



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:42 AM GMT

PDB ID : 3FOK
Title : Crystal Structure of Cgl0159 From *Corynebacterium glutamicum* (*Brevibacterium flavum*). Northeast Structural Genomics Target CgR115
Authors : Seetharaman, J.; Neely, H.; Wang, H.; Janjua, H.; Foote, E.L.; Xiao, R.; Everett, J.K.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-12-30
Resolution : 2.50 Å(reported)

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

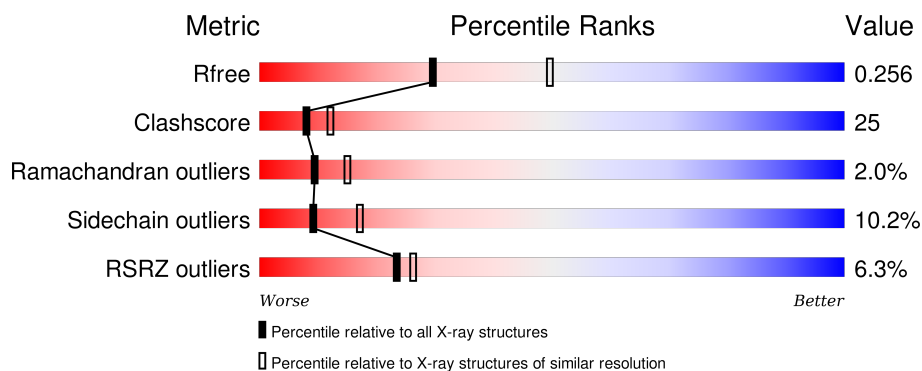
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 | 307 | <div> <div>5%</div> <div>63% 28% 6% .</div> </div> |
| 1 | B | 307 | <div> <div>5%</div> <div>65% 25% 6% .</div> </div> |
| 1 | C | 307 | <div> <div>4%</div> <div>61% 29% 6% .</div> </div> |
| 1 | D | 307 | <div> <div>6%</div> <div>64% 26% 6% .</div> </div> |
| 1 | E | 307 | <div> <div>6%</div> <div>65% 26% 6% .</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | F | 307 | <div><div></div><div>4%</div><div>64%</div><div>27%</div><div>6%</div><div></div></div> |
| 1 | G | 307 | <div><div></div><div>5%</div><div>64%</div><div>26%</div><div>6%</div><div></div></div> |
| 1 | H | 307 | <div><div></div><div>8%</div><div>63%</div><div>28%</div><div>6%</div><div></div></div> |
| 1 | I | 307 | <div><div></div><div>8%</div><div>62%</div><div>28%</div><div>6%</div><div></div></div> |
| 1 | J | 307 | <div><div></div><div>7%</div><div>62%</div><div>28%</div><div>7%</div><div></div></div> |

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 22795 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 uncharacterized protein Cgl0159.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | B | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | C | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | D | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | E | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | F | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | G | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | H | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | I | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |
| 1 | J | 295 | Total | C | N | O | Se | 0 | 0 | 0 |
| | | | 2208 | 1379 | 387 | 429 | 13 | | | |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 2 | A | 72 | Total | O | 0 | 0 |
| | | | 72 | 72 | | |
| 2 | B | 90 | Total | O | 0 | 0 |
| | | | 90 | 90 | | |
| 2 | C | 77 | Total | O | 0 | 0 |
| | | | 77 | 77 | | |
| 2 | D | 95 | Total | O | 0 | 0 |
| | | | 95 | 95 | | |

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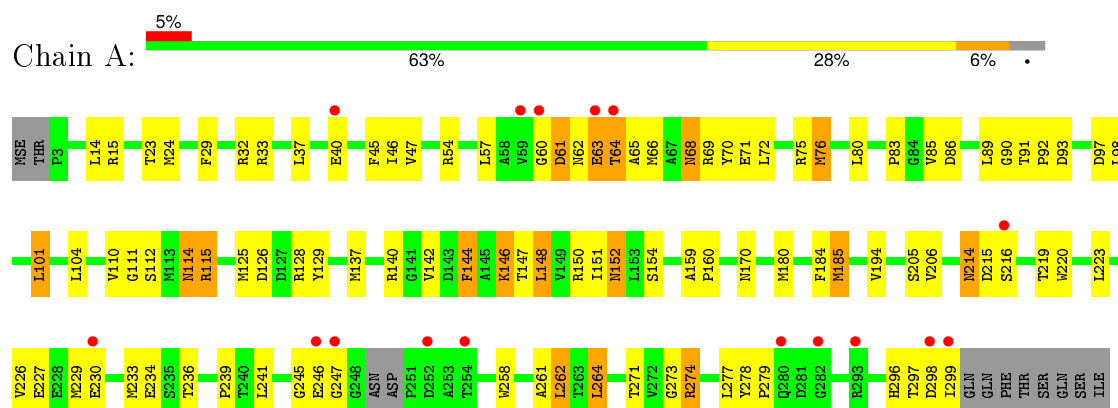
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 2 | E | 79 | Total 79 | O 79 | 0 | 0 |
| 2 | F | 62 | Total 62 | O 62 | 0 | 0 |
| 2 | G | 66 | Total 66 | O 66 | 0 | 0 |
| 2 | H | 74 | Total 74 | O 74 | 0 | 0 |
| 2 | I | 47 | Total 47 | O 47 | 0 | 0 |
| 2 | J | 53 | Total 53 | O 53 | 0 | 0 |

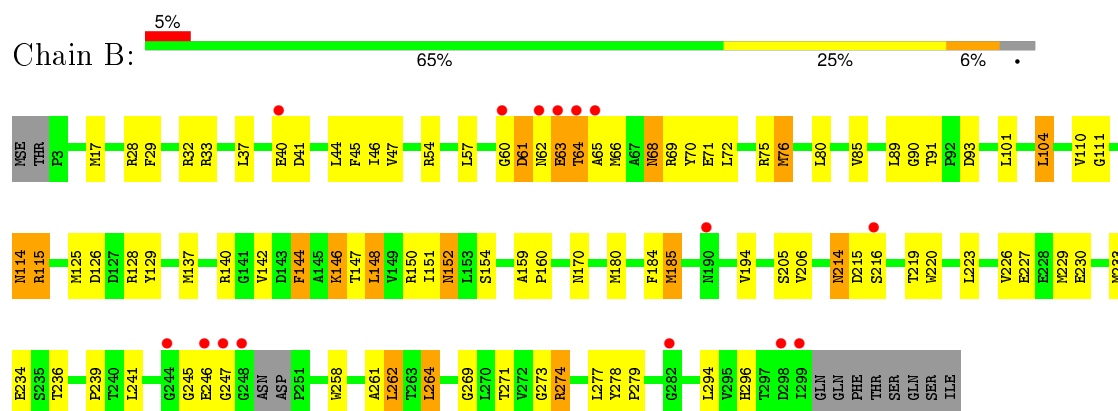
3 Residue-property plots [i](#)

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.

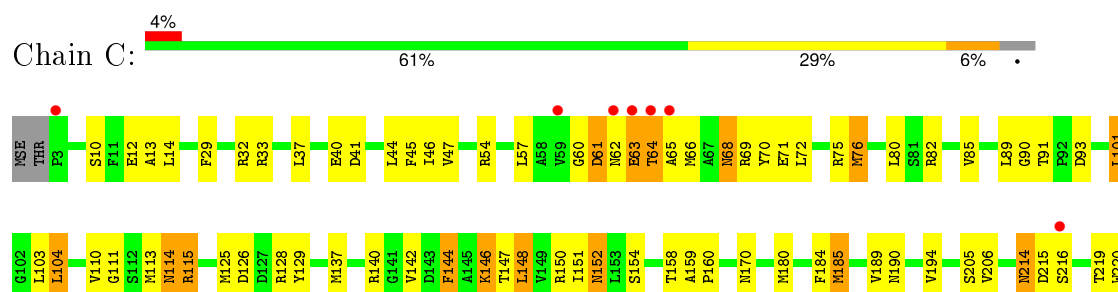
• Molecule 1: uncharacterized protein Cgl0159

