |
| 1:H:392:MET:HE3 | 4:H:1003:BEY:H12 | 1.93 | 0.51 |
| 1:K:357:LEU:HB2 | 1:K:425:PHE:HB2 | 1.91 | 0.51 |
| 1:H:423:ILE:HD11 | 1:H:600:VAL:HG13 | 1.93 | 0.51 |
| 1:B:180:ASP:C | 1:B:182:LYS:H | 2.15 | 0.51 |
| 1:C:489:GLY:N | 4:C:1003:BEY:O1 | 2.37 | 0.51 |
| 1:C:392:MET:CE | 4:C:1003:BEY:H12 | 2.40 | 0.50 |
| 1:C:238:PHE:HD2 | 1:C:239:LEU:HD12 | 1.76 | 0.50 |
| 1:G:235:PHE:CE2 | 1:G:277:TYR:HB3 | 2.46 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:129:ILE:HA | 1:K:188:GLY:O | 2.11 | 0.50 |
| 1:F:112:VAL:HG22 | 1:F:267:LEU:HB3 | 1.93 | 0.50 |
| 1:F:364:ASP:O | 1:F:420:ASN:HA | 2.11 | 0.50 |
| 1:B:176:TYR:CE2 | 1:F:156:PHE:HB2 | 2.46 | 0.50 |
| 1:D:219:LEU:HD22 | 7:D:2082:HOH:O | 2.12 | 0.50 |
| 1:A:240:GLU:OE2 | 1:A:287:TYR:CD2 | 2.65 | 0.50 |
| 1:C:176:TYR:CE2 | 1:E:156:PHE:HB2 | 2.45 | 0.50 |
| 1:H:230:VAL:O | 1:H:230:VAL:HG23 | 2.11 | 0.50 |
| 1:K:411:TYR:CE1 | 6:K:5:1PE:H142 | 2.46 | 0.50 |
| 1:H:135:PRO:HA | 1:H:196:ALA:HB2 | 1.93 | 0.50 |
| 1:A:357:LEU:HB2 | 1:A:425:PHE:HB2 | 1.92 | 0.50 |
| 1:A:476:LEU:CD1 | 7:A:645:HOH:O | 2.59 | 0.50 |
| 1:A:150:ASP:OD2 | 1:A:152:GLN:HB2 | 2.11 | 0.50 |
| 1:F:247:MET:HG2 | 1:F:288:TYR:OH | 2.11 | 0.50 |
| 1:E:92:VAL:HG23 | 1:E:94:LEU:H | 1.77 | 0.50 |
| 1:I:121:CYS:SG | 1:I:225:VAL:CG2 | 2.96 | 0.50 |
| 1:E:179:ASN:HB3 | 1:E:185:VAL:HG21 | 1.94 | 0.50 |
| 1:F:262:GLU:HA | 7:F:645:HOH:O | 2.11 | 0.50 |
| 1:C:321:LEU:CD1 | 1:C:411:TYR:HA | 2.41 | 0.50 |
| 1:L:423:ILE:HD11 | 1:L:600:VAL:CG1 | 2.42 | 0.50 |
| 1:B:240:GLU:OE2 | 1:B:287:TYR:CD2 | 2.65 | 0.50 |
| 1:E:442:GLY:O | 1:F:301:PRO:HB3 | 2.12 | 0.50 |
| 1:A:528:PRO:HB3 | 1:F:525:TRP:CZ3 | 2.47 | 0.50 |
| 1:J:372:VAL:O | 1:J:483:ASP:HA | 2.11 | 0.50 |
| 1:E:138:GLU:HA | 1:E:194:SER:OG | 2.11 | 0.50 |
| 1:H:230:VAL:O | 1:H:231:ASP:O | 2.30 | 0.50 |
| 1:E:357:LEU:HB2 | 1:E:425:PHE:HB2 | 1.93 | 0.50 |
| 1:I:192:CYS:HB3 | 1:I:198:LEU:HD21 | 1.93 | 0.50 |
| 1:H:150:ASP:HB3 | 1:H:153:VAL:HB | 1.94 | 0.49 |
| 1:I:320:LYS:HE2 | 6:I:21:1PE:H131 | 1.93 | 0.49 |
| 1:K:423:ILE:HD11 | 1:K:600:VAL:CG1 | 2.42 | 0.49 |
| 1:J:214:LEU:HD21 | 1:J:222:LEU:HD22 | 1.94 | 0.49 |
| 1:C:90:GLN:NE2 | 1:C:95:ASP:O | 2.33 | 0.49 |
| 1:D:211:VAL:HG21 | 1:D:245:GLU:HB2 | 1.93 | 0.49 |
| 1:F:321:LEU:CD1 | 1:F:411:TYR:HA | 2.41 | 0.49 |
| 1:D:536:THR:HG21 | 1:D:551:VAL:HG23 | 1.94 | 0.49 |
| 1:H:321:LEU:CD1 | 1:H:411:TYR:HA | 2.38 | 0.49 |
| 1:B:320:LYS:HZ1 | 6:B:61:1PE:H241 | 1.77 | 0.49 |
| 1:J:487:LEU:HD23 | 7:J:783:HOH:O | 2.12 | 0.49 |
| 1:C:156:PHE:O | 1:C:161:ASN:CB | 2.60 | 0.49 |
| 1:A:94:LEU:HD12 | 1:C:342:LEU:HD12 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:129:ILE:HG21 | 1:L:210:LEU:CD1 | 2.43 | 0.49 |
| 1:G:130:PHE:O | 1:G:189:TYR:HA | 2.12 | 0.49 |
| 1:H:481:ILE:O | 1:H:571:TRP:HA | 2.13 | 0.49 |
| 1:D:133:ASN:HB2 | 1:D:193:GLY:O | 2.13 | 0.49 |
| 1:E:214:LEU:HB3 | 1:E:246:TYR:CE1 | 2.47 | 0.49 |
| 1:D:226:PHE:CD2 | 1:D:230:VAL:HG11 | 2.47 | 0.49 |
| 1:I:146:SER:OG | 1:I:227:GLU:OE2 | 2.25 | 0.49 |
| 1:G:321:LEU:CD1 | 1:G:411:TYR:HA | 2.39 | 0.49 |
| 1:D:529:ILE:HG22 | 1:D:560:LEU:HD13 | 1.94 | 0.49 |
| 1:E:346:LYS:HE3 | 1:F:91:VAL:HG21 | 1.94 | 0.49 |
| 1:A:153:VAL:HG22 | 1:A:177:MET:SD | 2.53 | 0.49 |
| 1:H:142:VAL:HG23 | 1:H:162:MET:HB3 | 1.94 | 0.49 |
| 1:G:526:TRP:CZ3 | 6:G:30:1PE:H151 | 2.47 | 0.49 |
| 1:L:95:ASP:HB3 | 7:L:4971:HOH:O | 2.13 | 0.49 |
| 1:L:117:ILE:HG22 | 1:L:272:ASN:OD1 | 2.13 | 0.49 |
| 1:B:100:PRO:O | 1:B:251:ARG:HD2 | 2.12 | 0.49 |
| 1:I:364:ASP:O | 1:I:420:ASN:HA | 2.13 | 0.49 |
| 1:A:487:LEU:HD22 | 1:A:573:HIS:CE1 | 2.48 | 0.49 |
| 1:E:346:LYS:HE3 | 1:F:91:VAL:CG2 | 2.43 | 0.49 |
| 1:I:236:ARG:HD3 | 1:I:283:LYS:HD3 | 1.94 | 0.49 |
| 1:A:199:SER:O | 1:A:200:GLU:C | 2.51 | 0.49 |
| 1:K:88:VAL:HG21 | 1:K:97:THR:O | 2.13 | 0.49 |
| 1:G:117:ILE:CD1 | 1:G:226:PHE:O | 2.61 | 0.49 |
| 1:B:237:PHE:HA | 1:B:240:GLU:OE1 | 2.13 | 0.49 |
| 1:L:226:PHE:HE1 | 1:L:269:VAL:HG13 | 1.77 | 0.49 |
| 1:H:584:LYS:HB2 | 7:H:4904:HOH:O | 2.12 | 0.49 |
| 1:F:487:LEU:HD22 | 1:F:573:HIS:CE1 | 2.48 | 0.48 |
| 1:D:395:LEU:HD11 | 1:D:581:TRP:CG | 2.48 | 0.48 |
| 1:C:236:ARG:NE | 1:C:240:GLU:OE2 | 2.38 | 0.48 |
| 1:E:88:VAL:HG21 | 1:E:97:THR:O | 2.13 | 0.48 |
| 1:L:226:PHE:CE1 | 1:L:269:VAL:HG13 | 2.48 | 0.48 |
| 1:C:196:ALA:HB1 | 7:C:2678:HOH:O | 2.12 | 0.48 |
| 1:A:207:VAL:HG11 | 1:A:242:LEU:HA | 1.94 | 0.48 |
| 1:H:536:THR:HG21 | 1:H:551:VAL:HG23 | 1.95 | 0.48 |
| 1:D:273:ASN:HB3 | 1:D:276:THR:HG23 | 1.94 | 0.48 |
| 1:C:367:LYS:HG2 | 1:C:603:ASP:OD1 | 2.14 | 0.48 |
| 1:B:142:VAL:HG13 | 1:B:165:PHE:O | 2.13 | 0.48 |
| 1:J:124:GLU:HA | 1:J:179:ASN:HD22 | 1.79 | 0.48 |
| 1:J:133:ASN:OD1 | 1:J:135:PRO:HD3 | 2.13 | 0.48 |
| 1:J:134:ASN:ND2 | 1:J:141:PRO:HD2 | 2.28 | 0.48 |
| 1:L:440:ARG:NH2 | 7:L:4845:HOH:O | 2.46 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:364:ASP:O | 1:D:420:ASN:HA | 2.13 | 0.48 |
| 1:H:487:LEU:HD22 | 1:H:573:HIS:CE1 | 2.48 | 0.48 |
| 1:G:107:ILE:HA | 1:G:110:ILE:HD12 | 1.96 | 0.48 |
| 1:I:272:ASN:O | 1:I:273:ASN:HB2 | 2.14 | 0.48 |
| 1:H:451:LYS:HE3 | 1:H:564:GLU:O | 2.13 | 0.48 |
| 1:F:508:GLU:HB3 | 7:F:1215:HOH:O | 2.13 | 0.48 |
| 1:G:177:MET:HG2 | 1:G:185:VAL:HG23 | 1.96 | 0.48 |
| 1:D:144:ILE:HG13 | 1:D:157:LEU:HD22 | 1.96 | 0.48 |
| 1:D:121:CYS:HA | 1:D:270:TYR:CE2 | 2.48 | 0.48 |
| 1:I:321:LEU:CD1 | 1:I:411:TYR:HA | 2.42 | 0.48 |
| 1:J:487:LEU:O | 4:J:1003:BEY:H17A | 2.13 | 0.48 |
| 1:A:528:PRO:HD3 | 1:F:525:TRP:CE2 | 2.49 | 0.48 |
| 1:J:214:LEU:HB3 | 1:J:246:TYR:CE1 | 2.49 | 0.48 |
| 1:E:364:ASP:O | 1:E:420:ASN:HA | 2.14 | 0.48 |
| 1:H:160:GLU:O | 1:H:163:GLU:HG2 | 2.14 | 0.48 |
| 1:I:516:SER:OG | 1:I:599:PHE:HA | 2.14 | 0.48 |
| 1:C:364:ASP:O | 1:C:420:ASN:HA | 2.14 | 0.48 |
| 1:B:207:VAL:O | 1:B:211:VAL:HG23 | 2.14 | 0.48 |
| 1:F:423:ILE:HD11 | 1:F:600:VAL:CG1 | 2.44 | 0.48 |
| 1:A:423:ILE:HD11 | 1:A:600:VAL:HG13 | 1.96 | 0.48 |
| 1:E:316:GLU:HG3 | 6:E:612:1PE:H252 | 1.95 | 0.48 |
| 1:D:423:ILE:HD13 | 1:D:600:VAL:HG11 | 1.94 | 0.47 |
| 1:A:316:GLU:HG3 | 6:A:20:1PE:H231 | 1.96 | 0.47 |
| 1:B:222:LEU:HD23 | 1:B:267:LEU:HD13 | 1.94 | 0.47 |
| 1:E:133:ASN:OD1 | 1:E:135:PRO:HD3 | 2.14 | 0.47 |
| 1:A:207:VAL:CG1 | 1:A:242:LEU:HA | 2.43 | 0.47 |
| 1:D:199:SER:HB2 | 7:D:2343:HOH:O | 2.13 | 0.47 |
| 1:G:122:ASN:HD22 | 6:G:47:1PE:H142 | 1.78 | 0.47 |
| 1:J:99:ILE:HD11 | 1:J:310:LEU:HA | 1.96 | 0.47 |
| 1:I:357:LEU:HB2 | 1:I:425:PHE:HB2 | 1.96 | 0.47 |
| 1:J:272:ASN:O | 1:J:273:ASN:HB2 | 2.14 | 0.47 |
| 1:E:167:VAL:O | 1:E:168:LYS:C | 2.52 | 0.47 |
| 1:D:165:PHE:CD2 | 1:D:173:LYS:HG3 | 2.50 | 0.47 |
| 1:F:364:ASP:HB3 | 7:I:2655:HOH:O | 2.14 | 0.47 |
| 1:A:275:ASP:HB2 | 7:A:3251:HOH:O | 2.14 | 0.47 |
| 1:E:516:SER:OG | 1:E:599:PHE:HA | 2.14 | 0.47 |
| 1:J:487:LEU:O | 4:J:1003:BEY:C17 | 2.63 | 0.47 |
| 1:G:577:ALA:HB1 | 4:G:1003:BEY:H13 | 1.96 | 0.47 |
| 1:J:395:LEU:HD11 | 1:J:581:TRP:CG | 2.50 | 0.47 |
| 1:L:306:ASN:HB2 | 1:L:307:PRO:HD2 | 1.97 | 0.47 |
| 1:G:395:LEU:HD11 | 1:G:581:TRP:CG | 2.49 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:450:GLY:HA2 | 7:G:3308:HOH:O | 2.13 | 0.47 |
| 1:G:285:ARG:NH2 | 7:G:633:HOH:O | 2.45 | 0.47 |
| 1:I:551:VAL:HG12 | 1:I:553:ALA:H | 1.79 | 0.47 |
| 1:B:257:LYS:CB | 1:B:259:VAL:N | 2.77 | 0.47 |
| 1:I:230:VAL:HG23 | 1:I:234:LEU:HG | 1.95 | 0.47 |
| 1:D:423:ILE:CD1 | 1:D:600:VAL:HG11 | 2.44 | 0.47 |
| 1:A:499:TYR:CE2 | 1:A:523:PRO:CB | 2.97 | 0.47 |
| 1:A:139:ASN:ND2 | 1:A:168:LYS:HG3 | 2.29 | 0.47 |
| 1:C:423:ILE:HD11 | 1:C:600:VAL:CG1 | 2.45 | 0.47 |
| 1:I:395:LEU:HD11 | 1:I:581:TRP:CG | 2.50 | 0.47 |
| 1:L:236:ARG:HD3 | 1:L:283:LYS:HD3 | 1.96 | 0.47 |
| 1:A:557:VAL:HG11 | 7:A:37:HOH:O | 2.14 | 0.47 |
| 1:D:86:SER:HB2 | 1:D:308:VAL:HG13 | 1.95 | 0.47 |
| 1:C:131:LEU:HB3 | 1:C:192:CYS:SG | 2.54 | 0.47 |
| 6:I:22:1PE:H231 | 7:I:624:HOH:O | 2.15 | 0.47 |
| 1:K:108:HIS:NE2 | 6:K:5:1PE:H131 | 2.29 | 0.47 |
| 1:G:423:ILE:HD11 | 1:G:600:VAL:CG1 | 2.44 | 0.47 |
| 1:H:142:VAL:CG2 | 1:H:162:MET:HB3 | 2.44 | 0.47 |
| 1:E:381:GLY:HA2 | 1:E:459:ASP:OD1 | 2.15 | 0.47 |
| 1:D:440:ARG:CD | 1:E:302:SER:HB2 | 2.44 | 0.47 |
| 1:K:367:LYS:HD3 | 1:K:367:LYS:HA | 1.75 | 0.47 |
| 1:G:536:THR:HG21 | 1:G:551:VAL:HG23 | 1.97 | 0.47 |
| 1:D:133:ASN:OD1 | 1:D:135:PRO:HD3 | 2.15 | 0.47 |
| 1:G:150:ASP:OD2 | 1:G:153:VAL:N | 2.43 | 0.47 |