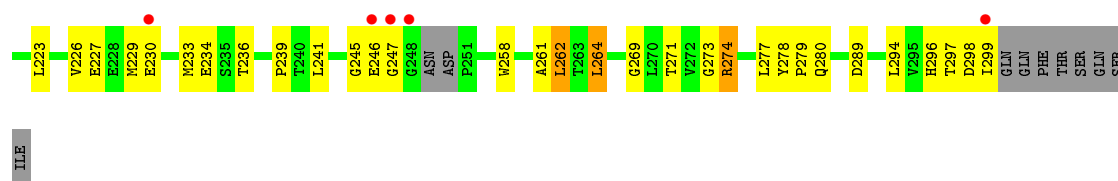


• Molecule 1: uncharacterized protein Cgl0159

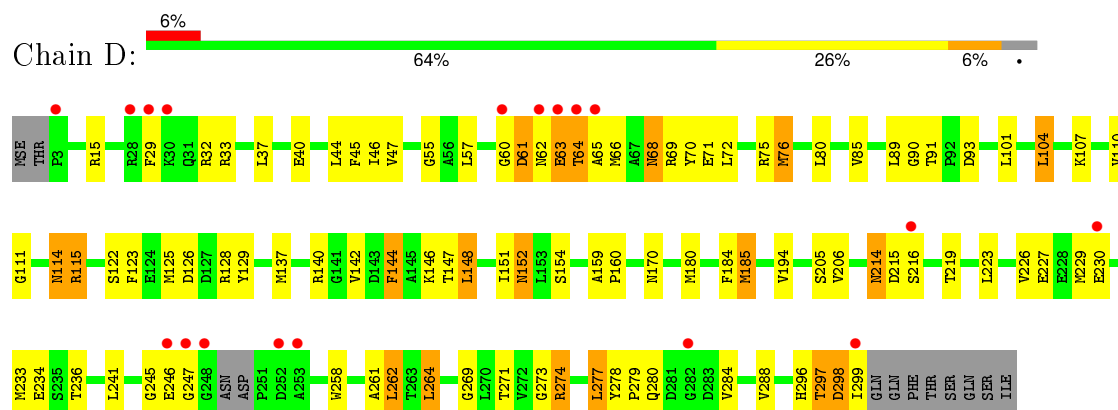


• Molecule 1: uncharacterized protein Cgl0159

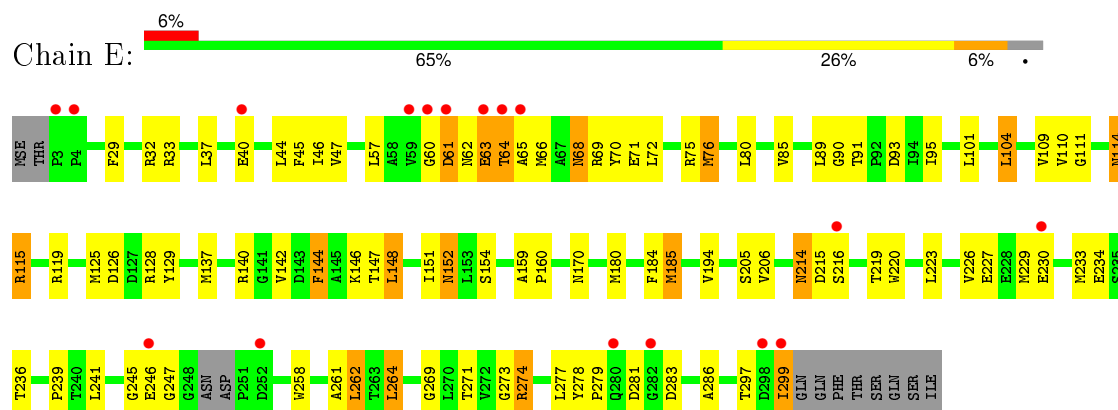




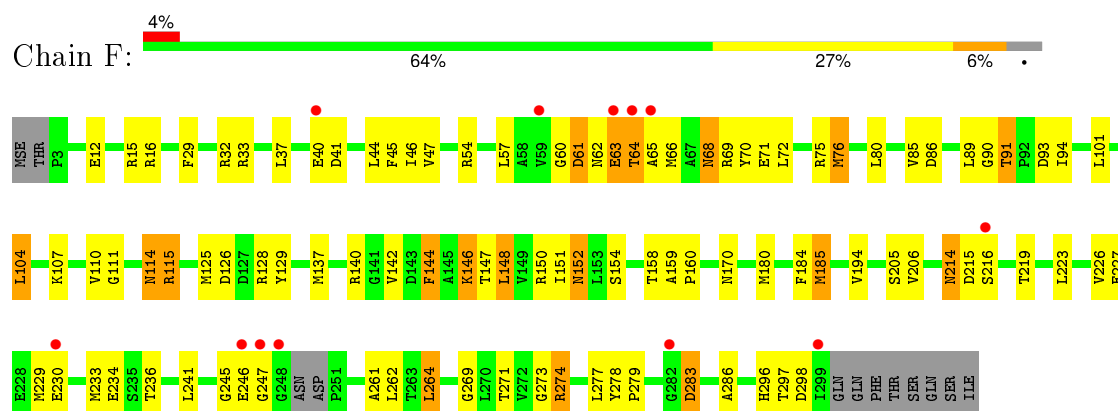
- Molecule 1: uncharacterized protein Cgl0159



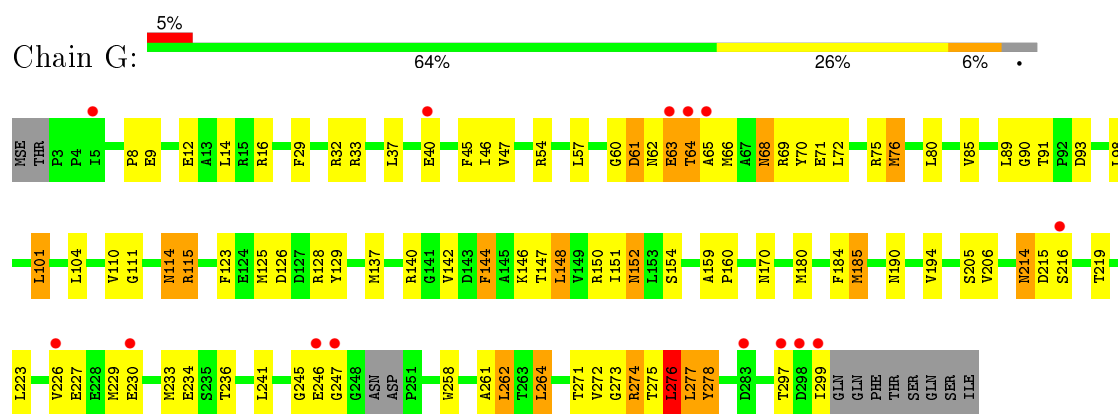
- Molecule 1: uncharacterized protein Cgl0159



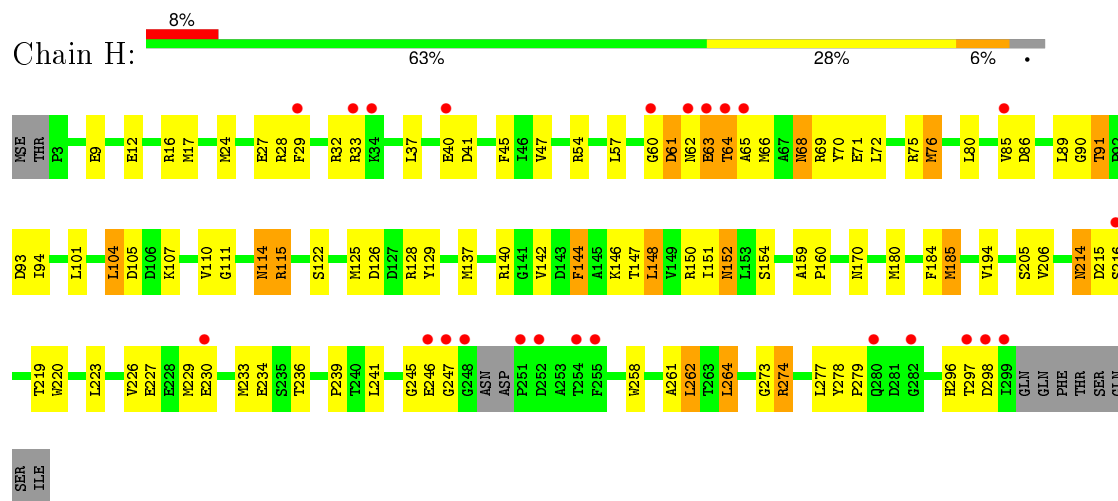
- Molecule 1: uncharacterized protein Cgl0159



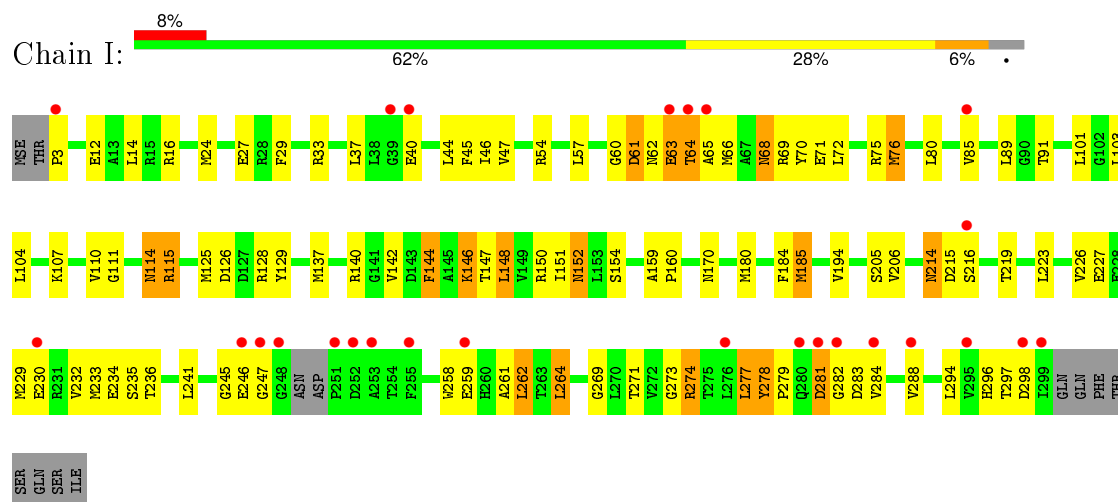
- Molecule 1: uncharacterized protein Cgl0159



• Molecule 1: uncharacterized protein Cgl0159

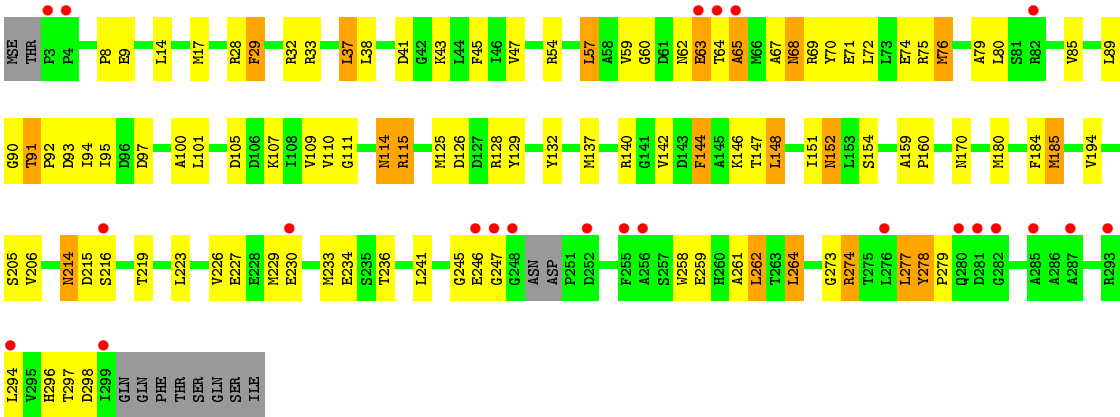


• Molecule 1: uncharacterized protein Cgl0159



• Molecule 1: uncharacterized protein Cgl0159





4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 94.00Å 176.21Å 104.24Å 90.00° 101.94° 90.00° | Depositor |
| Resolution (Å) | 39.00 – 2.50 49.50 – 2.39 | Depositor EDS |
| % Data completeness (in resolution range) | 94.9 (39.00-2.50) 97.4 (49.50-2.39) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.13 (at 2.39Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, R_{free} | 0.225 , 0.254 0.228 , 0.256 | Depositor DCC |
| R_{free} test set | 5276 reflections (4.91%) | DCC |
| Wilson B-factor (Å ²) | 23.7 | Xtriage |
| Anisotropy | 0.457 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.35 , 40.1 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Outliers | 1 of 255933 reflections (0.000%) | Xtriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 22795 | wwPDB-VP |
| Average B, all atoms (Å ²) | 27.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

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 | 0.30 | 0/2230 | 0.68 | 1/3005 (0.0%) |
| 1 | B | 0.30 | 0/2230 | 0.68 | 1/3005 (0.0%) |
| 1 | C | 0.30 | 0/2230 | 0.68 | 1/3005 (0.0%) |
| 1 | D | 0.31 | 0/2230 | 0.67 | 2/3005 (0.1%) |
| 1 | E | 0.30 | 0/2230 | 0.67 | 1/3005 (0.0%) |
| 1 | F | 0.30 | 0/2230 | 0.67 | 1/3005 (0.0%) |
| 1 | G | 0.69 | 11/2230 (0.5%) | 0.71 | 2/3005 (0.1%) |
| 1 | H | 0.30 | 0/2230 | 0.67 | 1/3005 (0.0%) |
| 1 | I | 0.57 | 7/2230 (0.3%) | 0.70 | 3/3005 (0.1%) |
| 1 | J | 0.76 | 10/2230 (0.4%) | 0.69 | 2/3005 (0.1%) |
| All | All | 0.45 | 28/22300 (0.1%) | 0.68 | 15/30050 (0.0%) |

All (28) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | J | 278 | TYR | CD1-CE1 | -17.43 | 1.13 | 1.39 |
| 1 | J | 278 | TYR | CD2-CE2 | -16.39 | 1.14 | 1.39 |
| 1 | G | 278 | TYR | CD1-CE1 | -14.28 | 1.18 | 1.39 |
| 1 | G | 278 | TYR | CD2-CE2 | -12.96 | 1.20 | 1.39 |
| 1 | J | 278 | TYR | CG-CD1 | -11.49 | 1.24 | 1.39 |
| 1 | J | 278 | TYR | CE2-CZ | -9.72 | 1.25 | 1.38 |
| 1 | J | 278 | TYR | CE1-CZ | -9.47 | 1.26 | 1.38 |
| 1 | I | 278 | TYR | CG-CD1 | -9.09 | 1.27 | 1.39 |
| 1 | I | 278 | TYR | CE2-CZ | -9.03 | 1.26 | 1.38 |
| 1 | I | 278 | TYR | CD2-CE2 | -8.61 | 1.26 | 1.39 |
| 1 | G | 278 | TYR | CE2-CZ | -8.20 | 1.27 | 1.38 |
| 1 | I | 278 | TYR | CD1-CE1 | -8.16 | 1.27 | 1.39 |
| 1 | G | 277 | LEU | CG-CD2 | -7.78 | 1.23 | 1.51 |
| 1 | G | 278 | TYR | CB-CG | -7.63 | 1.40 | 1.51 |
| 1 | I | 278 | TYR | CE1-CZ | -6.61 | 1.29 | 1.38 |
| 1 | J | 278 | TYR | CB-CG | -6.43 | 1.42 | 1.51 |
| 1 | J | 277 | LEU | CG-CD1 | -6.37 | 1.28 | 1.51 |
| 1 | J | 278 | TYR | CG-CD2 | -6.22 | 1.31 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | G | 276 | LEU | C-O | -6.07 | 1.11 | 1.23 |
| 1 | I | 278 | TYR | CG-CD2 | -5.99 | 1.31 | 1.39 |
| 1 | G | 277 | LEU | CG-CD1 | -5.97 | 1.29 | 1.51 |
| 1 | G | 278 | TYR | CG-CD1 | -5.82 | 1.31 | 1.39 |
| 1 | G | 278 | TYR | CG-CD2 | -5.56 | 1.31 | 1.39 |
| 1 | G | 276 | LEU | CG-CD2 | -5.43 | 1.31 | 1.51 |
| 1 | J | 277 | LEU | CG-CD2 | -5.20 | 1.32 | 1.51 |
| 1 | J | 278 | TYR | C-O | -5.18 | 1.13 | 1.23 |
| 1 | I | 277 | LEU | N-CA | -5.08 | 1.36 | 1.46 |
| 1 | G | 277 | LEU | N-CA | -5.05 | 1.36 | 1.46 |

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | J | 277 | LEU | CA-CB-CG | 7.91 | 133.49 | 115.30 |
| 1 | I | 277 | LEU | CA-CB-CG | 7.56 | 132.69 | 115.30 |
| 1 | G | 277 | LEU | CB-CG-CD1 | -6.85 | 99.36 | 111.00 |
| 1 | I | 277 | LEU | N-CA-C | -5.93 | 94.99 | 111.00 |
| 1 | D | 277 | LEU | N-CA-C | -5.57 | 95.96 | 111.00 |
| 1 | C | 185 | MSE | N-CA-C | -5.29 | 96.71 | 111.00 |
| 1 | A | 185 | MSE | N-CA-C | -5.29 | 96.73 | 111.00 |
| 1 | G | 185 | MSE | N-CA-C | -5.27 | 96.78 | 111.00 |
| 1 | J | 185 | MSE | N-CA-C | -5.26 | 96.80 | 111.00 |
| 1 | H | 185 | MSE | N-CA-C | -5.25 | 96.82 | 111.00 |
| 1 | I | 185 | MSE | N-CA-C | -5.25 | 96.83 | 111.00 |
| 1 | D | 185 | MSE | N-CA-C | -5.24 | 96.85 | 111.00 |
| 1 | F | 185 | MSE | N-CA-C | -5.23 | 96.89 | 111.00 |
| 1 | E | 185 | MSE | N-CA-C | -5.22 | 96.90 | 111.00 |
| 1 | B | 185 | MSE | N-CA-C | -5.21 | 96.93 | 111.00 |