| 1:C:150:ASP:OD1 | 1:C:179:ASN:HB2 | 2.14 | 0.47 |
| 1:H:203:MET:SD | 1:H:238:PHE:HD1 | 2.38 | 0.47 |
| 1:I:473:ALA:O | 1:I:476:LEU:HB2 | 2.15 | 0.47 |
| 1:B:209:SER:O | 1:B:212:THR:HB | 2.15 | 0.47 |
| 1:H:497:THR:HA | 1:H:578:GLY:O | 2.14 | 0.47 |
| 1:B:257:LYS:CA | 1:B:258:ASN:HB3 | 2.25 | 0.47 |
| 1:A:499:TYR:CG | 1:A:523:PRO:HB2 | 2.50 | 0.47 |
| 1:L:169:LEU:HD23 | 1:L:205:ARG:NH2 | 2.29 | 0.47 |
| 1:J:235:PHE:O | 1:J:238:PHE:HB3 | 2.14 | 0.47 |
| 1:F:374:LYS:HB3 | 7:F:622:HOH:O | 2.14 | 0.47 |
| 1:C:436:LYS:HG2 | 5:C:3:SO4:O3 | 2.14 | 0.47 |
| 1:J:364:ASP:O | 1:J:420:ASN:HA | 2.15 | 0.47 |
| 1:E:529:ILE:HG22 | 1:E:560:LEU:HD13 | 1.97 | 0.47 |
| 1:B:355:ILE:O | 1:B:426:LEU:HA | 2.14 | 0.47 |
| 1:K:364:ASP:O | 1:K:420:ASN:HA | 2.15 | 0.47 |
| 1:D:423:ILE:CD1 | 1:D:600:VAL:CG1 | 2.92 | 0.46 |
| 1:A:148:VAL:HG11 | 1:A:153:VAL:HG12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:H:215:HIS:O | 1:H:216:ASP:HB2 | 2.15 | 0.46 |
| 1:J:100:PRO:O | 1:J:251:ARG:HD2 | 2.14 | 0.46 |
| 1:H:236:ARG:HB2 | 1:H:280:GLU:HB3 | 1.97 | 0.46 |
| 1:E:200:GLU:OE1 | 1:E:523:PRO:HG3 | 2.14 | 0.46 |
| 1:G:256:ASP:O | 1:G:256:ASP:CG | 2.53 | 0.46 |
| 1:D:216:ASP:O | 1:D:216:ASP:CG | 2.53 | 0.46 |
| 1:J:451:LYS:HD3 | 7:J:3214:HOH:O | 2.15 | 0.46 |
| 1:J:261:MET:HG2 | 7:J:2991:HOH:O | 2.14 | 0.46 |
| 1:F:347:GLY:CA | 7:F:618:HOH:O | 2.63 | 0.46 |
| 1:J:246:TYR:CE2 | 1:J:264:ILE:HG12 | 2.50 | 0.46 |
| 1:G:124:GLU:O | 1:G:185:VAL:HG12 | 2.15 | 0.46 |
| 1:B:170:GLY:O | 1:B:209:SER:OG | 2.20 | 0.46 |
| 1:F:272:ASN:O | 1:F:273:ASN:HB2 | 2.14 | 0.46 |
| 1:K:221:LYS:HD3 | 7:K:1354:HOH:O | 2.16 | 0.46 |
| 4:I:1003:BEY:H10 | 4:I:1003:BEY:H18A | 1.74 | 0.46 |
| 1:C:273:ASN:O | 1:C:274:ALA:C | 2.54 | 0.46 |
| 1:D:487:LEU:O | 4:D:1003:BEY:C17 | 2.64 | 0.46 |
| 1:H:134:ASN:HA | 1:H:135:PRO:HD2 | 1.62 | 0.46 |
| 1:I:536:THR:HG21 | 1:I:551:VAL:HG23 | 1.98 | 0.46 |
| 1:E:169:LEU:HB3 | 7:E:5009:HOH:O | 2.15 | 0.46 |
| 1:I:222:LEU:O | 1:I:267:LEU:HA | 2.14 | 0.46 |
| 1:I:128:THR:O | 1:I:188:GLY:N | 2.47 | 0.46 |
| 1:B:395:LEU:HD11 | 1:B:581:TRP:CG | 2.50 | 0.46 |
| 1:A:128:THR:HG23 | 1:A:223:THR:HB | 1.96 | 0.46 |
| 1:K:138:GLU:HA | 1:K:194:SER:OG | 2.16 | 0.46 |
| 1:E:476:LEU:HD23 | 7:E:1550:HOH:O | 2.16 | 0.46 |
| 1:F:239:LEU:HB3 | 1:F:284:ALA:HB1 | 1.97 | 0.46 |
| 1:G:103:TYR:CD1 | 6:G:58:1PE:H151 | 2.51 | 0.46 |
| 1:B:257:LYS:CB | 1:B:259:VAL:H | 2.28 | 0.46 |
| 1:D:487:LEU:O | 4:D:1003:BEY:H17A | 2.15 | 0.46 |
| 1:G:254:SER:HB3 | 1:I:543:ASP:OD2 | 2.16 | 0.46 |
| 1:G:232:LYS:HB2 | 7:G:903:HOH:O | 2.16 | 0.46 |
| 1:G:307:PRO:HG2 | 7:G:622:HOH:O | 2.15 | 0.46 |
| 1:A:364:ASP:O | 1:A:420:ASN:HA | 2.16 | 0.46 |
| 2:D:1002:CO3:O2 | 4:D:1003:BEY:H17A | 2.16 | 0.46 |
| 1:J:246:TYR:HE2 | 1:J:264:ILE:HG12 | 1.80 | 0.46 |
| 1:J:273:ASN:HB3 | 1:J:276:THR:HG23 | 1.98 | 0.46 |
| 1:H:138:GLU:HA | 7:H:1925:HOH:O | 2.15 | 0.46 |
| 1:H:140:GLY:O | 1:H:166:ASN:HA | 2.16 | 0.46 |
| 1:A:169:LEU:HG | 1:A:205:ARG:HD2 | 1.97 | 0.46 |
| 1:K:101:ILE:HG21 | 1:K:103:TYR:CE2 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:167:VAL:O | 1:I:168:LYS:C | 2.53 | 0.46 |
| 1:L:516:SER:OG | 1:L:599:PHE:HA | 2.16 | 0.46 |
| 1:F:516:SER:OG | 1:F:599:PHE:HA | 2.16 | 0.46 |
| 1:K:167:VAL:HG12 | 1:K:192:CYS:H | 1.81 | 0.46 |
| 1:C:177:MET:O | 1:C:184:SER:HA | 2.16 | 0.46 |
| 1:L:224:VAL:N | 1:L:268:GLY:O | 2.42 | 0.46 |
| 1:H:602:ASN:HB2 | 7:H:2166:HOH:O | 2.16 | 0.46 |
| 1:G:121:CYS:HA | 1:G:270:TYR:CZ | 2.51 | 0.46 |
| 1:I:230:VAL:O | 1:I:277:TYR:CZ | 2.68 | 0.45 |
| 1:G:106:PRO:HD2 | 1:G:247:MET:SD | 2.56 | 0.45 |
| 1:J:128:THR:O | 1:J:187:VAL:HA | 2.16 | 0.45 |
| 1:J:125:GLU:CG | 1:J:221:LYS:HD2 | 2.46 | 0.45 |
| 1:F:207:VAL:HG12 | 1:F:207:VAL:O | 2.17 | 0.45 |
| 1:J:436:LYS:HG2 | 5:J:18:SO4:O2 | 2.17 | 0.45 |
| 1:I:130:PHE:CD2 | 1:I:225:VAL:HB | 2.50 | 0.45 |
| 1:H:217:ASN:ND2 | 1:L:165:PHE:HE2 | 2.14 | 0.45 |
| 1:B:577:ALA:HB1 | 4:B:1003:BEY:H13 | 1.98 | 0.45 |
| 1:G:217:ASN:OD1 | 1:G:219:LEU:HG | 2.16 | 0.45 |
| 1:D:451:LYS:HG3 | 6:D:44:1PE:H151 | 1.98 | 0.45 |
| 1:C:115:TYR:HB2 | 1:C:270:TYR:CD2 | 2.52 | 0.45 |
| 1:F:306:ASN:HB2 | 1:F:307:PRO:HD2 | 1.98 | 0.45 |
| 1:D:367:LYS:HD3 | 1:D:367:LYS:HA | 1.66 | 0.45 |
| 1:K:530:ILE:HD12 | 1:K:556:ILE:HD13 | 1.99 | 0.45 |
| 1:J:320:LYS:HZ3 | 6:J:3:1PE:C14 | 2.22 | 0.45 |
| 1:F:487:LEU:HD23 | 7:F:617:HOH:O | 2.17 | 0.45 |
| 1:G:230:VAL:O | 1:G:277:TYR:OH | 2.28 | 0.45 |
| 1:E:536:THR:HG21 | 1:E:551:VAL:HG23 | 1.98 | 0.45 |
| 1:E:530:ILE:HD12 | 1:E:556:ILE:HD13 | 1.98 | 0.45 |
| 1:B:451:LYS:HG2 | 1:C:255:THR:OG1 | 2.16 | 0.45 |
| 1:A:143:LYS:HG2 | 1:A:159:ASP:OD2 | 2.17 | 0.45 |
| 1:K:481:ILE:O | 1:K:571:TRP:HA | 2.17 | 0.45 |
| 1:B:375:GLY:O | 1:B:429:VAL:HA | 2.17 | 0.45 |
| 1:D:398:PHE:CD2 | 1:D:398:PHE:C | 2.89 | 0.45 |
| 1:K:244:TYR:CE1 | 1:K:291:THR:HG22 | 2.52 | 0.45 |
| 1:H:207:VAL:HG11 | 1:H:241:THR:HG22 | 1.99 | 0.45 |
| 1:B:536:THR:HG21 | 1:B:551:VAL:HG23 | 1.99 | 0.45 |
| 1:A:216:ASP:O | 1:D:173:LYS:CE | 2.60 | 0.45 |
| 1:K:165:PHE:CD2 | 1:K:173:LYS:HG3 | 2.52 | 0.45 |
| 1:B:142:VAL:CG2 | 1:B:162:MET:HB3 | 2.44 | 0.45 |
| 1:D:551:VAL:HG12 | 1:D:553:ALA:H | 1.81 | 0.45 |
| 1:L:167:VAL:O | 1:L:168:LYS:C | 2.53 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:141:PRO:HA | 1:A:165:PHE:O | 2.17 | 0.45 |
| 1:C:129:ILE:HA | 1:C:188:GLY:O | 2.16 | 0.45 |
| 1:J:164:LYS:HB2 | 1:J:164:LYS:HE3 | 1.65 | 0.45 |
| 1:C:153:VAL:HG12 | 1:C:157:LEU:HD12 | 1.96 | 0.45 |
| 4:E:1003:BEY:H18A | 4:E:1003:BEY:H10 | 1.76 | 0.45 |
| 1:F:487:LEU:O | 4:F:1003:BEY:H17A | 2.16 | 0.45 |
| 1:H:128:THR:HG23 | 1:H:223:THR:HB | 1.99 | 0.45 |
| 1:C:536:THR:HG21 | 1:C:551:VAL:HG23 | 1.99 | 0.45 |
| 1:A:249:ASP:CG | 1:A:251:ARG:HE | 2.20 | 0.45 |
| 1:D:497:THR:HA | 1:D:578:GLY:O | 2.17 | 0.45 |
| 1:K:130:PHE:O | 1:K:189:TYR:HA | 2.17 | 0.45 |
| 1:I:260:ASN:O | 1:I:262:GLU:N | 2.50 | 0.45 |
| 1:J:367:LYS:HD3 | 1:J:367:LYS:HA | 1.68 | 0.45 |
| 1:F:107:ILE:O | 1:F:107:ILE:HG22 | 2.17 | 0.45 |
| 5:E:7:SO4:O2 | 1:F:436:LYS:HG2 | 2.17 | 0.45 |
| 1:K:355:ILE:O | 1:K:426:LEU:HA | 2.17 | 0.45 |
| 1:J:536:THR:HG21 | 1:J:551:VAL:HG23 | 1.99 | 0.45 |
| 1:J:107:ILE:HG21 | 1:J:243:PHE:HB3 | 1.97 | 0.45 |
| 1:K:332:GLU:HG3 | 1:K:332:GLU:H | 1.45 | 0.45 |
| 1:H:487:LEU:O | 4:H:1003:BEY:H17 | 2.17 | 0.45 |
| 1:L:324:GLU:HA | 7:L:970:HOH:O | 2.16 | 0.45 |
| 1:C:528:PRO:HB3 | 1:D:525:TRP:CZ3 | 2.52 | 0.45 |
| 1:E:229:ASN:O | 1:E:230:VAL:CB | 2.57 | 0.44 |
| 1:K:381:GLY:HA2 | 1:K:459:ASP:OD1 | 2.16 | 0.44 |
| 1:G:332:GLU:HB2 | 7:G:5439:HOH:O | 2.16 | 0.44 |
| 1:B:586:ARG:HB3 | 7:B:2591:HOH:O | 2.17 | 0.44 |
| 1:J:487:LEU:HD22 | 1:J:573:HIS:CE1 | 2.53 | 0.44 |
| 1:J:100:PRO:O | 1:J:101:ILE:HD13 | 2.18 | 0.44 |
| 1:D:481:ILE:O | 1:D:571:TRP:HA | 2.16 | 0.44 |
| 1:A:444:ILE:HA | 1:A:453:ILE:O | 2.17 | 0.44 |
| 1:H:180:ASP:C | 1:H:182:LYS:H | 2.21 | 0.44 |
| 1:B:187:VAL:HG12 | 1:B:188:GLY:N | 2.31 | 0.44 |
| 1:F:202:ASP:O | 1:F:206:VAL:HG23 | 2.17 | 0.44 |
| 1:L:232:LYS:HB2 | 7:L:5173:HOH:O | 2.17 | 0.44 |
| 1:K:516:SER:OG | 1:K:599:PHE:HA | 2.17 | 0.44 |
| 1:H:307:PRO:HD3 | 1:H:377:THR:OG1 | 2.16 | 0.44 |
| 1:I:210:LEU:HD23 | 1:I:242:LEU:HD13 | 1.98 | 0.44 |
| 1:J:210:LEU:HA | 1:J:213:MET:HE3 | 1.98 | 0.44 |
| 1:C:514:LEU:O | 1:C:517:SER:HB3 | 2.17 | 0.44 |
| 1:B:481:ILE:O | 1:B:571:TRP:HA | 2.16 | 0.44 |
| 1:D:152:GLN:O | 1:D:155:GLU:HB3 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:103:TYR:CD1 | 6:K:4:1PE:H132 | 2.53 | 0.44 |
| 1:F:134:ASN:HB2 | 1:F:167:VAL:HG11 | 1.99 | 0.44 |
| 1:I:307:PRO:HD3 | 1:I:377:THR:OG1 | 2.18 | 0.44 |
| 1:I:100:PRO:O | 1:I:251:ARG:HD2 | 2.18 | 0.44 |
| 1:K:441:PRO:HG2 | 1:L:393:ILE:HG12 | 1.99 | 0.44 |
| 7:B:2359:HOH:O | 1:E:551:VAL:HG13 | 2.16 | 0.44 |
| 1:F:97:THR:O | 1:F:98:SER:HB3 | 2.17 | 0.44 |
| 1:E:395:LEU:HD11 | 1:E:581:TRP:CG | 2.53 | 0.44 |
| 1:I:528:PRO:HB3 | 1:J:525:TRP:CZ3 | 2.52 | 0.44 |
| 1:L:128:THR:HG23 | 1:L:223:THR:HB | 2.00 | 0.44 |
| 1:L:198:LEU:HD23 | 1:L:198:LEU:HA | 1.60 | 0.44 |
| 1:D:451:LYS:HE2 | 6:D:44:1PE:H261 | 1.99 | 0.44 |
| 1:A:138:GLU:HA | 1:A:194:SER:CB | 2.47 | 0.44 |
| 1:E:368:LYS:CE | 7:E:2241:HOH:O | 2.65 | 0.44 |
| 1:I:497:THR:HA | 1:I:578:GLY:O | 2.18 | 0.44 |
| 1:H:375:GLY:O | 1:H:429:VAL:HA | 2.18 | 0.44 |
| 1:I:243:PHE:HB3 | 1:I:288:TYR:CD1 | 2.53 | 0.44 |
| 1:F:586:ARG:NH2 | 7:F:2842:HOH:O | 2.36 | 0.44 |
| 1:J:544:ILE:CD1 | 1:J:564:GLU:HG3 | 2.47 | 0.44 |
| 1:K:451:LYS:CD | 6:K:42:1PE:H231 | 2.43 | 0.44 |
| 1:I:128:THR:HG23 | 1:I:223:THR:HB | 2.00 | 0.44 |
| 1:I:118:LYS:C | 1:I:120:GLY:H | 2.21 | 0.44 |
| 1:B:300:ALA:HA | 1:B:301:PRO:HD3 | 1.88 | 0.44 |
| 1:H:335:GLU:CB | 7:H:2588:HOH:O | 2.65 | 0.44 |
| 1:J:302:SER:HB3 | 7:J:1429:HOH:O | 2.18 | 0.44 |
| 1:K:438:SER:HA | 7:K:17:HOH:O | 2.18 | 0.44 |
| 1:C:532:GLU:HG3 | 1:D:201:ALA:HB1 | 1.99 | 0.44 |
| 1:B:218:LYS:HG2 | 1:B:262:GLU:CG | 2.48 | 0.44 |
| 1:D:198:LEU:HA | 1:D:198:LEU:HD12 | 1.86 | 0.44 |
| 1:L:451:LYS:CG | 6:L:612:1PE:H131 | 2.47 | 0.44 |
| 1:D:219:LEU:N | 1:D:219:LEU:HD22 | 2.33 | 0.43 |
| 1:C:392:MET:HE3 | 4:C:1003:BEY:H12 | 2.00 | 0.43 |
| 1:E:135:PRO:HA | 1:E:194:SER:O | 2.18 | 0.43 |
| 1:A:123:VAL:HG21 | 1:A:153:VAL:HG11 | 1.99 | 0.43 |
| 1:E:368:LYS:HE3 | 7:E:2241:HOH:O | 2.17 | 0.43 |
| 1:E:223:THR:HA | 1:E:268:GLY:O | 2.18 | 0.43 |
| 1:J:86:SER:HB2 | 7:J:1689:HOH:O | 2.18 | 0.43 |
| 1:K:208:LEU:HD13 | 1:K:245:GLU:HG3 | 2.00 | 0.43 |
| 1:F:395:LEU:HD11 | 1:F:581:TRP:CG | 2.53 | 0.43 |
| 1:G:214:LEU:HD21 | 1:G:222:LEU:HD22 | 1.99 | 0.43 |
| 1:A:326:LYS:HG2 | 1:A:328:LEU:HD12 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 4:A:1003:BEY:H18A | 4:A:1003:BEY:H10 | 1.63 | 0.43 |
| 1:C:156:PHE:CE2 | 1:C:175:PHE:HB3 | 2.54 | 0.43 |
| 1:L:300:ALA:HA | 1:L:301:PRO:HD3 | 1.84 | 0.43 |
| 1:C:207:VAL:CG1 | 1:C:242:LEU:HA | 2.48 | 0.43 |
| 1:H:355:ILE:O | 1:H:426:LEU:HA | 2.18 | 0.43 |
| 1:I:462:GLY:N | 2:I:1002:CO3:O1 | 2.52 | 0.43 |
| 1:G:198:LEU:HD22 | 1:G:202:ASP:HB2 | 1.99 | 0.43 |
| 1:J:541:TYR:HE1 | 1:K:249:ASP:HB3 | 1.83 | 0.43 |
| 1:B:423:ILE:HD11 | 1:B:600:VAL:CG1 | 2.48 | 0.43 |
| 1:B:180:ASP:C | 1:B:182:LYS:N | 2.72 | 0.43 |
| 1:J:99:ILE:HD12 | 1:J:313:ALA:HB2 | 1.99 | 0.43 |
| 1:H:594:ARG:HG3 | 7:H:781:HOH:O | 2.17 | 0.43 |
| 1:F:520:SER:HB3 | 1:F:598:GLU:HG3 | 1.99 | 0.43 |
| 1:G:528:PRO:HD3 | 1:L:525:TRP:CE2 | 2.53 | 0.43 |
| 1:E:216:ASP:C | 1:E:217:ASN:ND2 | 2.71 | 0.43 |
| 1:D:393:ILE:HG12 | 1:F:441:PRO:HG2 | 2.01 | 0.43 |
| 1:K:392:MET:HE1 | 4:K:1003:BEY:H12 | 2.00 | 0.43 |
| 1:F:150:ASP:HB3 | 1:F:153:VAL:HB | 2.00 | 0.43 |
| 1:K:395:LEU:HD11 | 1:K:581:TRP:CG | 2.54 | 0.43 |
| 1:B:440:ARG:HD2 | 1:C:302:SER:HB2 | 2.00 | 0.43 |
| 1:J:516:SER:OG | 1:J:599:PHE:HA | 2.18 | 0.43 |
| 1:E:355:ILE:O | 1:E:426:LEU:HA | 2.18 | 0.43 |
| 1:G:232:LYS:N | 7:G:903:HOH:O | 2.51 | 0.43 |
| 1:J:221:LYS:HE2 | 7:J:633:HOH:O | 2.17 | 0.43 |
| 1:A:214:LEU:HD11 | 1:A:222:LEU:HD22 | 1.99 | 0.43 |
| 1:J:520:SER:HB3 | 1:J:598:GLU:HG3 | 2.01 | 0.43 |
| 1:B:364:ASP:O | 1:B:420:ASN:HA | 2.17 | 0.43 |
| 1:I:381:GLY:HA2 | 1:I:459:ASP:OD1 | 2.18 | 0.43 |
| 1:E:157:LEU:HD23 | 1:E:157:LEU:HA | 1.87 | 0.43 |
| 1:I:320:LYS:NZ | 6:I:21:1PE:H131 | 2.34 | 0.43 |
| 1:G:222:LEU:O | 1:G:267:LEU:HD12 | 2.17 | 0.43 |
| 1:L:254:SER:OG | 1:L:254:SER:O | 2.36 | 0.43 |
| 1:I:182:LYS:HD3 | 1:I:182:LYS:N | 2.29 | 0.43 |
| 1:K:536:THR:HG21 | 1:K:551:VAL:HG23 | 2.00 | 0.43 |
| 1:A:536:THR:HG21 | 1:A:551:VAL:HG23 | 2.01 | 0.43 |
| 1:F:481:ILE:O | 1:F:571:TRP:HA | 2.19 | 0.43 |
| 1:E:106:PRO:HG2 | 1:E:263:TYR:CE2 | 2.54 | 0.43 |
| 1:J:108:HIS:HA | 1:J:285:ARG:HD2 | 2.00 | 0.43 |
| 1:G:516:SER:OG | 1:G:599:PHE:HA | 2.18 | 0.43 |
| 1:G:396:MET:HE3 | 7:G:2070:HOH:O | 2.19 | 0.43 |
| 1:L:150:ASP:HB3 | 1:L:153:VAL:HB | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:394:ASP:HB3 | 7:F:3100:HOH:O | 2.19 | 0.43 |
| 1:D:179:ASN:C | 1:D:181:ASN:H | 2.22 | 0.43 |
| 1:E:543:ASP:CG | 6:E:43:1PE:H142 | 2.39 | 0.43 |
| 1:F:423:ILE:HD13 | 1:F:600:VAL:HG11 | 2.01 | 0.43 |
| 1:I:168:LYS:O | 1:I:171:THR:HB | 2.19 | 0.43 |
| 1:C:208:LEU:O | 1:C:212:THR:HG23 | 2.19 | 0.43 |
| 1:K:159:ASP:O | 1:K:160:GLU:C | 2.53 | 0.43 |
| 1:K:246:TYR:CE2 | 1:K:263:TYR:HD1 | 2.37 | 0.43 |
| 1:I:530:ILE:HD12 | 1:I:556:ILE:HD13 | 2.01 | 0.43 |
| 1:G:423:ILE:HD13 | 1:G:600:VAL:HG11 | 2.01 | 0.43 |
| 1:G:95:ASP:HA | 1:G:96:PRO:HD2 | 1.90 | 0.43 |
| 1:G:112:VAL:HG22 | 1:G:267:LEU:HB3 | 2.00 | 0.43 |
| 1:H:131:LEU:O | 1:H:228:ILE:HG23 | 2.19 | 0.43 |
| 1:H:364:ASP:O | 1:H:420:ASN:HA | 2.18 | 0.43 |
| 1:F:103:TYR:HB2 | 5:F:21:SO4:O4 | 2.19 | 0.43 |
| 1:G:292:TYR:O | 1:G:295:SER:HB3 | 2.18 | 0.43 |
| 1:H:202:ASP:O | 1:H:206:VAL:HG23 | 2.19 | 0.43 |
| 1:I:324:GLU:H | 1:I:324:GLU:HG2 | 1.68 | 0.43 |
| 1:K:451:LYS:NZ | 6:K:42:1PE:H231 | 2.34 | 0.42 |
| 1:L:512:LYS:HD3 | 1:L:603:ASP:OD1 | 2.19 | 0.42 |
| 1:J:423:ILE:HD13 | 1:J:600:VAL:HG11 | 2.01 | 0.42 |
| 1:G:306:ASN:HB2 | 1:G:307:PRO:HD2 | 2.01 | 0.42 |
| 1:A:475:LYS:HD3 | 7:A:2808:HOH:O | 2.19 | 0.42 |
| 1:H:498:SER:HB3 | 1:H:499:TYR:HD2 | 1.84 | 0.42 |
| 4:C:1003:BEY:H8 | 4:C:1003:BEY:H2 | 1.66 | 0.42 |
| 1:B:229:ASN:ND2 | 7:B:2947:HOH:O | 2.52 | 0.42 |
| 1:J:103:TYR:HB2 | 5:J:20:SO4:O1 | 2.19 | 0.42 |
| 1:B:134:ASN:HB3 | 1:B:167:VAL:HG21 | 2.00 | 0.42 |
| 1:E:88:VAL:HA | 1:E:89:PRO:HD2 | 1.79 | 0.42 |
| 1:G:123:VAL:HG12 | 1:G:185:VAL:HG11 | 2.01 | 0.42 |
| 1:G:316:GLU:HG3 | 6:G:58:1PE:H131 | 2.01 | 0.42 |
| 1:K:106:PRO:HD2 | 1:K:247:MET:SD | 2.59 | 0.42 |
| 1:F:109:ASP:HB2 | 7:F:1094:HOH:O | 2.19 | 0.42 |
| 1:F:222:LEU:HB3 | 1:F:264:ILE:HD13 | 2.01 | 0.42 |
| 1:K:392:MET:CE | 4:K:1003:BEY:H12 | 2.49 | 0.42 |
| 6:D:44:1PE:H141 | 1:E:254:SER:C | 2.39 | 0.42 |
| 1:E:544:ILE:CD1 | 1:E:564:GLU:HG3 | 2.49 | 0.42 |
| 1:C:139:ASN:ND2 | 1:C:168:LYS:HB2 | 2.34 | 0.42 |
| 1:F:306:ASN:HB2 | 1:F:307:PRO:CD | 2.48 | 0.42 |
| 1:L:96:PRO:HB3 | 1:L:304:TYR:CE1 | 2.54 | 0.42 |
| 1:B:169:LEU:HD21 | 1:B:205:ARG:HD3 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:181:ASN:ND2 | 1:H:183:ASN:ND2 | 2.67 | 0.42 |
| 1:F:374:LYS:HB2 | 1:F:485:ALA:CB | 2.49 | 0.42 |
| 1:G:528:PRO:HD3 | 1:L:525:TRP:NE1 | 2.35 | 0.42 |
| 1:J:239:LEU:HB3 | 1:J:284:ALA:HB1 | 2.01 | 0.42 |
| 1:E:363:GLY:HA3 | 7:E:1962:HOH:O | 2.19 | 0.42 |
| 1:F:95:ASP:O | 1:F:96:PRO:C | 2.56 | 0.42 |
| 1:I:137:LYS:CB | 7:I:5069:HOH:O | 2.66 | 0.42 |
| 1:K:107:ILE:O | 1:K:109:ASP:N | 2.52 | 0.42 |
| 1:A:114:VAL:HA | 1:A:269:VAL:O | 2.20 | 0.42 |
| 1:H:543:ASP:HA | 1:I:256:ASP:HB3 | 2.00 | 0.42 |
| 1:K:248:THR:HG23 | 7:K:2935:HOH:O | 2.19 | 0.42 |
| 1:J:317:LEU:HG | 1:J:321:LEU:HD12 | 2.02 | 0.42 |
| 1:D:219:LEU:N | 1:D:219:LEU:HD13 | 2.26 | 0.42 |
| 1:J:440:ARG:CD | 1:K:302:SER:HB2 | 2.49 | 0.42 |
| 1:H:423:ILE:HD11 | 1:H:600:VAL:CG1 | 2.49 | 0.42 |
| 1:E:362:LYS:N | 7:E:1815:HOH:O | 2.52 | 0.42 |
| 1:F:544:ILE:CD1 | 1:F:564:GLU:HG3 | 2.49 | 0.42 |
| 1:J:321:LEU:CD1 | 1:J:411:TYR:HA | 2.47 | 0.42 |
| 1:I:423:ILE:HD11 | 1:I:600:VAL:CG1 | 2.50 | 0.42 |
| 1:J:273:ASN:HB2 | 1:J:277:TYR:HE2 | 1.83 | 0.42 |
| 1:E:440:ARG:NH2 | 7:E:663:HOH:O | 2.52 | 0.42 |
| 1:K:121:CYS:HA | 1:K:270:TYR:CE2 | 2.54 | 0.42 |
| 1:C:395:LEU:HD11 | 1:C:581:TRP:CG | 2.55 | 0.42 |
| 1:F:444:ILE:HA | 1:F:453:ILE:O | 2.18 | 0.42 |
| 1:A:112:VAL:HA | 1:A:267:LEU:O | 2.19 | 0.42 |
| 1:J:320:LYS:CE | 6:J:3:1PE:H142 | 2.49 | 0.42 |
| 1:J:393:ILE:HG12 | 1:L:441:PRO:HG2 | 2.02 | 0.42 |
| 1:J:207:VAL:HG13 | 1:J:242:LEU:HA | 2.00 | 0.42 |
| 1:G:445:ILE:HA | 7:G:866:HOH:O | 2.19 | 0.42 |
| 1:J:423:ILE:CD1 | 1:J:600:VAL:CG1 | 2.98 | 0.42 |
| 1:E:169:LEU:HD12 | 1:E:192:CYS:HA | 2.01 | 0.42 |
| 1:F:134:ASN:CB | 1:F:167:VAL:HG11 | 2.50 | 0.42 |
| 1:A:92:VAL:O | 1:A:95:ASP:HB2 | 2.19 | 0.42 |
| 1:C:316:GLU:HG3 | 6:C:17:1PE:H221 | 2.02 | 0.42 |
| 1:G:398:PHE:CD2 | 1:G:398:PHE:C | 2.93 | 0.42 |
| 1:D:179:ASN:O | 1:D:182:LYS:N | 2.51 | 0.42 |
| 1:D:272:ASN:O | 1:D:273:ASN:HB2 | 2.20 | 0.42 |
| 1:F:240:GLU:HG3 | 1:F:240:GLU:H | 1.60 | 0.42 |
| 1:C:168:LYS:O | 1:C:169:LEU:C | 2.57 | 0.42 |
| 1:C:392:MET:HE1 | 4:C:1003:BEY:H12 | 2.01 | 0.42 |
| 1:D:133:ASN:C | 1:D:133:ASN:OD1 | 2.57 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:L:150:ASP:OD1 | 1:L:179:ASN:HB2 | 2.19 | 0.42 |
| 1:E:129:ILE:HA | 1:E:188:GLY:O | 2.20 | 0.42 |
| 1:F:533:TYR:HB2 | 1:F:560:LEU:CD1 | 2.49 | 0.42 |
| 1:E:222:LEU:O | 1:E:267:LEU:HA | 2.19 | 0.42 |
| 1:G:134:ASN:O | 1:G:194:SER:HB2 | 2.20 | 0.42 |
| 1:H:381:GLY:HA2 | 1:H:459:ASP:OD1 | 2.19 | 0.42 |
| 1:K:207:VAL:CG1 | 1:K:242:LEU:HA | 2.50 | 0.42 |
| 1:J:195:VAL:HG12 | 1:J:195:VAL:O | 2.20 | 0.42 |
| 1:A:528:PRO:HD3 | 1:F:525:TRP:NE1 | 2.35 | 0.41 |