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 | 2208 | 0 | 2202 | 109 | 0 |
| 1 | B | 2208 | 0 | 2202 | 105 | 0 |
| 1 | C | 2208 | 0 | 2202 | 118 | 0 |
| 1 | D | 2208 | 0 | 2202 | 112 | 0 |
| 1 | E | 2208 | 0 | 2202 | 103 | 0 |
| 1 | F | 2208 | 0 | 2202 | 108 | 0 |
| 1 | G | 2208 | 0 | 2202 | 114 | 0 |
| 1 | H | 2208 | 0 | 2202 | 107 | 0 |
| 1 | I | 2208 | 0 | 2202 | 109 | 0 |
| 1 | J | 2208 | 0 | 2202 | 115 | 0 |
| 2 | A | 72 | 0 | 0 | 4 | 0 |
| 2 | B | 90 | 0 | 0 | 1 | 0 |
| 2 | C | 77 | 0 | 0 | 4 | 0 |
| 2 | D | 95 | 0 | 0 | 3 | 0 |
| 2 | E | 79 | 0 | 0 | 2 | 0 |
| 2 | F | 62 | 0 | 0 | 4 | 0 |
| 2 | G | 66 | 0 | 0 | 6 | 0 |
| 2 | H | 74 | 0 | 0 | 2 | 0 |
| 2 | I | 47 | 0 | 0 | 2 | 0 |
| 2 | J | 53 | 0 | 0 | 1 | 0 |
| All | All | 22795 | 0 | 22020 | 1090 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1090) 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:J:76:MSE:CE | 1:J:277:LEU:HD21 | 1.71 | 1.20 |
| 1:C:137:MSE:HE2 | 1:C:142:VAL:HG21 | 1.20 | 1.16 |
| 1:F:137:MSE:HE2 | 1:F:142:VAL:HG21 | 1.22 | 1.15 |
| 1:A:137:MSE:HE2 | 1:A:142:VAL:HG21 | 1.22 | 1.14 |
| 1:J:137:MSE:HE2 | 1:J:142:VAL:HG21 | 1.23 | 1.12 |
| 1:G:137:MSE:HE2 | 1:G:142:VAL:HG21 | 1.22 | 1.11 |
| 1:I:137:MSE:HE2 | 1:I:142:VAL:HG21 | 1.23 | 1.11 |
| 1:D:137:MSE:HE2 | 1:D:142:VAL:HG21 | 1.23 | 1.11 |
| 1:B:137:MSE:HE2 | 1:B:142:VAL:HG21 | 1.21 | 1.10 |
| 1:H:137:MSE:HE2 | 1:H:142:VAL:HG21 | 1.21 | 1.10 |
| 1:E:137:MSE:HE2 | 1:E:142:VAL:HG21 | 1.22 | 1.09 |
| 1:C:190:ASN:OD1 | 1:H:122:SER:HA | 1.54 | 1.08 |
| 1:J:76:MSE:HE3 | 1:J:277:LEU:HD21 | 1.39 | 0.99 |
| 1:J:76:MSE:HE2 | 1:J:277:LEU:HD21 | 1.47 | 0.94 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:190:ASN:OD1 | 1:H:122:SER:CA | 2.19 | 0.90 |
| 1:C:111:GLY:HA3 | 1:C:137:MSE:HE3 | 1.52 | 0.90 |
| 1:C:189:VAL:HG12 | 1:C:190:ASN:ND2 | 1.86 | 0.90 |
| 1:J:114:ASN:HD22 | 1:J:114:ASN:H | 1.20 | 0.89 |
| 1:E:111:GLY:HA3 | 1:E:137:MSE:HE3 | 1.54 | 0.89 |
| 1:I:76:MSE:HE3 | 1:I:277:LEU:HD21 | 1.56 | 0.88 |
| 1:A:111:GLY:HA3 | 1:A:137:MSE:HE3 | 1.56 | 0.87 |
| 1:G:76:MSE:HA | 1:G:76:MSE:HE2 | 1.57 | 0.86 |
| 1:E:76:MSE:HA | 1:E:76:MSE:HE2 | 1.58 | 0.86 |
| 1:F:76:MSE:HA | 1:F:76:MSE:HE2 | 1.57 | 0.86 |
| 1:A:76:MSE:HA | 1:A:76:MSE:HE2 | 1.58 | 0.86 |
| 1:H:76:MSE:HA | 1:H:76:MSE:HE2 | 1.58 | 0.86 |
| 1:C:137:MSE:HE2 | 1:C:142:VAL:CG2 | 2.06 | 0.85 |
| 1:I:76:MSE:HA | 1:I:76:MSE:HE2 | 1.57 | 0.85 |
| 1:D:122:SER:HA | 1:G:190:ASN:OD1 | 1.76 | 0.85 |
| 1:C:76:MSE:HE2 | 1:C:76:MSE:HA | 1.58 | 0.85 |
| 1:I:12:GLU:HG3 | 1:I:16:ARG:HH12 | 1.40 | 0.84 |
| 1:C:189:VAL:HG12 | 1:C:190:ASN:HD22 | 1.41 | 0.84 |
| 1:A:137:MSE:CE | 1:A:142:VAL:HG21 | 2.07 | 0.84 |
| 1:A:114:ASN:HD22 | 1:A:114:ASN:H | 1.24 | 0.84 |
| 1:H:75:ARG:HH21 | 1:H:278:TYR:HA | 1.43 | 0.83 |
| 1:E:137:MSE:HE2 | 1:E:142:VAL:CG2 | 2.07 | 0.83 |
| 1:D:76:MSE:HA | 1:D:76:MSE:HE2 | 1.58 | 0.83 |
| 1:B:137:MSE:CE | 1:B:142:VAL:HG21 | 2.07 | 0.83 |
| 1:F:137:MSE:HE2 | 1:F:142:VAL:CG2 | 2.08 | 0.83 |
| 1:G:137:MSE:HE2 | 1:G:142:VAL:CG2 | 2.08 | 0.83 |
| 1:J:68:ASN:HD22 | 1:J:68:ASN:C | 1.83 | 0.83 |
| 1:A:223:LEU:HD12 | 1:A:233:MSE:HE1 | 1.61 | 0.83 |
| 1:B:137:MSE:HE2 | 1:B:142:VAL:CG2 | 2.07 | 0.83 |
| 1:H:137:MSE:HE2 | 1:H:142:VAL:CG2 | 2.07 | 0.82 |
| 1:B:76:MSE:HE2 | 1:B:76:MSE:HA | 1.57 | 0.82 |
| 1:B:223:LEU:HD12 | 1:B:233:MSE:HE1 | 1.61 | 0.82 |
| 1:I:137:MSE:HE2 | 1:I:142:VAL:CG2 | 2.09 | 0.82 |
| 1:B:274:ARG:H | 1:B:274:ARG:HE | 1.28 | 0.82 |
| 1:F:223:LEU:HD12 | 1:F:233:MSE:HE1 | 1.62 | 0.82 |
| 1:E:223:LEU:HD12 | 1:E:233:MSE:HE1 | 1.62 | 0.82 |
| 1:A:151:ILE:HD12 | 1:A:185:MSE:HE1 | 1.61 | 0.82 |
| 1:G:111:GLY:HA3 | 1:G:137:MSE:HE3 | 1.62 | 0.82 |
| 1:F:274:ARG:H | 1:F:274:ARG:HE | 1.27 | 0.82 |
| 1:I:137:MSE:CE | 1:I:142:VAL:HG21 | 2.08 | 0.81 |
| 1:I:274:ARG:HE | 1:I:274:ARG:H | 1.28 | 0.81 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:137:MSE:HE2 | 1:A:142:VAL:CG2 | 2.08 | 0.81 |
| 1:H:137:MSE:CE | 1:H:142:VAL:HG21 | 2.07 | 0.81 |
| 1:B:114:ASN:HD22 | 1:B:114:ASN:H | 1.28 | 0.81 |
| 1:C:151:ILE:HD12 | 1:C:185:MSE:HE1 | 1.62 | 0.81 |
| 1:D:223:LEU:HD12 | 1:D:233:MSE:HE1 | 1.62 | 0.81 |
| 1:E:151:ILE:HD12 | 1:E:185:MSE:HE1 | 1.61 | 0.81 |
| 1:J:63:GLU:HG3 | 1:J:64:THR:H | 1.44 | 0.81 |
| 1:B:151:ILE:HD12 | 1:B:185:MSE:HE1 | 1.61 | 0.81 |
| 1:F:151:ILE:HD12 | 1:F:185:MSE:HE1 | 1.62 | 0.81 |
| 1:C:137:MSE:CE | 1:C:142:VAL:HG21 | 2.06 | 0.81 |
| 1:H:274:ARG:H | 1:H:274:ARG:HE | 1.27 | 0.81 |
| 1:D:151:ILE:HD12 | 1:D:185:MSE:HE1 | 1.61 | 0.81 |
| 1:G:223:LEU:HD12 | 1:G:233:MSE:HE1 | 1.62 | 0.81 |
| 1:G:114:ASN:HD22 | 1:G:114:ASN:H | 1.29 | 0.81 |
| 1:J:137:MSE:HB3 | 1:J:142:VAL:HG22 | 1.63 | 0.81 |
| 1:D:274:ARG:H | 1:D:274:ARG:HE | 1.27 | 0.81 |
| 1:D:137:MSE:CE | 1:D:142:VAL:HG21 | 2.09 | 0.80 |
| 1:F:137:MSE:HB3 | 1:F:142:VAL:HG22 | 1.63 | 0.80 |