| 1:E:118:LYS:C | 1:E:120:GLY:H | 2.23 | 0.41 |
| 1:I:444:ILE:HA | 1:I:453:ILE:O | 2.20 | 0.41 |
| 1:A:395:LEU:HD11 | 1:A:581:TRP:CG | 2.54 | 0.41 |
| 1:L:162:MET:CE | 1:L:165:PHE:HE1 | 2.32 | 0.41 |
| 1:D:544:ILE:CD1 | 1:D:564:GLU:HG3 | 2.50 | 0.41 |
| 1:L:214:LEU:HD21 | 1:L:222:LEU:HD22 | 2.02 | 0.41 |
| 1:G:234:LEU:HD12 | 1:G:234:LEU:O | 2.20 | 0.41 |
| 1:J:350:TYR:HE1 | 1:L:440:ARG:HH21 | 1.68 | 0.41 |
| 1:F:239:LEU:HD23 | 1:F:281:VAL:HA | 2.01 | 0.41 |
| 1:J:307:PRO:HD3 | 1:J:377:THR:OG1 | 2.20 | 0.41 |
| 1:A:516:SER:OG | 1:A:599:PHE:HA | 2.20 | 0.41 |
| 1:F:178:PHE:HD1 | 1:F:182:LYS:O | 2.03 | 0.41 |
| 1:A:346:LYS:HB3 | 1:A:437:ASN:O | 2.19 | 0.41 |
| 1:B:381:GLY:HA2 | 1:B:459:ASP:OD1 | 2.19 | 0.41 |
| 1:F:198:LEU:HD12 | 1:F:198:LEU:HA | 1.84 | 0.41 |
| 1:C:532:GLU:HB2 | 7:D:4750:HOH:O | 2.20 | 0.41 |
| 1:L:142:VAL:HG23 | 1:L:165:PHE:O | 2.20 | 0.41 |
| 1:L:235:PHE:HE1 | 1:L:269:VAL:HG11 | 1.86 | 0.41 |
| 1:F:375:GLY:O | 1:F:429:VAL:HA | 2.19 | 0.41 |
| 1:B:520:SER:HB3 | 1:B:598:GLU:HG3 | 2.01 | 0.41 |
| 1:A:300:ALA:HA | 1:A:301:PRO:HD3 | 1.87 | 0.41 |
| 1:J:90:GLN:NE2 | 1:J:95:ASP:O | 2.53 | 0.41 |
| 1:J:91:VAL:HB | 1:L:346:LYS:HE3 | 2.02 | 0.41 |
| 1:B:528:PRO:HB3 | 1:E:525:TRP:CZ3 | 2.54 | 0.41 |
| 1:D:346:LYS:HB3 | 1:D:437:ASN:O | 2.19 | 0.41 |
| 1:E:158:LYS:O | 1:E:161:ASN:HB3 | 2.20 | 0.41 |
| 1:E:161:ASN:ND2 | 7:E:1724:HOH:O | 2.53 | 0.41 |
| 1:E:208:LEU:HA | 1:E:208:LEU:HD12 | 1.90 | 0.41 |
| 1:I:225:VAL:HG22 | 1:I:270:TYR:HB2 | 2.01 | 0.41 |
| 1:A:142:VAL:HG21 | 1:A:189:TYR:CZ | 2.56 | 0.41 |
| 1:G:487:LEU:HD22 | 1:G:573:HIS:CE1 | 2.56 | 0.41 |
| 1:F:307:PRO:HD3 | 1:F:377:THR:OG1 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:J:494:SER:HB3 | 7:J:1288:HOH:O | 2.19 | 0.41 |
| 1:G:174:HIS:HB3 | 1:J:175:PHE:CD2 | 2.56 | 0.41 |
| 1:K:307:PRO:HD3 | 1:K:377:THR:OG1 | 2.20 | 0.41 |
| 1:D:168:LYS:O | 1:D:169:LEU:C | 2.57 | 0.41 |
| 1:C:181:ASN:ND2 | 1:C:183:ASN:ND2 | 2.67 | 0.41 |
| 1:J:514:LEU:O | 1:J:518:LYS:HG2 | 2.21 | 0.41 |
| 1:K:237:PHE:O | 1:K:240:GLU:HB2 | 2.20 | 0.41 |
| 1:K:221:LYS:HG3 | 1:K:266:HIS:HB2 | 2.03 | 0.41 |
| 1:F:207:VAL:HG11 | 1:F:241:THR:HG22 | 2.03 | 0.41 |
| 1:B:541:TYR:OH | 1:C:587:LYS:HB2 | 2.21 | 0.41 |
| 1:J:323:LEU:HD23 | 1:J:323:LEU:HA | 1.78 | 0.41 |
| 1:H:487:LEU:O | 4:H:1003:BEY:H17A | 2.19 | 0.41 |
| 1:L:232:LYS:HE2 | 1:L:276:THR:O | 2.20 | 0.41 |
| 1:I:207:VAL:HG11 | 1:I:242:LEU:N | 2.36 | 0.41 |
| 1:I:497:THR:HB | 7:I:4920:HOH:O | 2.20 | 0.41 |
| 1:C:481:ILE:O | 1:C:571:TRP:HA | 2.20 | 0.41 |
| 1:E:219:LEU:O | 1:E:264:ILE:HG22 | 2.20 | 0.41 |
| 1:I:230:VAL:CG2 | 1:I:234:LEU:HG | 2.51 | 0.41 |
| 1:B:441:PRO:HG2 | 1:C:393:ILE:HG12 | 2.03 | 0.41 |
| 1:H:178:PHE:HZ | 1:L:155:GLU:HG2 | 1.84 | 0.41 |
| 1:I:111:LYS:HE2 | 1:I:266:HIS:NE2 | 2.36 | 0.41 |
| 1:C:346:LYS:HB3 | 1:C:437:ASN:O | 2.20 | 0.41 |
| 1:G:88:VAL:HA | 1:G:89:PRO:HD2 | 1.88 | 0.41 |
| 1:D:440:ARG:HD3 | 1:E:302:SER:HB2 | 2.01 | 0.41 |
| 1:G:528:PRO:HD3 | 1:L:525:TRP:CD1 | 2.56 | 0.41 |
| 1:B:167:VAL:O | 1:B:168:LYS:C | 2.59 | 0.41 |
| 1:A:301:PRO:CG | 1:C:444:ILE:HD12 | 2.50 | 0.41 |
| 1:C:487:LEU:HD22 | 1:C:573:HIS:CE1 | 2.56 | 0.41 |
| 1:J:481:ILE:O | 1:J:571:TRP:HA | 2.20 | 0.41 |
| 1:G:522:GLU:HA | 1:G:523:PRO:HD3 | 1.92 | 0.41 |
| 1:L:364:ASP:O | 1:L:420:ASN:HA | 2.21 | 0.41 |
| 1:L:536:THR:HG21 | 1:L:551:VAL:HG23 | 2.02 | 0.41 |
| 1:E:481:ILE:O | 1:E:571:TRP:HA | 2.20 | 0.41 |
| 1:H:520:SER:HB3 | 1:H:598:GLU:HG3 | 2.02 | 0.41 |
| 1:A:176:TYR:CE2 | 1:D:156:PHE:HB2 | 2.55 | 0.41 |
| 1:K:544:ILE:CD1 | 1:K:564:GLU:HG3 | 2.51 | 0.41 |
| 1:L:103:TYR:HB3 | 6:L:1:1PE:H252 | 2.03 | 0.41 |
| 1:J:219:LEU:HB3 | 1:J:220:SER:H | 1.62 | 0.41 |
| 1:F:105:THR:C | 1:F:107:ILE:N | 2.74 | 0.41 |
| 1:D:487:LEU:HD22 | 1:D:573:HIS:CE1 | 2.56 | 0.41 |
| 1:A:393:ILE:HG12 | 1:C:441:PRO:HG2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 4:A:1003:BEY:H17 | 4:A:1003:BEY:H18 | 1.78 | 0.41 |
| 1:C:551:VAL:HG12 | 1:C:553:ALA:H | 1.86 | 0.41 |
| 1:I:203:MET:O | 1:I:207:VAL:HG23 | 2.21 | 0.41 |
| 1:I:487:LEU:HD12 | 1:I:487:LEU:HA | 1.95 | 0.41 |
| 1:H:219:LEU:O | 1:H:264:ILE:HG22 | 2.21 | 0.41 |
| 1:A:263:TYR:N | 7:A:2776:HOH:O | 2.43 | 0.41 |
| 1:H:552:LYS:HE3 | 1:K:492:LEU:HD13 | 2.03 | 0.41 |
| 1:F:126:GLY:HA3 | 1:F:221:LYS:O | 2.20 | 0.41 |
| 1:H:156:PHE:CD2 | 1:H:156:PHE:C | 2.94 | 0.41 |
| 1:B:360:LYS:HE3 | 1:B:365:VAL:HG21 | 2.03 | 0.41 |
| 1:F:367:LYS:HA | 1:F:367:LYS:HD3 | 1.83 | 0.41 |
| 1:I:139:ASN:O | 1:I:166:ASN:HB2 | 2.21 | 0.41 |
| 1:G:177:MET:O | 1:G:184:SER:HA | 2.21 | 0.41 |
| 1:G:374:LYS:HB3 | 7:G:636:HOH:O | 2.20 | 0.41 |
| 1:L:207:VAL:O | 1:L:211:VAL:HG23 | 2.20 | 0.41 |
| 1:A:235:PHE:HE1 | 1:A:269:VAL:HG11 | 1.84 | 0.40 |
| 1:E:129:ILE:HA | 1:E:129:ILE:HD13 | 1.84 | 0.40 |
| 1:A:198:LEU:HB3 | 1:A:202:ASP:HB2 | 2.03 | 0.40 |
| 1:J:375:GLY:O | 1:J:429:VAL:HA | 2.21 | 0.40 |
| 1:K:440:ARG:CD | 1:L:302:SER:HB2 | 2.51 | 0.40 |
| 1:G:481:ILE:O | 1:G:571:TRP:HA | 2.21 | 0.40 |
| 1:I:265:LYS:HA | 1:I:265:LYS:HE2 | 2.03 | 0.40 |
| 1:D:128:THR:O | 1:D:129:ILE:HD13 | 2.21 | 0.40 |
| 1:H:441:PRO:HG2 | 1:I:393:ILE:HG12 | 2.03 | 0.40 |
| 1:D:301:PRO:HB2 | 1:D:303:ASN:OD1 | 2.21 | 0.40 |
| 1:C:239:LEU:HD21 | 1:C:281:VAL:HG22 | 2.03 | 0.40 |
| 1:K:366:LYS:HG3 | 1:K:420:ASN:HB3 | 2.03 | 0.40 |
| 1:H:138:GLU:O | 1:H:140:GLY:N | 2.50 | 0.40 |
| 1:G:301:PRO:HB3 | 1:I:442:GLY:O | 2.20 | 0.40 |
| 1:J:475:LYS:HB3 | 7:J:4358:HOH:O | 2.21 | 0.40 |
| 1:A:349:MET:HG2 | 7:C:1438:HOH:O | 2.21 | 0.40 |
| 1:B:442:GLY:O | 1:C:301:PRO:HB3 | 2.21 | 0.40 |
| 1:C:292:TYR:O | 1:C:295:SER:HB3 | 2.22 | 0.40 |
| 1:C:176:TYR:CE1 | 1:C:184:SER:HB2 | 2.56 | 0.40 |
| 1:J:350:TYR:HA | 1:J:351:PRO:HD3 | 1.97 | 0.40 |
| 1:I:487:LEU:HD22 | 1:I:573:HIS:CE1 | 2.56 | 0.40 |
| 1:L:505:ASN:HA | 7:L:2672:HOH:O | 2.21 | 0.40 |
| 1:I:88:VAL:HG21 | 1:I:97:THR:O | 2.21 | 0.40 |
| 1:B:190:VAL:HG11 | 1:B:206:VAL:HG13 | 2.02 | 0.40 |
| 1:D:522:GLU:HA | 1:D:523:PRO:HD3 | 1.94 | 0.40 |
| 1:I:223:THR:HA | 1:I:268:GLY:O | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:326:LYS:HG2 | 1:A:328:LEU:CD1 | 2.51 | 0.40 |
| 1:G:393:ILE:HG12 | 1:I:441:PRO:HG2 | 2.03 | 0.40 |
| 1:C:178:PHE:CZ | 1:E:155:GLU:HG2 | 2.52 | 0.40 |
| 1:A:200:GLU:HB2 | 1:A:521:ASN:OD1 | 2.21 | 0.40 |
| 1:B:125:GLU:HG2 | 1:B:126:GLY:N | 2.36 | 0.40 |
| 1:K:127:LEU:HA | 1:K:186:ALA:O | 2.20 | 0.40 |
| 1:B:460:ALA:O | 1:B:546:GLN:NE2 | 2.54 | 0.40 |
| 1:K:157:LEU:HA | 1:K:157:LEU:HD23 | 1.88 | 0.40 |
| 1:C:156:PHE:CZ | 1:C:175:PHE:HB3 | 2.56 | 0.40 |
| 1:I:399:ASP:OD1 | 4:I:1003:BEY:N | 2.55 | 0.40 |
| 1:G:115:TYR:O | 1:G:270:TYR:HA | 2.21 | 0.40 |
| 1:L:123:VAL:HG11 | 1:L:153:VAL:HG21 | 2.04 | 0.40 |
| 1:G:239:LEU:HD23 | 1:G:239:LEU:HA | 1.86 | 0.40 |
| 1:G:159:ASP:N | 1:G:159:ASP:OD1 | 2.55 | 0.40 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|-----------------------|--------------------------|-------------------|
| 1:B:366:LYS:NZ | 7:D:3762:HOH:O[4_555] | 1.84 | 0.36 |

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 | 514/528 (97%) | 493 (96%) | 19 (4%) | 2 (0%) | 39 62 |
| 1 | B | 516/528 (98%) | 488 (95%) | 25 (5%) | 3 (1%) | 30 52 |
| 1 | C | 516/528 (98%) | 495 (96%) | 18 (4%) | 3 (1%) | 30 52 |
| 1 | D | 509/528 (96%) | 492 (97%) | 16 (3%) | 1 (0%) | 52 74 |
| 1 | E | 506/528 (96%) | 487 (96%) | 17 (3%) | 2 (0%) | 39 62 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | F | 504/528 (96%) | 484 (96%) | 14 (3%) | 6 (1%) | 16 | 30 |
| 1 | G | 512/528 (97%) | 483 (94%) | 27 (5%) | 2 (0%) | 39 | 62 |
| 1 | H | 503/528 (95%) | 477 (95%) | 21 (4%) | 5 (1%) | 19 | 36 |
| 1 | I | 516/528 (98%) | 493 (96%) | 22 (4%) | 1 (0%) | 52 | 74 |
| 1 | J | 509/528 (96%) | 483 (95%) | 24 (5%) | 2 (0%) | 39 | 62 |
| 1 | K | 503/528 (95%) | 479 (95%) | 22 (4%) | 2 (0%) | 39 | 62 |
| 1 | L | 509/528 (96%) | 484 (95%) | 24 (5%) | 1 (0%) | 52 | 74 |
| All | All | 6117/6336 (96%) | 5838 (95%) | 249 (4%) | 30 (0%) | 34 | 57 |

All (30) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 217 | ASN |
| 1 | B | 149 | ASN |
| 1 | E | 230 | VAL |
| 1 | H | 139 | ASN |
| 1 | B | 273 | ASN |
| 1 | C | 274 | ALA |
| 1 | E | 137 | LYS |
| 1 | H | 231 | ASP |
| 1 | I | 261 | MET |
| 1 | K | 108 | HIS |
| 1 | D | 180 | ASP |
| 1 | F | 163 | GLU |
| 1 | F | 184 | SER |
| 1 | F | 274 | ALA |
| 1 | J | 149 | ASN |
| 1 | C | 139 | ASN |
| 1 | F | 149 | ASN |
| 1 | F | 179 | ASN |
| 1 | G | 149 | ASN |
| 1 | J | 251 | ARG |
| 1 | K | 139 | ASN |
| 1 | L | 168 | LYS |
| 1 | A | 200 | GLU |
| 1 | B | 254 | SER |
| 1 | F | 168 | LYS |
| 1 | G | 218 | LYS |
| 1 | H | 117 | ILE |
| 1 | H | 181 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 117 | ILE |
| 1 | H | 195 | VAL |

5.3.2 Protein sidechains ⓘ

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 | 426/455 (94%) | 407 (96%) | 19 (4%) | 34 | 58 |
| 1 | B | 412/455 (90%) | 403 (98%) | 9 (2%) | 60 | 82 |
| 1 | C | 419/455 (92%) | 406 (97%) | 13 (3%) | 47 | 73 |
| 1 | D | 417/455 (92%) | 395 (95%) | 22 (5%) | 28 | 49 |
| 1 | E | 414/455 (91%) | 396 (96%) | 18 (4%) | 35 | 60 |
| 1 | F | 409/455 (90%) | 385 (94%) | 24 (6%) | 24 | 44 |
| 1 | G | 435/455 (96%) | 418 (96%) | 17 (4%) | 39 | 64 |
| 1 | H | 430/455 (94%) | 412 (96%) | 18 (4%) | 36 | 61 |
| 1 | I | 437/455 (96%) | 414 (95%) | 23 (5%) | 28 | 49 |
| 1 | J | 430/455 (94%) | 404 (94%) | 26 (6%) | 24 | 43 |
| 1 | K | 427/455 (94%) | 412 (96%) | 15 (4%) | 43 | 68 |
| 1 | L | 421/455 (92%) | 403 (96%) | 18 (4%) | 35 | 60 |
| All | All | 5077/5460 (93%) | 4855 (96%) | 222 (4%) | 35 | 59 |

All (222) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 86 | SER |
| 1 | A | 132 | VAL |
| 1 | A | 159 | ASP |
| 1 | A | 160 | GLU |
| 1 | A | 166 | ASN |
| 1 | A | 168 | LYS |
| 1 | A | 194 | SER |
| 1 | A | 197 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 198 | LEU |
| 1 | A | 288 | TYR |
| 1 | A | 310 | LEU |
| 1 | A | 330 | VAL |
| 1 | A | 367 | LYS |
| 1 | A | 398 | PHE |
| 1 | A | 439 | TYR |
| 1 | A | 476 | LEU |
| 1 | A | 498 | SER |
| 1 | A | 579 | VAL |
| 1 | A | 603 | ASP |
| 1 | B | 104 | ASN |
| 1 | B | 200 | GLU |
| 1 | B | 210 | LEU |
| 1 | B | 288 | TYR |
| 1 | B | 310 | LEU |
| 1 | B | 332 | GLU |
| 1 | B | 398 | PHE |
| 1 | B | 439 | TYR |
| 1 | B | 498 | SER |
| 1 | C | 86 | SER |
| 1 | C | 145 | SER |
| 1 | C | 146 | SER |
| 1 | C | 163 | GLU |
| 1 | C | 177 | MET |
| 1 | C | 181 | ASN |
| 1 | C | 185 | VAL |
| 1 | C | 194 | SER |
| 1 | C | 208 | LEU |
| 1 | C | 229 | ASN |
| 1 | C | 288 | TYR |
| 1 | C | 398 | PHE |
| 1 | C | 439 | TYR |
| 1 | D | 90 | GLN |
| 1 | D | 111 | LYS |
| 1 | D | 132 | VAL |
| 1 | D | 198 | LEU |
| 1 | D | 210 | LEU |
| 1 | D | 219 | LEU |
| 1 | D | 231 | ASP |
| 1 | D | 248 | THR |
| 1 | D | 261 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 262 | GLU |
| 1 | D | 276 | THR |
| 1 | D | 288 | TYR |
| 1 | D | 310 | LEU |
| 1 | D | 322 | ASN |
| 1 | D | 367 | LYS |
| 1 | D | 398 | PHE |
| 1 | D | 400 | MET |
| 1 | D | 439 | TYR |
| 1 | D | 518 | LYS |
| 1 | D | 532 | GLU |
| 1 | D | 560 | LEU |
| 1 | D | 579 | VAL |
| 1 | E | 172 | SER |
| 1 | E | 185 | VAL |
| 1 | E | 208 | LEU |
| 1 | E | 217 | ASN |
| 1 | E | 220 | SER |
| 1 | E | 230 | VAL |
| 1 | E | 236 | ARG |
| 1 | E | 238 | PHE |
| 1 | E | 248 | THR |
| 1 | E | 267 | LEU |
| 1 | E | 288 | TYR |
| 1 | E | 310 | LEU |
| 1 | E | 398 | PHE |
| 1 | E | 407 | LEU |
| 1 | E | 413 | VAL |
| 1 | E | 439 | TYR |
| 1 | E | 483 | ASP |
| 1 | E | 560 | LEU |
| 1 | F | 86 | SER |
| 1 | F | 92 | VAL |
| 1 | F | 93 | SER |
| 1 | F | 102 | GLU |
| 1 | F | 114 | VAL |
| 1 | F | 117 | ILE |
| 1 | F | 161 | ASN |
| 1 | F | 198 | LEU |
| 1 | F | 200 | GLU |
| 1 | F | 217 | ASN |
| 1 | F | 239 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 240 | GLU |
| 1 | F | 248 | THR |
| 1 | F | 288 | TYR |
| 1 | F | 310 | LEU |
| 1 | F | 330 | VAL |
| 1 | F | 364 | ASP |
| 1 | F | 367 | LYS |
| 1 | F | 398 | PHE |
| 1 | F | 439 | TYR |
| 1 | F | 476 | LEU |
| 1 | F | 507 | GLU |
| 1 | F | 508 | GLU |
| 1 | F | 579 | VAL |
| 1 | G | 101 | ILE |
| 1 | G | 154 | SER |
| 1 | G | 159 | ASP |
| 1 | G | 164 | LYS |
| 1 | G | 182 | LYS |
| 1 | G | 185 | VAL |
| 1 | G | 195 | VAL |
| 1 | G | 229 | ASN |
| 1 | G | 288 | TYR |
| 1 | G | 310 | LEU |
| 1 | G | 367 | LYS |
| 1 | G | 398 | PHE |
| 1 | G | 400 | MET |
| 1 | G | 439 | TYR |
| 1 | G | 476 | LEU |
| 1 | G | 515 | GLN |
| 1 | G | 579 | VAL |
| 1 | H | 155 | GLU |
| 1 | H | 158 | LYS |
| 1 | H | 173 | LYS |
| 1 | H | 200 | GLU |
| 1 | H | 212 | THR |
| 1 | H | 213 | MET |
| 1 | H | 276 | THR |
| 1 | H | 279 | GLU |
| 1 | H | 288 | TYR |
| 1 | H | 310 | LEU |
| 1 | H | 331 | LYS |
| 1 | H | 398 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 439 | TYR |
| 1 | H | 476 | LEU |
| 1 | H | 498 | SER |
| 1 | H | 508 | GLU |
| 1 | H | 515 | GLN |
| 1 | H | 579 | VAL |
| 1 | I | 121 | CYS |
| 1 | I | 145 | SER |
| 1 | I | 154 | SER |
| 1 | I | 163 | GLU |
| 1 | I | 171 | THR |
| 1 | I | 181 | ASN |
| 1 | I | 182 | LYS |
| 1 | I | 198 | LEU |
| 1 | I | 199 | SER |
| 1 | I | 200 | GLU |
| 1 | I | 208 | LEU |
| 1 | I | 229 | ASN |
| 1 | I | 239 | LEU |
| 1 | I | 288 | TYR |
| 1 | I | 310 | LEU |
| 1 | I | 324 | GLU |
| 1 | I | 398 | PHE |
| 1 | I | 439 | TYR |
| 1 | I | 476 | LEU |
| 1 | I | 483 | ASP |
| 1 | I | 508 | GLU |
| 1 | I | 579 | VAL |
| 1 | I | 603 | ASP |
| 1 | J | 86 | SER |
| 1 | J | 111 | LYS |
| 1 | J | 123 | VAL |
| 1 | J | 143 | LYS |
| 1 | J | 184 | SER |
| 1 | J | 195 | VAL |
| 1 | J | 197 | ASP |
| 1 | J | 208 | LEU |
| 1 | J | 239 | LEU |
| 1 | J | 246 | TYR |
| 1 | J | 248 | THR |
| 1 | J | 261 | MET |
| 1 | J | 276 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | J | 279 | GLU |
| 1 | J | 288 | TYR |
| 1 | J | 310 | LEU |
| 1 | J | 322 | ASN |
| 1 | J | 367 | LYS |
| 1 | J | 398 | PHE |
| 1 | J | 400 | MET |
| 1 | J | 439 | TYR |
| 1 | J | 476 | LEU |
| 1 | J | 483 | ASP |
| 1 | J | 518 | LYS |
| 1 | J | 579 | VAL |
| 1 | J | 603 | ASP |
| 1 | K | 86 | SER |
| 1 | K | 102 | GLU |
| 1 | K | 132 | VAL |
| 1 | K | 208 | LEU |
| 1 | K | 218 | LYS |
| 1 | K | 248 | THR |
| 1 | K | 265 | LYS |
| 1 | K | 288 | TYR |
| 1 | K | 310 | LEU |
| 1 | K | 367 | LYS |
| 1 | K | 398 | PHE |
| 1 | K | 439 | TYR |
| 1 | K | 476 | LEU |
| 1 | K | 579 | VAL |
| 1 | K | 603 | ASP |
| 1 | L | 86 | SER |
| 1 | L | 92 | VAL |
| 1 | L | 161 | ASN |
| 1 | L | 165 | PHE |
| 1 | L | 167 | VAL |
| 1 | L | 184 | SER |
| 1 | L | 200 | GLU |
| 1 | L | 275 | ASP |
| 1 | L | 288 | TYR |
| 1 | L | 310 | LEU |
| 1 | L | 367 | LYS |
| 1 | L | 398 | PHE |
| 1 | L | 439 | TYR |
| 1 | L | 508 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | L | 518 | LYS |
| 1 | L | 579 | VAL |
| 1 | L | 584 | LYS |
| 1 | L | 605 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 152 | GLN |
| 1 | B | 113 | GLN |
| 1 | B | 181 | ASN |
| 1 | B | 229 | ASN |
| 1 | C | 181 | ASN |
| 1 | C | 215 | HIS |
| 1 | E | 161 | ASN |
| 1 | E | 181 | ASN |
| 1 | E | 272 | ASN |
| 1 | E | 531 | ASN |
| 1 | F | 217 | ASN |
| 1 | G | 122 | ASN |
| 1 | G | 567 | GLN |
| 1 | H | 183 | ASN |
| 1 | H | 511 | ASN |
| 1 | I | 139 | ASN |
| 1 | I | 166 | ASN |
| 1 | I | 602 | ASN |
| 1 | K | 181 | ASN |
| 1 | K | 322 | ASN |
| 1 | K | 602 | ASN |
| 1 | L | 420 | ASN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 24 are monoatomic - leaving 76 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 | $\# Z > 2$ |
| 5 | SO4 | A | 1 | - | 4,4,4 | 0.20 | 0 | 6,6,6 | 0.29 | 0 |
| 2 | CO3 | A | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | A | 1003 | 3 | 19,26,26 | 0.73 | 0 | 22,35,35 | 1.14 | 2 (9%) |
| 6 | 1PE | A | 19 | - | 8,8,15 | 0.61 | 0 | 7,7,14 | 0.21 | 0 |
| 5 | SO4 | A | 2 | - | 4,4,4 | 0.32 | 0 | 6,6,6 | 0.47 | 0 |
| 6 | 1PE | A | 20 | - | 11,11,15 | 0.64 | 0 | 10,10,14 | 0.35 | 0 |
| 5 | SO4 | A | 24 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.32 | 0 |
| 2 | CO3 | B | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | B | 1003 | 3 | 19,26,26 | 0.87 | 0 | 22,35,35 | 1.29 | 2 (9%) |
| 6 | 1PE | B | 60 | - | 9,9,15 | 0.55 | 0 | 8,8,14 | 0.28 | 0 |
| 6 | 1PE | B | 61 | - | 9,9,15 | 0.72 | 0 | 8,8,14 | 0.93 | 0 |
| 6 | 1PE | B | 62 | - | 9,9,15 | 0.69 | 0 | 8,8,14 | 0.45 | 0 |
| 2 | CO3 | C | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | C | 1003 | 3 | 19,26,26 | 1.21 | 1 (5%) | 22,35,35 | 1.42 | 3 (13%) |
| 6 | 1PE | C | 17 | - | 12,12,15 | 0.92 | 0 | 11,11,14 | 1.07 | 1 (9%) |