| 1:C:223:LEU:HD12 | 1:C:233:MSE:HE1 | 1.62 | 0.80 |
| 1:F:114:ASN:HD21 | 1:F:148:LEU:H | 1.25 | 0.80 |
| 1:J:274:ARG:H | 1:J:274:ARG:HE | 1.29 | 0.80 |
| 1:D:137:MSE:HE2 | 1:D:142:VAL:CG2 | 2.09 | 0.80 |
| 1:I:114:ASN:H | 1:I:114:ASN:HD22 | 1.29 | 0.80 |
| 1:H:223:LEU:HD12 | 1:H:233:MSE:HE1 | 1.62 | 0.80 |
| 1:B:137:MSE:HB3 | 1:B:142:VAL:HG22 | 1.63 | 0.80 |
| 1:A:274:ARG:HE | 1:A:274:ARG:H | 1.27 | 0.80 |
| 1:H:151:ILE:HD12 | 1:H:185:MSE:HE1 | 1.61 | 0.80 |
| 1:J:137:MSE:HE2 | 1:J:142:VAL:CG2 | 2.09 | 0.80 |
| 1:J:151:ILE:HD12 | 1:J:185:MSE:HE1 | 1.62 | 0.80 |
| 1:G:137:MSE:HB3 | 1:G:142:VAL:HG22 | 1.63 | 0.80 |
| 1:D:137:MSE:HB3 | 1:D:142:VAL:HG22 | 1.64 | 0.80 |
| 1:C:125:MSE:HE2 | 1:C:152:ASN:HB2 | 1.64 | 0.80 |
| 1:I:125:MSE:HE2 | 1:I:152:ASN:HB2 | 1.63 | 0.80 |
| 1:F:137:MSE:CE | 1:F:142:VAL:HG21 | 2.08 | 0.79 |
| 1:I:151:ILE:HD12 | 1:I:185:MSE:HE1 | 1.62 | 0.79 |
| 1:C:137:MSE:HB3 | 1:C:142:VAL:HG22 | 1.65 | 0.79 |
| 1:C:114:ASN:HD22 | 1:C:114:ASN:H | 1.29 | 0.79 |
| 1:G:151:ILE:HD12 | 1:G:185:MSE:HE1 | 1.62 | 0.79 |
| 1:J:223:LEU:HD12 | 1:J:233:MSE:HE1 | 1.62 | 0.79 |
| 1:E:137:MSE:HB3 | 1:E:142:VAL:HG22 | 1.63 | 0.79 |
| 1:I:137:MSE:HB3 | 1:I:142:VAL:HG22 | 1.64 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:137:MSE:HB3 | 1:H:142:VAL:HG22 | 1.63 | 0.79 |
| 1:C:274:ARG:HE | 1:C:274:ARG:H | 1.27 | 0.79 |
| 1:A:125:MSE:HE2 | 1:A:152:ASN:HB2 | 1.63 | 0.79 |
| 1:G:125:MSE:HE2 | 1:G:152:ASN:HB2 | 1.64 | 0.79 |
| 1:G:137:MSE:CE | 1:G:142:VAL:HG21 | 2.08 | 0.79 |
| 1:I:223:LEU:HD12 | 1:I:233:MSE:HE1 | 1.63 | 0.79 |
| 1:C:14:LEU:HD13 | 1:C:101:LEU:HD13 | 1.63 | 0.79 |
| 1:J:137:MSE:CE | 1:J:142:VAL:HG21 | 2.09 | 0.79 |
| 1:B:111:GLY:HA3 | 1:B:137:MSE:HE3 | 1.64 | 0.79 |
| 1:D:125:MSE:HE2 | 1:D:152:ASN:HB2 | 1.65 | 0.79 |
| 1:J:125:MSE:HE2 | 1:J:152:ASN:HB2 | 1.64 | 0.78 |
| 1:F:125:MSE:HE2 | 1:F:152:ASN:HB2 | 1.64 | 0.78 |
| 1:H:111:GLY:HA3 | 1:H:137:MSE:HE3 | 1.64 | 0.78 |
| 1:H:125:MSE:HE2 | 1:H:152:ASN:HB2 | 1.63 | 0.78 |
| 1:J:71:GLU:O | 1:J:75:ARG:HG3 | 1.83 | 0.78 |
| 1:A:137:MSE:HB3 | 1:A:142:VAL:HG22 | 1.63 | 0.78 |
| 1:G:274:ARG:H | 1:G:274:ARG:HE | 1.28 | 0.78 |
| 1:E:274:ARG:H | 1:E:274:ARG:HE | 1.28 | 0.77 |
| 1:E:137:MSE:CE | 1:E:142:VAL:HG21 | 2.08 | 0.77 |
| 2:I:312:HOH:O | 1:J:93:ASP:HA | 1.84 | 0.77 |
| 1:I:76:MSE:CE | 1:I:277:LEU:HD21 | 2.14 | 0.77 |
| 1:A:185:MSE:HE3 | 1:A:205:SER:CB | 2.14 | 0.77 |
| 1:D:114:ASN:H | 1:D:114:ASN:HD22 | 1.32 | 0.77 |
| 1:F:111:GLY:HA3 | 1:F:137:MSE:HE3 | 1.66 | 0.76 |
| 1:E:111:GLY:HA3 | 1:E:137:MSE:CE | 2.15 | 0.76 |
| 1:E:185:MSE:HE3 | 1:E:205:SER:CB | 2.15 | 0.76 |
| 1:G:114:ASN:HD21 | 1:G:148:LEU:H | 1.32 | 0.76 |
| 1:H:185:MSE:HE3 | 1:H:205:SER:CB | 2.15 | 0.76 |
| 1:D:110:VAL:HG22 | 1:D:144:PHE:HB3 | 1.67 | 0.76 |
| 1:B:125:MSE:HE2 | 1:B:152:ASN:HB2 | 1.65 | 0.76 |
| 1:D:114:ASN:HD21 | 1:D:148:LEU:H | 1.32 | 0.76 |
| 1:E:125:MSE:HE2 | 1:E:152:ASN:HB2 | 1.65 | 0.76 |
| 1:D:32:ARG:HD2 | 1:D:104:LEU:HB3 | 1.67 | 0.76 |
| 1:E:63:GLU:HG3 | 1:E:64:THR:H | 1.51 | 0.76 |
| 1:D:122:SER:CB | 1:G:190:ASN:OD1 | 2.33 | 0.76 |
| 1:J:185:MSE:HE3 | 1:J:205:SER:CB | 2.15 | 0.76 |
| 1:C:185:MSE:HE3 | 1:C:205:SER:CB | 2.15 | 0.76 |
| 1:B:63:GLU:HG3 | 1:B:64:THR:H | 1.51 | 0.75 |
| 1:B:114:ASN:HD21 | 1:B:148:LEU:H | 1.31 | 0.75 |
| 1:G:185:MSE:HE3 | 1:G:205:SER:CB | 2.15 | 0.75 |
| 1:F:63:GLU:HG3 | 1:F:64:THR:H | 1.51 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:185:MSE:HE3 | 1:B:205:SER:CB | 2.16 | 0.75 |
| 1:D:185:MSE:HE3 | 1:D:205:SER:CB | 2.15 | 0.75 |
| 1:I:185:MSE:HE3 | 1:I:205:SER:CB | 2.16 | 0.75 |
| 1:B:76:MSE:HE3 | 1:B:277:LEU:HD11 | 1.67 | 0.75 |
| 1:F:185:MSE:HE3 | 1:F:205:SER:CB | 2.15 | 0.75 |
| 1:A:111:GLY:HA3 | 1:A:137:MSE:CE | 2.17 | 0.75 |
| 1:D:63:GLU:HG3 | 1:D:64:THR:H | 1.51 | 0.75 |
| 1:D:76:MSE:CE | 1:D:277:LEU:HD21 | 2.17 | 0.74 |
| 1:J:14:LEU:HD22 | 1:J:101:LEU:HD11 | 1.70 | 0.74 |
| 1:A:63:GLU:HG3 | 1:A:64:THR:H | 1.51 | 0.74 |
| 1:C:63:GLU:HG3 | 1:C:64:THR:H | 1.52 | 0.74 |
| 1:C:111:GLY:HA3 | 1:C:137:MSE:CE | 2.16 | 0.74 |
| 1:G:63:GLU:HG3 | 1:G:64:THR:H | 1.52 | 0.73 |
| 1:F:41:ASP:OD2 | 1:F:296:HIS:HD2 | 1.71 | 0.73 |
| 1:G:272:VAL:HG13 | 2:G:549:HOH:O | 1.87 | 0.73 |
| 1:H:63:GLU:HG3 | 1:H:64:THR:H | 1.51 | 0.73 |
| 1:A:93:ASP:HA | 2:A:308:HOH:O | 1.87 | 0.73 |
| 1:I:63:GLU:HG3 | 1:I:64:THR:H | 1.52 | 0.73 |
| 1:C:114:ASN:HD21 | 1:C:148:LEU:H | 1.34 | 0.73 |
| 1:A:226:VAL:HG12 | 1:A:227:GLU:N | 2.04 | 0.72 |
| 1:B:226:VAL:HG12 | 1:B:227:GLU:N | 2.05 | 0.72 |
| 1:F:226:VAL:HG12 | 1:F:227:GLU:N | 2.04 | 0.72 |
| 1:H:33:ARG:HH11 | 1:H:33:ARG:HG3 | 1.54 | 0.72 |
| 1:I:226:VAL:HG12 | 1:I:227:GLU:N | 2.05 | 0.72 |
| 1:D:226:VAL:HG12 | 1:D:227:GLU:N | 2.04 | 0.72 |
| 1:I:33:ARG:HH11 | 1:I:33:ARG:HG3 | 1.55 | 0.72 |
| 1:H:226:VAL:HG12 | 1:H:227:GLU:N | 2.04 | 0.72 |