| 6 | 1PE | C | 18 | - | 8,8,15 | 0.59 | 0 | 7,7,14 | 0.37 | 0 |
| 5 | SO4 | C | 3 | - | 4,4,4 | 0.38 | 0 | 6,6,6 | 0.23 | 0 |
| 2 | CO3 | D | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | D | 1003 | 3 | 19,26,26 | 0.96 | 1 (5%) | 22,35,35 | 0.97 | 1 (4%) |
| 6 | 1PE | D | 44 | - | 10,10,15 | 0.71 | 0 | 9,9,14 | 0.45 | 0 |
| 5 | SO4 | D | 5 | - | 4,4,4 | 0.20 | 0 | 6,6,6 | 0.13 | 0 |
| 6 | 1PE | D | 63 | - | 9,9,15 | 0.71 | 0 | 8,8,14 | 0.42 | 0 |
| 6 | 1PE | D | 67 | - | 6,6,15 | 0.73 | 0 | 5,5,14 | 0.37 | 0 |
| 6 | 1PE | D | 9 | - | 9,9,15 | 0.61 | 0 | 8,8,14 | 0.58 | 0 |
| 2 | CO3 | E | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | E | 1003 | 3 | 19,26,26 | 0.73 | 0 | 22,35,35 | 1.57 | 3 (13%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 5 | SO4 | E | 22 | - | 4,4,4 | 0.30 | 0 | 6,6,6 | 0.40 | 0 |
| 6 | 1PE | E | 43 | - | 7,7,15 | 0.47 | 0 | 6,6,14 | 0.50 | 0 |
| 6 | 1PE | E | 612 | - | 11,11,15 | 0.61 | 0 | 10,10,14 | 0.42 | 0 |
| 5 | SO4 | E | 7 | - | 4,4,4 | 0.43 | 0 | 6,6,6 | 0.37 | 0 |
| 6 | 1PE | E | 8 | - | 11,11,15 | 0.53 | 0 | 10,10,14 | 0.44 | 0 |
| 2 | CO3 | F | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | F | 1003 | 3 | 19,26,26 | 1.11 | 1 (5%) | 22,35,35 | 1.27 | 1 (4%) |
| 5 | SO4 | F | 21 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.15 | 0 |
| 6 | 1PE | F | 31 | - | 9,9,15 | 0.50 | 0 | 8,8,14 | 0.50 | 0 |
| 6 | 1PE | F | 32 | - | 9,9,15 | 0.66 | 0 | 8,8,14 | 0.42 | 0 |
| 6 | 1PE | F | 33 | - | 9,9,15 | 0.62 | 0 | 8,8,14 | 0.25 | 0 |
| 2 | CO3 | G | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | G | 1003 | 3 | 19,26,26 | 0.94 | 0 | 22,35,35 | 1.50 | 1 (4%) |
| 6 | 1PE | G | 12 | - | 8,8,15 | 0.50 | 0 | 7,7,14 | 0.20 | 0 |
| 5 | SO4 | G | 23 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.21 | 0 |
| 5 | SO4 | G | 26 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.08 | 0 |
| 6 | 1PE | G | 30 | - | 6,6,15 | 0.55 | 0 | 5,5,14 | 0.41 | 0 |
| 6 | 1PE | G | 47 | - | 5,5,15 | 0.41 | 0 | 4,4,14 | 0.27 | 0 |
| 6 | 1PE | G | 48 | - | 5,5,15 | 0.64 | 0 | 4,4,14 | 0.76 | 0 |
| 6 | 1PE | G | 58 | - | 14,14,15 | 0.74 | 0 | 13,13,14 | 0.54 | 0 |
| 2 | CO3 | H | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | H | 1003 | 3 | 19,26,26 | 0.80 | 0 | 22,35,35 | 1.31 | 2 (9%) |
| 6 | 1PE | H | 64 | - | 9,9,15 | 0.63 | 0 | 8,8,14 | 0.25 | 0 |
| 6 | 1PE | H | 65 | - | 9,9,15 | 0.60 | 0 | 8,8,14 | 0.24 | 0 |
| 2 | CO3 | I | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | I | 1003 | 3 | 19,26,26 | 0.79 | 1 (5%) | 22,35,35 | 1.65 | 4 (18%) |
| 5 | SO4 | I | 17 | - | 4,4,4 | 0.22 | 0 | 6,6,6 | 0.16 | 0 |
| 6 | 1PE | I | 21 | - | 14,14,15 | 0.73 | 0 | 13,13,14 | 0.51 | 0 |
| 6 | 1PE | I | 22 | - | 10,10,15 | 0.58 | 0 | 9,9,14 | 0.54 | 0 |
| 6 | 1PE | I | 66 | - | 6,6,15 | 0.62 | 0 | 5,5,14 | 0.53 | 0 |
| 2 | CO3 | J | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | J | 1003 | 3 | 19,26,26 | 0.84 | 0 | 22,35,35 | 0.98 | 1 (4%) |
| 5 | SO4 | J | 18 | - | 4,4,4 | 0.63 | 0 | 6,6,6 | 0.20 | 0 |
| 6 | 1PE | J | 2 | - | 10,10,15 | 0.61 | 0 | 9,9,14 | 0.37 | 0 |
| 5 | SO4 | J | 20 | - | 4,4,4 | 0.25 | 0 | 6,6,6 | 0.26 | 0 |
| 6 | 1PE | J | 3 | - | 9,9,15 | 0.59 | 0 | 8,8,14 | 0.53 | 0 |
| 6 | 1PE | J | 45 | - | 9,9,15 | 0.68 | 0 | 8,8,14 | 0.53 | 0 |
| 2 | CO3 | K | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | K | 1003 | 3 | 19,26,26 | 0.62 | 0 | 22,35,35 | 2.03 | 5 (22%) |
| 5 | SO4 | K | 19 | - | 4,4,4 | 0.26 | 0 | 6,6,6 | 0.13 | 0 |
| 6 | 1PE | K | 4 | - | 11,11,15 | 0.74 | 0 | 10,10,14 | 0.64 | 0 |
| 6 | 1PE | K | 42 | - | 10,10,15 | 0.59 | 0 | 9,9,14 | 0.34 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 6 | 1PE | K | 5 | - | 11,11,15 | 0.52 | 0 | 10,10,14 | 0.43 | 0 |
| 6 | 1PE | K | 50 | - | 5,5,15 | 0.68 | 0 | 4,4,14 | 0.48 | 0 |
| 6 | 1PE | L | 1 | - | 9,9,15 | 0.52 | 0 | 8,8,14 | 0.36 | 0 |
| 2 | CO3 | L | 1002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | BEY | L | 1003 | 3 | 19,26,26 | 0.86 | 1 (5%) | 22,35,35 | 1.20 | 2 (9%) |
| 5 | SO4 | L | 25 | - | 4,4,4 | 0.18 | 0 | 6,6,6 | 0.35 | 0 |
| 6 | 1PE | L | 56 | - | 10,10,15 | 0.77 | 0 | 9,9,14 | 0.47 | 0 |
| 6 | 1PE | L | 612 | - | 11,11,15 | 0.66 | 0 | 10,10,14 | 0.33 | 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 |
|-----|------|-------|------|------|---------|------------|---------|
| 5 | SO4 | A | 1 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | CO3 | A | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | A | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | A | 19 | - | - | 0/6/6/13 | 0/0/0/0 |
| 5 | SO4 | A | 2 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | A | 20 | - | - | 0/9/9/13 | 0/0/0/0 |
| 5 | SO4 | A | 24 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | CO3 | B | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | B | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | B | 60 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | B | 61 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | B | 62 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | C | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | C | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | C | 17 | - | - | 0/10/10/13 | 0/0/0/0 |
| 6 | 1PE | C | 18 | - | - | 0/6/6/13 | 0/0/0/0 |
| 5 | SO4 | C | 3 | - | - | 0/0/0/0 | 0/0/0/0 |
| 2 | CO3 | D | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | D | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | D | 44 | - | - | 0/8/8/13 | 0/0/0/0 |
| 5 | SO4 | D | 5 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | D | 63 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | D | 67 | - | - | 0/4/4/13 | 0/0/0/0 |
| 6 | 1PE | D | 9 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | E | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | E | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | E | 22 | - | - | 0/0/0/0 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 6 | 1PE | E | 43 | - | - | 0/5/5/13 | 0/0/0/0 |
| 6 | 1PE | E | 612 | - | - | 0/9/9/13 | 0/0/0/0 |
| 5 | SO4 | E | 7 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | E | 8 | - | - | 0/9/9/13 | 0/0/0/0 |
| 2 | CO3 | F | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | F | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | F | 21 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | F | 31 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | F | 32 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | F | 33 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | G | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | G | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | G | 12 | - | - | 0/6/6/13 | 0/0/0/0 |
| 5 | SO4 | G | 23 | - | - | 0/0/0/0 | 0/0/0/0 |
| 5 | SO4 | G | 26 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | G | 30 | - | - | 0/4/4/13 | 0/0/0/0 |
| 6 | 1PE | G | 47 | - | - | 0/3/3/13 | 0/0/0/0 |
| 6 | 1PE | G | 48 | - | - | 0/3/3/13 | 0/0/0/0 |
| 6 | 1PE | G | 58 | - | - | 0/12/12/13 | 0/0/0/0 |
| 2 | CO3 | H | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | H | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 6 | 1PE | H | 64 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | H | 65 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | I | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | I | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | I | 17 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | I | 21 | - | - | 0/12/12/13 | 0/0/0/0 |
| 6 | 1PE | I | 22 | - | - | 0/8/8/13 | 0/0/0/0 |
| 6 | 1PE | I | 66 | - | - | 0/4/4/13 | 0/0/0/0 |
| 2 | CO3 | J | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | J | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | J | 18 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | J | 2 | - | - | 0/8/8/13 | 0/0/0/0 |
| 5 | SO4 | J | 20 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | J | 3 | - | - | 0/7/7/13 | 0/0/0/0 |
| 6 | 1PE | J | 45 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | K | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | K | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | K | 19 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | K | 4 | - | - | 0/9/9/13 | 0/0/0/0 |