| 1:I:259:GLU:HB2 | 1:I:294:LEU:HD11 | 1.71 | 0.72 |
| 1:I:14:LEU:HD22 | 1:I:101:LEU:HD11 | 1.70 | 0.71 |
| 1:J:226:VAL:HG12 | 1:J:227:GLU:N | 2.04 | 0.71 |
| 1:H:114:ASN:HD21 | 1:H:148:LEU:H | 1.35 | 0.71 |
| 1:G:226:VAL:HG12 | 1:G:227:GLU:N | 2.05 | 0.71 |
| 1:D:75:ARG:HH21 | 1:D:278:TYR:HA | 1.55 | 0.71 |
| 1:C:226:VAL:HG12 | 1:C:227:GLU:N | 2.04 | 0.71 |
| 1:J:111:GLY:HA3 | 1:J:137:MSE:HE3 | 1.73 | 0.71 |
| 1:I:71:GLU:O | 1:I:75:ARG:HG3 | 1.91 | 0.71 |
| 1:H:68:ASN:HD22 | 1:H:68:ASN:C | 1.95 | 0.71 |
| 1:F:33:ARG:HG3 | 1:F:33:ARG:HH11 | 1.56 | 0.71 |
| 1:C:68:ASN:HD22 | 1:C:68:ASN:C | 1.94 | 0.70 |
| 1:E:33:ARG:HH11 | 1:E:33:ARG:HG3 | 1.56 | 0.70 |
| 1:E:226:VAL:HG12 | 1:E:227:GLU:N | 2.04 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:111:GLY:HA3 | 1:D:137:MSE:HE3 | 1.71 | 0.70 |
| 2:G:308:HOH:O | 1:H:93:ASP:HA | 1.91 | 0.70 |
| 1:J:45:PHE:CE2 | 1:J:85:VAL:HG12 | 2.26 | 0.70 |
| 1:A:68:ASN:HD22 | 1:A:68:ASN:C | 1.95 | 0.70 |
| 1:C:33:ARG:HG3 | 1:C:33:ARG:HH11 | 1.56 | 0.70 |
| 1:D:122:SER:CA | 1:G:190:ASN:OD1 | 2.39 | 0.70 |
| 1:F:68:ASN:HD22 | 1:F:68:ASN:C | 1.94 | 0.70 |
| 1:I:68:ASN:HD22 | 1:I:68:ASN:C | 1.94 | 0.70 |
| 1:A:33:ARG:HH11 | 1:A:33:ARG:HG3 | 1.55 | 0.70 |
| 1:G:71:GLU:O | 1:G:75:ARG:HG3 | 1.92 | 0.70 |
| 1:A:71:GLU:O | 1:A:75:ARG:HG3 | 1.91 | 0.70 |
| 1:E:68:ASN:C | 1:E:68:ASN:HD22 | 1.95 | 0.70 |
| 1:F:230:GLU:O | 1:F:234:GLU:HG3 | 1.92 | 0.70 |
| 1:G:33:ARG:HG3 | 1:G:33:ARG:HH11 | 1.57 | 0.70 |
| 1:D:71:GLU:O | 1:D:75:ARG:HG3 | 1.91 | 0.70 |
| 1:C:230:GLU:O | 1:C:234:GLU:HG3 | 1.92 | 0.70 |
| 1:A:114:ASN:HD21 | 1:A:148:LEU:H | 1.39 | 0.70 |
| 1:I:230:GLU:O | 1:I:234:GLU:HG3 | 1.92 | 0.70 |
| 1:J:230:GLU:O | 1:J:234:GLU:HG3 | 1.92 | 0.70 |
| 1:B:33:ARG:HG3 | 1:B:33:ARG:HH11 | 1.56 | 0.70 |
| 1:H:71:GLU:O | 1:H:75:ARG:HG3 | 1.92 | 0.69 |
| 2:A:317:HOH:O | 1:B:93:ASP:HA | 1.91 | 0.69 |
| 1:H:230:GLU:O | 1:H:234:GLU:HG3 | 1.92 | 0.69 |
| 1:B:68:ASN:C | 1:B:68:ASN:HD22 | 1.96 | 0.69 |
| 1:B:230:GLU:O | 1:B:234:GLU:HG3 | 1.91 | 0.69 |
| 1:A:230:GLU:O | 1:A:234:GLU:HG3 | 1.92 | 0.69 |
| 1:E:230:GLU:O | 1:E:234:GLU:HG3 | 1.92 | 0.69 |
| 1:G:230:GLU:O | 1:G:234:GLU:HG3 | 1.92 | 0.69 |
| 1:D:68:ASN:C | 1:D:68:ASN:HD22 | 1.95 | 0.69 |
| 1:J:114:ASN:HD22 | 1:J:114:ASN:N | 1.91 | 0.69 |
| 1:D:33:ARG:HH11 | 1:D:33:ARG:HG3 | 1.56 | 0.69 |
| 1:G:68:ASN:C | 1:G:68:ASN:HD22 | 1.95 | 0.69 |
| 1:D:230:GLU:O | 1:D:234:GLU:HG3 | 1.92 | 0.69 |
| 1:F:114:ASN:HD22 | 1:F:114:ASN:H | 1.40 | 0.69 |
| 1:A:76:MSE:HE3 | 1:A:277:LEU:HD21 | 1.75 | 0.69 |
| 1:E:71:GLU:O | 1:E:75:ARG:HG3 | 1.93 | 0.69 |
| 1:D:76:MSE:HE3 | 1:D:277:LEU:HD21 | 1.75 | 0.68 |
| 1:F:71:GLU:O | 1:F:75:ARG:HG3 | 1.92 | 0.68 |
| 1:C:80:LEU:HA | 1:C:85:VAL:HG21 | 1.76 | 0.68 |
| 1:C:71:GLU:O | 1:C:75:ARG:HG3 | 1.93 | 0.68 |
| 1:F:93:ASP:HA | 2:F:309:HOH:O | 1.92 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:80:LEU:HA | 1:B:85:VAL:HG21 | 1.76 | 0.68 |
| 1:B:71:GLU:O | 1:B:75:ARG:HG3 | 1.93 | 0.68 |
| 1:D:80:LEU:HA | 1:D:85:VAL:HG21 | 1.76 | 0.68 |
| 1:J:76:MSE:HE3 | 1:J:277:LEU:HD11 | 1.76 | 0.68 |
| 1:I:111:GLY:HA3 | 1:I:137:MSE:HE3 | 1.75 | 0.68 |
| 1:I:80:LEU:HA | 1:I:85:VAL:HG21 | 1.76 | 0.68 |
| 1:C:111:GLY:H | 1:C:137:MSE:HE1 | 1.60 | 0.67 |
| 1:A:137:MSE:HB3 | 1:A:142:VAL:CG2 | 2.25 | 0.67 |
| 1:J:151:ILE:HB | 1:J:185:MSE:CE | 2.25 | 0.67 |
| 1:E:151:ILE:HB | 1:E:185:MSE:CE | 2.25 | 0.66 |
| 1:F:226:VAL:CG1 | 1:F:227:GLU:N | 2.59 | 0.66 |
| 1:H:137:MSE:HB3 | 1:H:142:VAL:CG2 | 2.26 | 0.66 |
| 1:J:114:ASN:HD21 | 1:J:148:LEU:H | 1.43 | 0.66 |
| 1:E:226:VAL:CG1 | 1:E:227:GLU:N | 2.59 | 0.66 |
| 1:C:190:ASN:OD1 | 1:H:122:SER:CB | 2.42 | 0.66 |
| 1:A:151:ILE:HB | 1:A:185:MSE:CE | 2.25 | 0.66 |
| 1:H:226:VAL:CG1 | 1:H:227:GLU:N | 2.58 | 0.66 |
| 1:G:274:ARG:NH2 | 2:G:549:HOH:O | 2.27 | 0.66 |
| 1:E:114:ASN:HD22 | 1:E:114:ASN:H | 1.42 | 0.66 |
| 1:F:137:MSE:HB3 | 1:F:142:VAL:CG2 | 2.25 | 0.66 |
| 1:G:137:MSE:HB3 | 1:G:142:VAL:CG2 | 2.26 | 0.66 |
| 1:B:137:MSE:HB3 | 1:B:142:VAL:CG2 | 2.26 | 0.66 |
| 1:D:122:SER:HB2 | 1:G:190:ASN:OD1 | 1.95 | 0.66 |
| 1:A:80:LEU:HA | 1:A:85:VAL:HG21 | 1.76 | 0.66 |
| 1:H:151:ILE:HB | 1:H:185:MSE:CE | 2.26 | 0.66 |
| 1:H:32:ARG:HD2 | 1:H:104:LEU:HB3 | 1.77 | 0.66 |
| 1:G:80:LEU:HA | 1:G:85:VAL:HG21 | 1.76 | 0.66 |
| 1:F:80:LEU:HA | 1:F:85:VAL:HG21 | 1.77 | 0.66 |
| 1:G:151:ILE:HB | 1:G:185:MSE:CE | 2.25 | 0.66 |
| 1:I:226:VAL:CG1 | 1:I:227:GLU:N | 2.59 | 0.66 |
| 1:D:226:VAL:CG1 | 1:D:227:GLU:N | 2.59 | 0.66 |
| 1:J:68:ASN:HD21 | 1:J:70:TYR:HB2 | 1.61 | 0.66 |
| 1:J:226:VAL:CG1 | 1:J:227:GLU:N | 2.58 | 0.66 |
| 1:D:111:GLY:H | 1:D:137:MSE:HE1 | 1.60 | 0.66 |
| 1:C:226:VAL:CG1 | 1:C:227:GLU:N | 2.59 | 0.66 |
| 1:B:226:VAL:CG1 | 1:B:227:GLU:N | 2.59 | 0.66 |
| 1:E:80:LEU:HA | 1:E:85:VAL:HG21 | 1.76 | 0.66 |
| 1:C:151:ILE:HB | 1:C:185:MSE:CE | 2.26 | 0.65 |
| 1:F:151:ILE:HB | 1:F:185:MSE:CE | 2.26 | 0.65 |
| 1:D:110:VAL:HG22 | 1:D:144:PHE:CB | 2.26 | 0.65 |
| 1:E:226:VAL:O | 1:E:229:MSE:HG2 | 1.97 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:H:75:ARG:NH2 | 1:H:278:TYR:HA | 2.11 | 0.65 |
| 1:A:226:VAL:CG1 | 1:A:227:GLU:N | 2.59 | 0.65 |
| 1:G:226:VAL:CG1 | 1:G:227:GLU:N | 2.59 | 0.65 |
| 1:E:137:MSE:HB3 | 1:E:142:VAL:CG2 | 2.25 | 0.65 |
| 1:F:32:ARG:HD2 | 1:F:104:LEU:HB3 | 1.76 | 0.65 |
| 1:J:137:MSE:HB3 | 1:J:142:VAL:CG2 | 2.26 | 0.65 |
| 1:G:111:GLY:H | 1:G:137:MSE:HE1 | 1.61 | 0.65 |
| 1:B:151:ILE:HB | 1:B:185:MSE:CE | 2.26 | 0.65 |
| 1:I:151:ILE:HB | 1:I:185:MSE:CE | 2.26 | 0.65 |
| 1:H:80:LEU:HA | 1:H:85:VAL:HG21 | 1.76 | 0.65 |
| 1:B:111:GLY:H | 1:B:137:MSE:HE1 | 1.62 | 0.65 |
| 1:B:151:ILE:CD1 | 1:B:185:MSE:HE1 | 2.27 | 0.65 |
| 1:D:151:ILE:HB | 1:D:185:MSE:CE | 2.26 | 0.65 |
| 1:I:125:MSE:HE2 | 1:I:152:ASN:CB | 2.27 | 0.65 |
| 1:F:226:VAL:O | 1:F:229:MSE:HG2 | 1.97 | 0.65 |
| 1:I:226:VAL:O | 1:I:229:MSE:HG2 | 1.97 | 0.65 |
| 2:F:310:HOH:O | 1:G:93:ASP:HA | 1.96 | 0.65 |
| 1:H:151:ILE:CD1 | 1:H:185:MSE:HE1 | 2.27 | 0.65 |
| 1:A:76:MSE:CE | 1:A:277:LEU:HD21 | 2.27 | 0.65 |
| 1:H:76:MSE:CE | 1:H:277:LEU:HD21 | 2.27 | 0.64 |
| 1:E:151:ILE:CD1 | 1:E:185:MSE:HE1 | 2.27 | 0.64 |
| 1:D:151:ILE:CD1 | 1:D:185:MSE:HE1 | 2.28 | 0.64 |
| 1:A:151:ILE:CD1 | 1:A:185:MSE:HE1 | 2.28 | 0.64 |
| 1:F:151:ILE:CD1 | 1:F:185:MSE:HE1 | 2.28 | 0.64 |
| 1:I:151:ILE:CD1 | 1:I:185:MSE:HE1 | 2.28 | 0.64 |
| 1:G:151:ILE:CD1 | 1:G:185:MSE:HE1 | 2.27 | 0.64 |
| 1:J:125:MSE:HE2 | 1:J:152:ASN:CB | 2.27 | 0.64 |
| 1:D:226:VAL:O | 1:D:229:MSE:HG2 | 1.96 | 0.64 |
| 1:D:137:MSE:HB3 | 1:D:142:VAL:CG2 | 2.26 | 0.64 |
| 1:J:226:VAL:O | 1:J:229:MSE:HG2 | 1.98 | 0.64 |
| 1:F:125:MSE:HE2 | 1:F:152:ASN:CB | 2.27 | 0.64 |
| 1:B:226:VAL:O | 1:B:229:MSE:HG2 | 1.97 | 0.64 |
| 1:C:76:MSE:HE3 | 1:C:277:LEU:HD11 | 1.80 | 0.64 |
| 1:G:125:MSE:HE2 | 1:G:152:ASN:CB | 2.27 | 0.64 |
| 1:A:114:ASN:N | 1:A:114:ASN:HD22 | 1.94 | 0.64 |
| 1:C:151:ILE:CD1 | 1:C:185:MSE:HE1 | 2.28 | 0.64 |
| 1:D:125:MSE:HE2 | 1:D:152:ASN:CB | 2.28 | 0.64 |
| 1:E:93:ASP:HA | 2:J:308:HOH:O | 1.97 | 0.64 |
| 1:C:137:MSE:HB3 | 1:C:142:VAL:CG2 | 2.26 | 0.64 |
| 1:I:137:MSE:HB3 | 1:I:142:VAL:CG2 | 2.26 | 0.64 |
| 1:D:278:TYR:N | 1:D:279:PRO:HD3 | 2.12 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:226:VAL:O | 1:C:229:MSE:HG2 | 1.98 | 0.64 |
| 1:A:125:MSE:HE2 | 1:A:152:ASN:CB | 2.28 | 0.63 |
| 1:H:226:VAL:O | 1:H:229:MSE:HG2 | 1.98 | 0.63 |
| 1:J:151:ILE:CD1 | 1:J:185:MSE:HE1 | 2.28 | 0.63 |
| 1:B:125:MSE:HE2 | 1:B:152:ASN:CB | 2.28 | 0.63 |
| 1:H:125:MSE:HE2 | 1:H:152:ASN:CB | 2.27 | 0.63 |
| 1:A:226:VAL:O | 1:A:229:MSE:HG2 | 1.98 | 0.63 |
| 1:G:111:GLY:HA3 | 1:G:137:MSE:CE | 2.28 | 0.63 |
| 1:I:278:TYR:N | 1:I:279:PRO:HD3 | 2.13 | 0.63 |
| 1:C:125:MSE:HE2 | 1:C:152:ASN:CB | 2.28 | 0.63 |
| 1:E:125:MSE:HE2 | 1:E:152:ASN:CB | 2.28 | 0.63 |
| 1:F:111:GLY:H | 1:F:137:MSE:HE1 | 1.64 | 0.62 |
| 1:A:185:MSE:HE3 | 1:A:205:SER:HB3 | 1.81 | 0.62 |
| 1:G:226:VAL:O | 1:G:229:MSE:HG2 | 1.98 | 0.62 |
| 1:H:111:GLY:H | 1:H:137:MSE:HE1 | 1.65 | 0.62 |
| 1:D:93:ASP:HA | 2:D:310:HOH:O | 1.97 | 0.62 |
| 1:H:111:GLY:HA3 | 1:H:137:MSE:CE | 2.28 | 0.62 |
| 1:G:54:ARG:HH21 | 1:G:150:ARG:HH12 | 1.46 | 0.62 |
| 1:B:151:ILE:HD12 | 1:B:185:MSE:CE | 2.30 | 0.62 |
| 1:D:277:LEU:O | 1:D:278:TYR:HB2 | 1.98 | 0.62 |
| 1:H:114:ASN:HD22 | 1:H:114:ASN:H | 1.46 | 0.62 |
| 1:G:151:ILE:HD12 | 1:G:185:MSE:CE | 2.30 | 0.62 |
| 1:E:278:TYR:N | 1:E:279:PRO:HD3 | 2.14 | 0.62 |
| 1:C:93:ASP:HA | 2:E:308:HOH:O | 1.99 | 0.62 |
| 1:C:185:MSE:HE3 | 1:C:205:SER:HB3 | 1.81 | 0.61 |
| 1:D:151:ILE:HD12 | 1:D:185:MSE:CE | 2.29 | 0.61 |
| 1:J:97:ASP:O | 1:J:101:LEU:HD13 | 2.00 | 0.61 |
| 1:F:185:MSE:HE3 | 1:F:205:SER:HB3 | 1.82 | 0.61 |
| 1:B:185:MSE:HE3 | 1:B:205:SER:HB3 | 1.82 | 0.61 |
| 1:J:63:GLU:HG3 | 1:J:64:THR:N | 2.13 | 0.61 |
| 1:F:151:ILE:HD12 | 1:F:185:MSE:CE | 2.30 | 0.61 |
| 1:G:185:MSE:HE3 | 1:G:205:SER:HB3 | 1.82 | 0.61 |
| 1:B:111:GLY:HA3 | 1:B:137:MSE:CE | 2.29 | 0.61 |
| 1:E:114:ASN:HD21 | 1:E:148:LEU:H | 1.47 | 0.61 |
| 1:H:110:VAL:HG13 | 1:H:144:PHE:HB3 | 1.82 | 0.61 |
| 1:I:111:GLY:H | 1:I:137:MSE:HE1 | 1.65 | 0.61 |
| 1:H:185:MSE:HE3 | 1:H:205:SER:HB3 | 1.81 | 0.61 |
| 1:E:151:ILE:HD12 | 1:E:185:MSE:CE | 2.30 | 0.60 |
| 1:E:76:MSE:HE3 | 1:E:277:LEU:HD21 | 1.82 | 0.60 |
| 1:H:76:MSE:HE3 | 1:H:277:LEU:HD21 | 1.82 | 0.60 |
| 1:D:185:MSE:HE3 | 1:D:205:SER:HB3 | 1.81 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:151:ILE:HD12 | 1:J:185:MSE:CE | 2.31 | 0.60 |
| 1:J:185:MSE:HE3 | 1:J:205:SER:HB3 | 1.82 | 0.60 |
| 1:C:114:ASN:N | 1:C:114:ASN:HD22 | 1.98 | 0.60 |
| 1:G:246:GLU:HG2 | 1:G:247:GLY:H | 1.67 | 0.60 |
| 1:E:76:MSE:CE | 1:E:277:LEU:HD21 | 2.31 | 0.60 |
| 1:C:76:MSE:CE | 1:C:277:LEU:HD21 | 2.30 | 0.60 |