| 6 | 1PE | K | 42 | - | - | 0/8/8/13 | 0/0/0/0 |
| 6 | 1PE | K | 5 | - | - | 0/9/9/13 | 0/0/0/0 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 6 | 1PE | K | 50 | - | - | 0/3/3/13 | 0/0/0/0 |
| 6 | 1PE | L | 1 | - | - | 0/7/7/13 | 0/0/0/0 |
| 2 | CO3 | L | 1002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | BEY | L | 1003 | 3 | - | 0/14/24/24 | 0/2/2/2 |
| 5 | SO4 | L | 25 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | 1PE | L | 56 | - | - | 0/8/8/13 | 0/0/0/0 |
| 6 | 1PE | L | 612 | - | - | 0/9/9/13 | 0/0/0/0 |

All (5) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 4 | I | 1003 | BEY | P-C17 | 2.21 | 1.81 | 1.79 |
| 4 | L | 1003 | BEY | P-C17 | 2.43 | 1.82 | 1.79 |
| 4 | F | 1003 | BEY | P-C17 | 2.69 | 1.82 | 1.79 |
| 4 | D | 1003 | BEY | P-C17 | 2.86 | 1.82 | 1.79 |
| 4 | C | 1003 | BEY | P-C17 | 3.97 | 1.83 | 1.79 |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4 | C | 1003 | BEY | C7-C8-C9 | -4.48 | 102.27 | 111.03 |
| 4 | K | 1003 | BEY | C17-C8-C7 | -4.44 | 103.30 | 110.83 |
| 4 | B | 1003 | BEY | C17-C8-C7 | -4.08 | 103.92 | 110.83 |
| 4 | E | 1003 | BEY | C17-C8-C7 | -4.05 | 103.97 | 110.83 |
| 4 | L | 1003 | BEY | C17-C8-C7 | -3.32 | 105.20 | 110.83 |
| 4 | C | 1003 | BEY | C1-C7-C8 | -3.00 | 109.58 | 113.92 |
| 4 | H | 1003 | BEY | C17-C8-C7 | -2.47 | 106.63 | 110.83 |
| 4 | I | 1003 | BEY | C17-C8-C7 | -2.13 | 107.21 | 110.83 |
| 4 | D | 1003 | BEY | C1-C7-C8 | -2.13 | 110.83 | 113.92 |
| 4 | K | 1003 | BEY | C18-C19-N | -2.03 | 104.77 | 110.52 |
| 4 | C | 1003 | BEY | C5-C1-C2 | 2.00 | 121.34 | 118.13 |
| 4 | L | 1003 | BEY | C1-C7-C8 | 2.02 | 116.83 | 113.92 |
| 6 | C | 17 | 1PE | OH4-C24-C14 | 2.09 | 119.64 | 110.36 |
| 4 | A | 1003 | BEY | C13-C16-C10 | 2.14 | 121.55 | 118.13 |
| 4 | E | 1003 | BEY | C7-C8-C9 | 2.14 | 115.21 | 111.03 |
| 4 | I | 1003 | BEY | O3-P-O4 | 2.50 | 117.57 | 113.72 |
| 4 | A | 1003 | BEY | O3-P-O4 | 2.75 | 117.95 | 113.72 |
| 4 | B | 1003 | BEY | O3-P-O4 | 2.78 | 117.99 | 113.72 |
| 4 | I | 1003 | BEY | C7-C8-C9 | 3.28 | 117.44 | 111.03 |
| 4 | J | 1003 | BEY | O3-P-O4 | 3.74 | 119.47 | 113.72 |
| 4 | K | 1003 | BEY | O3-P-O4 | 3.82 | 119.59 | 113.72 |
| 4 | H | 1003 | BEY | O3-P-O4 | 3.98 | 119.84 | 113.72 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4 | F | 1003 | BEY | O3-P-O4 | 4.17 | 120.14 | 113.72 |
| 4 | E | 1003 | BEY | O3-P-O4 | 4.43 | 120.53 | 113.72 |
| 4 | K | 1003 | BEY | C1-C7-C8 | 4.45 | 120.36 | 113.92 |
| 4 | K | 1003 | BEY | C7-C8-C9 | 4.48 | 119.79 | 111.03 |
| 4 | I | 1003 | BEY | C1-C7-C8 | 5.37 | 121.69 | 113.92 |
| 4 | G | 1003 | BEY | O3-P-O4 | 5.41 | 122.04 | 113.72 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

49 monomers are involved in 99 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | A | 1003 | BEY | 4 | 0 |
| 6 | A | 20 | 1PE | 2 | 0 |
| 4 | B | 1003 | BEY | 2 | 0 |
| 6 | B | 60 | 1PE | 1 | 0 |
| 6 | B | 61 | 1PE | 2 | 0 |
| 4 | C | 1003 | BEY | 5 | 0 |
| 6 | C | 17 | 1PE | 1 | 0 |
| 5 | C | 3 | SO4 | 1 | 0 |
| 2 | D | 1002 | CO3 | 2 | 0 |
| 4 | D | 1003 | BEY | 6 | 0 |
| 6 | D | 44 | 1PE | 4 | 0 |
| 6 | D | 63 | 1PE | 1 | 0 |
| 4 | E | 1003 | BEY | 2 | 0 |
| 5 | E | 22 | SO4 | 1 | 0 |
| 6 | E | 43 | 1PE | 2 | 0 |
| 6 | E | 612 | 1PE | 1 | 0 |
| 5 | E | 7 | SO4 | 2 | 0 |
| 4 | F | 1003 | BEY | 2 | 0 |
| 5 | F | 21 | SO4 | 1 | 0 |
| 6 | F | 31 | 1PE | 1 | 0 |
| 4 | G | 1003 | BEY | 2 | 0 |
| 6 | G | 30 | 1PE | 1 | 0 |
| 6 | G | 47 | 1PE | 1 | 0 |
| 6 | G | 58 | 1PE | 2 | 0 |
| 2 | H | 1002 | CO3 | 1 | 0 |
| 4 | H | 1003 | BEY | 7 | 0 |
| 6 | H | 65 | 1PE | 1 | 0 |
| 2 | I | 1002 | CO3 | 1 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 4 | I | 1003 | BEY | 2 | 0 |
| 5 | I | 17 | SO4 | 1 | 0 |
| 6 | I | 21 | 1PE | 4 | 0 |
| 6 | I | 22 | 1PE | 1 | 0 |
| 2 | J | 1002 | CO3 | 1 | 0 |
| 4 | J | 1003 | BEY | 3 | 0 |
| 5 | J | 18 | SO4 | 1 | 0 |
| 6 | J | 2 | 1PE | 2 | 0 |
| 5 | J | 20 | SO4 | 1 | 0 |
| 6 | J | 3 | 1PE | 5 | 0 |
| 6 | J | 45 | 1PE | 2 | 0 |
| 2 | K | 1002 | CO3 | 2 | 0 |
| 4 | K | 1003 | BEY | 4 | 0 |
| 6 | K | 4 | 1PE | 1 | 0 |
| 6 | K | 42 | 1PE | 3 | 0 |
| 6 | K | 5 | 1PE | 3 | 0 |
| 6 | K | 50 | 1PE | 1 | 0 |
| 6 | L | 1 | 1PE | 2 | 0 |
| 2 | L | 1002 | CO3 | 1 | 0 |
| 4 | L | 1003 | BEY | 2 | 0 |
| 6 | L | 612 | 1PE | 3 | 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, 95th 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 | 518/528 (98%) | 0.17 | 12 (2%) 64 62 | 13, 25, 45, 61 | 1 (0%) |
| 1 | B | 518/528 (98%) | 0.22 | 10 (1%) 70 68 | 13, 29, 64, 77 | 0 |
| 1 | C | 518/528 (98%) | 0.17 | 2 (0%) 93 93 | 11, 26, 49, 59 | 0 |
| 1 | D | 513/528 (97%) | 0.00 | 4 (0%) 87 87 | 15, 25, 45, 66 | 0 |
| 1 | E | 510/528 (96%) | 0.04 | 5 (0%) 84 84 | 11, 24, 40, 59 | 0 |
| 1 | F | 510/528 (96%) | 0.53 | 48 (9%) 11 9 | 18, 30, 60, 72 | 0 |
| 1 | G | 516/528 (97%) | 0.23 | 9 (1%) 73 71 | 13, 25, 44, 62 | 0 |
| 1 | H | 509/528 (96%) | 0.16 | 7 (1%) 78 77 | 14, 28, 60, 72 | 0 |
| 1 | I | 518/528 (98%) | 0.20 | 9 (1%) 73 71 | 15, 26, 52, 64 | 0 |
| 1 | J | 513/528 (97%) | 0.07 | 5 (0%) 84 84 | 12, 25, 46, 69 | 0 |
| 1 | K | 509/528 (96%) | 0.02 | 3 (0%) 90 90 | 13, 24, 42, 58 | 0 |
| 1 | L | 513/528 (97%) | 0.32 | 21 (4%) 41 38 | 16, 28, 55, 63 | 0 |
| All | All | 6165/6336 (97%) | 0.18 | 135 (2%) 65 64 | 11, 26, 53, 77 | 1 (0%) |

All (135) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 363 | GLY | 5.9 |
| 1 | F | 362 | LYS | 5.7 |
| 1 | B | 259 | VAL | 4.9 |
| 1 | F | 140 | GLY | 4.8 |
| 1 | F | 156 | PHE | 4.8 |
| 1 | F | 113 | GLN | 4.6 |
| 1 | J | 260 | ASN | 4.3 |
| 1 | L | 145 | SER | 4.1 |
| 1 | B | 257 | LYS | 4.1 |
| 1 | F | 165 | PHE | 4.0 |
| 1 | F | 126 | GLY | 3.9 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 267 | LEU | 3.8 |
| 1 | F | 364 | ASP | 3.7 |
| 1 | B | 258 | ASN | 3.6 |
| 1 | F | 132 | VAL | 3.6 |
| 1 | L | 165 | PHE | 3.5 |
| 1 | F | 121 | CYS | 3.5 |
| 1 | L | 132 | VAL | 3.5 |
| 1 | A | 364 | ASP | 3.5 |
| 1 | F | 222 | LEU | 3.5 |
| 1 | F | 270 | TYR | 3.4 |
| 1 | B | 260 | ASN | 3.4 |
| 1 | L | 163 | GLU | 3.3 |
| 1 | F | 276 | THR | 3.3 |
| 1 | G | 183 | ASN | 3.3 |
| 1 | F | 157 | LEU | 3.3 |
| 1 | F | 148 | VAL | 3.3 |
| 1 | L | 141 | PRO | 3.2 |
| 1 | G | 148 | VAL | 3.2 |
| 1 | G | 602 | ASN | 3.2 |
| 1 | F | 127 | LEU | 3.2 |
| 1 | F | 187 | VAL | 3.1 |
| 1 | F | 223 | THR | 3.1 |
| 1 | K | 603 | ASP | 3.1 |
| 1 | F | 114 | VAL | 3.1 |
| 1 | A | 121 | CYS | 3.0 |
| 1 | G | 119 | GLY | 3.0 |
| 1 | H | 603 | ASP | 3.0 |
| 1 | A | 601 | LEU | 3.0 |
| 1 | L | 604 | ALA | 3.0 |
| 1 | F | 185 | VAL | 2.9 |
| 1 | L | 119 | GLY | 2.9 |
| 1 | F | 159 | ASP | 2.9 |
| 1 | F | 139 | ASN | 2.9 |
| 1 | F | 161 | ASN | 2.9 |
| 1 | D | 219 | LEU | 2.9 |
| 1 | L | 115 | TYR | 2.8 |
| 1 | F | 128 | THR | 2.8 |
| 1 | F | 160 | GLU | 2.8 |
| 1 | A | 603 | ASP | 2.8 |
| 1 | L | 144 | ILE | 2.8 |
| 1 | B | 603 | ASP | 2.8 |
| 1 | J | 261 | MET | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | F | 141 | PRO | 2.8 |
| 1 | F | 271 | ILE | 2.7 |
| 1 | B | 421 | VAL | 2.7 |
| 1 | F | 119 | GLY | 2.7 |
| 1 | J | 603 | ASP | 2.7 |
| 1 | F | 115 | TYR | 2.7 |
| 1 | F | 130 | PHE | 2.6 |
| 1 | L | 130 | PHE | 2.6 |
| 1 | L | 140 | GLY | 2.6 |
| 1 | I | 103 | TYR | 2.6 |
| 1 | H | 196 | ALA | 2.6 |
| 1 | L | 360 | LYS | 2.5 |
| 1 | F | 549 | SER | 2.5 |
| 1 | B | 176 | TYR | 2.5 |
| 1 | E | 456 | GLY | 2.5 |
| 1 | L | 363 | GLY | 2.5 |
| 1 | A | 277 | TYR | 2.5 |
| 1 | A | 119 | GLY | 2.5 |
| 1 | F | 183 | ASN | 2.5 |
| 1 | J | 599 | PHE | 2.5 |
| 1 | F | 145 | SER | 2.5 |
| 1 | D | 419 | GLU | 2.4 |
| 1 | F | 146 | SER | 2.4 |
| 1 | E | 366 | LYS | 2.4 |
| 1 | I | 421 | VAL | 2.4 |
| 1 | I | 259 | VAL | 2.4 |
| 1 | D | 261 | MET | 2.4 |
| 1 | B | 269 | VAL | 2.4 |
| 1 | F | 210 | LEU | 2.4 |
| 1 | E | 361 | SER | 2.3 |
| 1 | I | 418 | PRO | 2.3 |
| 1 | J | 136 | GLY | 2.3 |
| 1 | L | 146 | SER | 2.3 |
| 1 | L | 362 | LYS | 2.3 |
| 1 | F | 112 | VAL | 2.3 |
| 1 | A | 180 | ASP | 2.3 |
| 1 | C | 419 | GLU | 2.3 |
| 1 | C | 603 | ASP | 2.3 |
| 1 | F | 144 | ILE | 2.3 |
| 1 | H | 178 | PHE | 2.3 |
| 1 | E | 363 | GLY | 2.3 |
| 1 | H | 175 | PHE | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | F | 195 | VAL | 2.3 |
| 1 | I | 195 | VAL | 2.3 |
| 1 | A | 148 | VAL | 2.3 |
| 1 | G | 195 | VAL | 2.3 |
| 1 | G | 225 | VAL | 2.3 |
| 1 | G | 601 | LEU | 2.2 |
| 1 | K | 373 | GLY | 2.2 |
| 1 | F | 217 | ASN | 2.2 |
| 1 | E | 480 | TYR | 2.2 |
| 1 | B | 154 | SER | 2.2 |
| 1 | I | 420 | ASN | 2.2 |
| 1 | A | 602 | ASN | 2.2 |
| 1 | L | 158 | LYS | 2.1 |
| 1 | B | 263 | TYR | 2.1 |
| 1 | H | 163 | GLU | 2.1 |
| 1 | G | 118 | LYS | 2.1 |
| 1 | F | 413 | VAL | 2.1 |
| 1 | F | 150 | ASP | 2.1 |
| 1 | F | 229 | ASN | 2.1 |
| 1 | H | 109 | ASP | 2.1 |
| 1 | F | 176 | TYR | 2.1 |
| 1 | K | 324 | GLU | 2.1 |
| 1 | L | 162 | MET | 2.1 |
| 1 | A | 226 | PHE | 2.1 |
| 1 | F | 184 | SER | 2.1 |
| 1 | G | 364 | ASP | 2.1 |
| 1 | I | 318 | ALA | 2.1 |
| 1 | A | 136 | GLY | 2.1 |
| 1 | L | 157 | LEU | 2.1 |
| 1 | I | 304 | TYR | 2.0 |
| 1 | L | 176 | TYR | 2.0 |
| 1 | F | 420 | ASN | 2.0 |
| 1 | A | 118 | LYS | 2.0 |
| 1 | F | 478 | VAL | 2.0 |
| 1 | I | 120 | GLY | 2.0 |
| 1 | H | 421 | VAL | 2.0 |
| 1 | D | 279 | GLU | 2.0 |
| 1 | F | 155 | GLU | 2.0 |
| 1 | L | 323 | LEU | 2.0 |
| 1 | L | 270 | TYR | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|------|----------------------------|-------|
| 6 | 1PE | D | 67 | 7/16 | 0.82 | 0.29 | 7.05 | 30,41,53,54 | 0 |
| 6 | 1PE | L | 612 | 12/16 | 0.85 | 0.28 | 6.51 | 41,59,63,64 | 0 |
| 6 | 1PE | F | 33 | 10/16 | 0.86 | 0.23 | 5.45 | 33,61,63,64 | 0 |
| 5 | SO4 | G | 26 | 5/5 | 0.93 | 0.41 | 5.34 | 30,30,30,30 | 0 |
| 6 | 1PE | D | 44 | 11/16 | 0.80 | 0.26 | 4.99 | 37,51,60,63 | 0 |
| 2 | CO3 | J | 1002 | 4/4 | 0.98 | 0.18 | 3.82 | 27,27,29,31 | 0 |
| 6 | 1PE | K | 50 | 6/16 | 0.88 | 0.21 | 3.48 | 11,25,55,55 | 0 |
| 6 | 1PE | B | 60 | 10/16 | 0.90 | 0.25 | 3.32 | 33,48,74,75 | 0 |
| 6 | 1PE | F | 31 | 10/16 | 0.86 | 0.22 | 2.96 | 36,44,74,74 | 0 |
| 6 | 1PE | G | 58 | 15/16 | 0.88 | 0.21 | 2.51 | 43,47,56,56 | 0 |
| 6 | 1PE | A | 20 | 12/16 | 0.88 | 0.21 | 2.31 | 49,54,58,58 | 0 |
| 6 | 1PE | H | 64 | 10/16 | 0.88 | 0.23 | 2.02 | 43,47,52,53 | 0 |
| 6 | 1PE | G | 47 | 6/16 | 0.96 | 0.27 | 1.91 | 15,22,28,39 | 0 |
| 4 | BEY | A | 1003 | 25/25 | 0.94 | 0.19 | 1.68 | 17,33,63,65 | 0 |
| 2 | CO3 | F | 1002 | 4/4 | 0.98 | 0.18 | 1.66 | 35,38,39,44 | 0 |
| 4 | BEY | L | 1003 | 25/25 | 0.92 | 0.20 | 1.62 | 36,57,69,71 | 0 |
| 5 | SO4 | A | 2 | 5/5 | 0.84 | 0.19 | 1.33 | 60,62,74,74 | 0 |
| 2 | CO3 | L | 1002 | 4/4 | 0.97 | 0.18 | 1.29 | 27,27,28,33 | 0 |
| 2 | CO3 | A | 1002 | 4/4 | 0.95 | 0.16 | 1.19 | 39,42,43,46 | 0 |
| 6 | 1PE | J | 2 | 11/16 | 0.94 | 0.21 | 1.08 | 12,25,44,48 | 0 |
| 4 | BEY | K | 1003 | 25/25 | 0.95 | 0.18 | 1.05 | 19,30,45,54 | 0 |
| 4 | BEY | I | 1003 | 25/25 | 0.94 | 0.17 | 1.03 | 21,33,40,50 | 0 |
| 2 | CO3 | B | 1002 | 4/4 | 0.97 | 0.18 | 1.02 | 11,14,16,19 | 0 |
| 4 | BEY | F | 1003 | 25/25 | 0.92 | 0.18 | 0.95 | 23,35,51,55 | 0 |
| 2 | CO3 | H | 1002 | 4/4 | 0.96 | 0.17 | 0.93 | 15,23,23,28 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 4 | BEY | H | 1003 | 25/25 | 0.90 | 0.18 | 0.91 | 26,38,46,50 | 0 |
| 2 | CO3 | E | 1002 | 4/4 | 0.96 | 0.16 | 0.87 | 31,33,34,34 | 0 |
| 2 | CO3 | G | 1002 | 4/4 | 0.97 | 0.17 | 0.80 | 19,20,22,26 | 0 |
| 6 | 1PE | E | 43 | 8/16 | 0.86 | 0.22 | 0.76 | 43,45,55,55 | 0 |
| 4 | BEY | J | 1003 | 25/25 | 0.93 | 0.17 | 0.59 | 28,42,55,57 | 0 |
| 2 | CO3 | K | 1002 | 4/4 | 0.95 | 0.17 | 0.58 | 25,30,31,37 | 0 |
| 4 | BEY | D | 1003 | 25/25 | 0.93 | 0.17 | 0.53 | 20,40,59,61 | 0 |
| 4 | BEY | E | 1003 | 25/25 | 0.94 | 0.17 | 0.45 | 22,42,59,61 | 0 |
| 4 | BEY | C | 1003 | 25/25 | 0.94 | 0.17 | 0.31 | 16,33,43,47 | 0 |
| 5 | SO4 | J | 18 | 5/5 | 0.99 | 0.17 | 0.22 | 22,28,36,37 | 0 |
| 4 | BEY | G | 1003 | 25/25 | 0.94 | 0.16 | 0.12 | 13,29,59,61 | 0 |
| 4 | BEY | B | 1003 | 25/25 | 0.94 | 0.15 | 0.04 | 26,38,48,50 | 0 |
| 6 | 1PE | I | 22 | 11/16 | 0.91 | 0.21 | 0.03 | 30,47,62,67 | 0 |
| 6 | 1PE | K | 42 | 11/16 | 0.87 | 0.16 | -0.12 | 30,44,49,51 | 0 |
| 6 | 1PE | D | 9 | 10/16 | 0.91 | 0.17 | -0.16 | 27,38,45,48 | 0 |
| 5 | SO4 | A | 24 | 5/5 | 0.94 | 0.16 | -0.31 | 53,57,63,64 | 0 |
| 6 | 1PE | E | 8 | 12/16 | 0.93 | 0.15 | -0.33 | 18,34,63,63 | 0 |
| 6 | 1PE | K | 5 | 12/16 | 0.92 | 0.16 | -0.47 | 23,35,52,53 | 0 |
| 2 | CO3 | C | 1002 | 4/4 | 0.96 | 0.15 | -0.65 | 13,21,22,28 | 0 |
| 6 | 1PE | A | 19 | 9/16 | 0.93 | 0.14 | -0.76 | 20,25,34,41 | 0 |
| 6 | 1PE | I | 66 | 7/16 | 0.91 | 0.17 | -0.79 | 26,35,44,46 | 0 |
| 5 | SO4 | C | 3 | 5/5 | 0.99 | 0.14 | -0.86 | 17,18,25,26 | 0 |
| 2 | CO3 | D | 1002 | 4/4 | 0.97 | 0.14 | -1.00 | 22,24,25,27 | 0 |
| 6 | 1PE | L | 1 | 10/16 | 0.95 | 0.13 | -1.10 | 15,23,33,35 | 0 |
| 5 | SO4 | E | 7 | 5/5 | 0.99 | 0.12 | -1.45 | 16,24,35,37 | 0 |
| 6 | 1PE | G | 12 | 9/16 | 0.94 | 0.14 | -1.51 | 20,25,41,44 | 0 |
| 6 | 1PE | G | 48 | 6/16 | 0.95 | 0.16 | -2.09 | 16,22,26,26 | 0 |
| 5 | SO4 | I | 17 | 5/5 | 0.99 | 0.10 | -2.14 | 8,10,15,22 | 0 |
| 2 | CO3 | I | 1002 | 4/4 | 0.98 | 0.12 | -2.41 | 18,19,22,23 | 0 |
| 3 | ZN | E | 1001 | 1/1 | 0.99 | 0.06 | -2.46 | 30,30,30,30 | 0 |
| 3 | ZN | F | 1001 | 1/1 | 0.99 | 0.08 | -2.49 | 29,29,29,29 | 0 |
| 3 | ZN | E | 1004 | 1/1 | 0.99 | 0.04 | -3.07 | 45,45,45,45 | 0 |
| 3 | ZN | H | 1001 | 1/1 | 0.99 | 0.07 | -3.29 | 39,39,39,39 | 0 |
| 3 | ZN | J | 1004 | 1/1 | 0.99 | 0.05 | -3.79 | 46,46,46,46 | 0 |
| 3 | ZN | G | 1004 | 1/1 | 0.98 | 0.08 | -3.80 | 35,35,35,35 | 0 |
| 3 | ZN | K | 1001 | 1/1 | 1.00 | 0.05 | -3.85 | 23,23,23,23 | 0 |
| 3 | ZN | B | 1001 | 1/1 | 0.99 | 0.06 | -3.99 | 35,35,35,35 | 0 |
| 3 | ZN | L | 1001 | 1/1 | 0.99 | 0.08 | -4.27 | 29,29,29,29 | 0 |
| 3 | ZN | C | 1001 | 1/1 | 0.99 | 0.07 | -4.28 | 26,26,26,26 | 0 |
| 6 | 1PE | C | 18 | 9/16 | 0.92 | 0.13 | -4.31 | 27,36,38,45 | 0 |
| 3 | ZN | G | 1001 | 1/1 | 1.00 | 0.06 | -4.36 | 28,28,28,28 | 0 |
| 3 | ZN | C | 1004 | 1/1 | 0.97 | 0.05 | -4.40 | 42,42,42,42 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 3 | ZN | D | 1004 | 1/1 | 0.99 | 0.06 | -4.48 | 39,39,39,39 | 0 |
| 3 | ZN | H | 1004 | 1/1 | 0.98 | 0.04 | -4.60 | 32,32,32,32 | 0 |
| 3 | ZN | B | 1004 | 1/1 | 0.97 | 0.05 | -4.65 | 36,36,36,36 | 0 |
| 3 | ZN | K | 1004 | 1/1 | 0.96 | 0.04 | -4.65 | 39,39,39,39 | 0 |
| 3 | ZN | A | 1004 | 1/1 | 0.99 | 0.06 | -4.75 | 37,37,37,37 | 0 |
| 3 | ZN | F | 1004 | 1/1 | 0.99 | 0.05 | -4.88 | 37,37,37,37 | 0 |
| 3 | ZN | J | 1001 | 1/1 | 0.98 | 0.06 | -5.15 | 39,39,39,39 | 0 |
| 3 | ZN | A | 1001 | 1/1 | 0.99 | 0.07 | -5.76 | 30,30,30,30 | 0 |
| 3 | ZN | L | 1004 | 1/1 | 0.99 | 0.05 | -6.22 | 39,39,39,39 | 0 |
| 3 | ZN | I | 1004 | 1/1 | 0.99 | 0.06 | -6.69 | 35,35,35,35 | 0 |
| 3 | ZN | I | 1001 | 1/1 | 0.99 | 0.07 | -7.30 | 26,26,26,26 | 0 |
| 3 | ZN | D | 1001 | 1/1 | 0.97 | 0.05 | -7.38 | 41,41,41,41 | 0 |
| 5 | SO4 | K | 19 | 5/5 | 0.97 | 0.33 | - | 71,71,76,77 | 0 |
| 5 | SO4 | G | 23 | 5/5 | 0.97 | 0.20 | - | 45,45,49,50 | 0 |
| 5 | SO4 | E | 22 | 5/5 | 0.89 | 0.36 | - | 90,90,94,97 | 0 |
| 6 | 1PE | I | 21 | 15/16 | 0.91 | 0.20 | - | 25,34,53,54 | 0 |
| 6 | 1PE | C | 17 | 13/16 | 0.90 | 0.20 | - | 15,36,43,43 | 0 |
| 6 | 1PE | B | 62 | 10/16 | 0.44 | 0.47 | - | 74,89,91,92 | 0 |
| 5 | SO4 | A | 1 | 5/5 | 0.94 | 0.18 | - | 61,62,66,66 | 0 |
| 6 | 1PE | L | 56 | 11/16 | 0.82 | 0.19 | - | 30,44,50,50 | 0 |
| 6 | 1PE | E | 612 | 12/16 | 0.88 | 0.26 | - | 31,46,54,55 | 0 |
| 6 | 1PE | H | 65 | 10/16 | 0.90 | 0.20 | - | 42,49,54,55 | 0 |
| 5 | SO4 | L | 25 | 5/5 | 0.93 | 0.15 | - | 68,71,75,76 | 0 |
| 6 | 1PE | B | 61 | 10/16 | 0.86 | 0.21 | - | 34,46,48,51 | 0 |
| 6 | 1PE | J | 45 | 10/16 | 0.66 | 0.35 | - | 50,68,73,75 | 0 |
| 6 | 1PE | G | 30 | 7/16 | 0.94 | 0.16 | - | 24,39,53,57 | 0 |
| 6 | 1PE | F | 32 | 10/16 | 0.92 | 0.14 | - | 33,42,45,46 | 0 |
| 6 | 1PE | J | 3 | 10/16 | 0.89 | 0.30 | - | 33,50,53,54 | 0 |
| 6 | 1PE | K | 4 | 12/16 | 0.82 | 0.21 | - | 27,44,55,55 | 0 |
| 5 | SO4 | D | 5 | 5/5 | 0.94 | 0.30 | - | 92,94,97,97 | 0 |
| 5 | SO4 | F | 21 | 5/5 | 0.95 | 0.17 | - | 69,70,71,75 | 0 |
| 6 | 1PE | D | 63 | 10/16 | 0.88 | 0.19 | - | 37,42,46,53 | 0 |
| 5 | SO4 | J | 20 | 5/5 | 0.93 | 0.41 | - | 72,74,78,81 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.