| 1:C:151:ILE:HD12 | 1:C:185:MSE:CE | 2.31 | 0.60 |
| 1:E:185:MSE:HE3 | 1:E:205:SER:HB3 | 1.82 | 0.60 |
| 1:H:151:ILE:HD12 | 1:H:185:MSE:CE | 2.29 | 0.60 |
| 1:F:75:ARG:HH21 | 1:F:278:TYR:HA | 1.67 | 0.60 |
| 1:E:246:GLU:HG2 | 1:E:247:GLY:H | 1.67 | 0.60 |
| 1:J:151:ILE:HB | 1:J:185:MSE:HE2 | 1.84 | 0.60 |
| 1:H:24:MSE:HE1 | 1:H:27:GLU:OE1 | 2.01 | 0.60 |
| 1:D:246:GLU:HG2 | 1:D:247:GLY:H | 1.67 | 0.60 |
| 1:A:151:ILE:HB | 1:A:185:MSE:HE2 | 1.82 | 0.60 |
| 1:F:110:VAL:HG22 | 1:F:144:PHE:HB3 | 1.84 | 0.60 |
| 1:J:68:ASN:ND2 | 1:J:68:ASN:C | 2.55 | 0.60 |
| 1:F:246:GLU:HG2 | 1:F:247:GLY:H | 1.67 | 0.60 |
| 1:B:76:MSE:CE | 1:B:277:LEU:HD21 | 2.31 | 0.60 |
| 1:I:151:ILE:HD12 | 1:I:185:MSE:CE | 2.30 | 0.60 |
| 1:C:47:VAL:HG11 | 1:C:76:MSE:HE1 | 1.84 | 0.59 |
| 1:A:151:ILE:HD12 | 1:A:185:MSE:CE | 2.30 | 0.59 |
| 1:G:32:ARG:HD2 | 1:G:104:LEU:HB3 | 1.83 | 0.59 |
| 1:J:47:VAL:HB | 1:J:76:MSE:HE1 | 1.84 | 0.59 |
| 1:B:273:GLY:N | 1:B:274:ARG:HH21 | 2.00 | 0.59 |
| 1:C:85:VAL:HG23 | 1:C:85:VAL:O | 2.03 | 0.59 |
| 1:F:111:GLY:HA3 | 1:F:137:MSE:CE | 2.31 | 0.59 |
| 1:H:47:VAL:HG11 | 1:H:76:MSE:HE1 | 1.84 | 0.59 |
| 1:E:151:ILE:HB | 1:E:185:MSE:HE2 | 1.83 | 0.59 |
| 1:I:185:MSE:HE3 | 1:I:205:SER:HB3 | 1.83 | 0.59 |
| 1:E:75:ARG:HH21 | 1:E:278:TYR:HA | 1.67 | 0.59 |
| 1:H:246:GLU:HG2 | 1:H:247:GLY:H | 1.67 | 0.59 |
| 1:I:246:GLU:HG2 | 1:I:247:GLY:H | 1.67 | 0.59 |
| 1:C:273:GLY:H | 1:C:274:ARG:HH21 | 1.51 | 0.59 |
| 1:D:226:VAL:CG1 | 1:D:227:GLU:H | 2.16 | 0.59 |
| 1:I:85:VAL:O | 1:I:85:VAL:HG23 | 2.03 | 0.59 |
| 1:H:273:GLY:H | 1:H:274:ARG:HH21 | 1.51 | 0.59 |
| 1:B:274:ARG:O | 1:B:277:LEU:O | 2.21 | 0.59 |
| 1:C:190:ASN:OD1 | 1:H:122:SER:HB2 | 2.03 | 0.59 |
| 1:F:273:GLY:N | 1:F:274:ARG:HH21 | 2.00 | 0.59 |
| 1:C:273:GLY:N | 1:C:274:ARG:HH21 | 2.01 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:151:ILE:HB | 1:C:185:MSE:HE2 | 1.85 | 0.59 |
| 1:J:226:VAL:CG1 | 1:J:227:GLU:H | 2.16 | 0.59 |
| 1:E:261:ALA:HA | 1:E:264:LEU:HD22 | 1.85 | 0.59 |
| 1:J:80:LEU:HA | 1:J:85:VAL:HG21 | 1.85 | 0.59 |
| 1:A:111:GLY:H | 1:A:137:MSE:HE1 | 1.67 | 0.59 |
| 1:D:151:ILE:HB | 1:D:185:MSE:HE2 | 1.85 | 0.59 |
| 1:A:246:GLU:HG2 | 1:A:247:GLY:H | 1.67 | 0.59 |
| 1:J:246:GLU:HG2 | 1:J:247:GLY:H | 1.67 | 0.59 |
| 1:F:151:ILE:HB | 1:F:185:MSE:HE2 | 1.84 | 0.58 |
| 1:E:152:ASN:HD22 | 1:E:152:ASN:C | 2.06 | 0.58 |
| 1:E:46:ILE:HD13 | 1:E:110:VAL:HG21 | 1.83 | 0.58 |
| 1:I:151:ILE:HB | 1:I:185:MSE:HE2 | 1.85 | 0.58 |
| 1:I:226:VAL:CG1 | 1:I:227:GLU:H | 2.16 | 0.58 |
| 1:E:226:VAL:CG1 | 1:E:227:GLU:H | 2.16 | 0.58 |
| 1:J:76:MSE:HE2 | 1:J:277:LEU:CD2 | 2.26 | 0.58 |
| 1:B:278:TYR:N | 1:B:279:PRO:HD3 | 2.18 | 0.58 |
| 1:G:85:VAL:O | 1:G:85:VAL:HG23 | 2.03 | 0.58 |
| 1:C:261:ALA:HA | 1:C:264:LEU:HD22 | 1.86 | 0.58 |
| 1:I:152:ASN:C | 1:I:152:ASN:HD22 | 2.07 | 0.58 |
| 1:F:226:VAL:CG1 | 1:F:227:GLU:H | 2.16 | 0.58 |
| 1:I:273:GLY:N | 1:I:274:ARG:HH21 | 2.02 | 0.58 |
| 1:F:47:VAL:HG11 | 1:F:76:MSE:HE1 | 1.85 | 0.58 |
| 1:A:226:VAL:CG1 | 1:A:227:GLU:H | 2.16 | 0.58 |
| 1:G:151:ILE:HB | 1:G:185:MSE:HE2 | 1.84 | 0.58 |
| 1:H:261:ALA:HA | 1:H:264:LEU:HD22 | 1.86 | 0.58 |
| 1:C:246:GLU:HG2 | 1:C:247:GLY:H | 1.67 | 0.58 |
| 1:E:47:VAL:HG11 | 1:E:76:MSE:HE1 | 1.86 | 0.58 |
| 1:C:226:VAL:CG1 | 1:C:227:GLU:H | 2.16 | 0.58 |
| 1:D:261:ALA:HA | 1:D:264:LEU:HD22 | 1.85 | 0.58 |
| 1:F:85:VAL:O | 1:F:85:VAL:HG23 | 2.03 | 0.58 |
| 1:H:85:VAL:O | 1:H:85:VAL:HG23 | 2.03 | 0.58 |
| 1:B:274:ARG:H | 1:B:274:ARG:NE | 2.01 | 0.58 |
| 1:B:151:ILE:HB | 1:B:185:MSE:HE2 | 1.85 | 0.58 |
| 1:B:246:GLU:HG2 | 1:B:247:GLY:H | 1.67 | 0.58 |
| 1:C:54:ARG:HH21 | 1:C:150:ARG:HH12 | 1.52 | 0.58 |
| 1:G:261:ALA:HA | 1:G:264:LEU:HD22 | 1.85 | 0.58 |
| 1:H:273:GLY:N | 1:H:274:ARG:HH21 | 2.01 | 0.57 |
| 1:D:273:GLY:N | 1:D:274:ARG:HH21 | 2.02 | 0.57 |
| 1:I:114:ASN:HD21 | 1:I:148:LEU:H | 1.52 | 0.57 |
| 1:B:261:ALA:HA | 1:B:264:LEU:HD22 | 1.86 | 0.57 |
| 1:B:152:ASN:C | 1:B:152:ASN:HD22 | 2.07 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:85:VAL:O | 1:B:85:VAL:HG23 | 2.04 | 0.57 |
| 1:C:111:GLY:CA | 1:C:137:MSE:CE | 2.82 | 0.57 |
| 1:F:273:GLY:H | 1:F:274:ARG:HH21 | 1.51 | 0.57 |
| 1:H:274:ARG:NE | 1:H:274:ARG:H | 2.01 | 0.57 |
| 1:G:152:ASN:C | 1:G:152:ASN:HD22 | 2.06 | 0.57 |
| 1:H:226:VAL:CG1 | 1:H:227:GLU:H | 2.16 | 0.57 |
| 1:C:75:ARG:HH21 | 1:C:278:TYR:HA | 1.69 | 0.57 |
| 1:E:85:VAL:HG23 | 1:E:85:VAL:O | 2.03 | 0.57 |
| 1:J:76:MSE:HE2 | 1:J:76:MSE:HA | 1.86 | 0.57 |
| 1:A:76:MSE:HA | 1:A:76:MSE:CE | 2.33 | 0.57 |
| 1:B:47:VAL:HG11 | 1:B:76:MSE:HE1 | 1.86 | 0.57 |
| 1:H:151:ILE:HB | 1:H:185:MSE:HE2 | 1.85 | 0.57 |
| 1:C:152:ASN:C | 1:C:152:ASN:HD22 | 2.07 | 0.57 |
| 1:H:41:ASP:OD2 | 1:H:296:HIS:HD2 | 1.86 | 0.57 |
| 1:A:273:GLY:N | 1:A:274:ARG:HH21 | 2.02 | 0.57 |
| 1:F:152:ASN:C | 1:F:152:ASN:HD22 | 2.06 | 0.57 |
| 1:B:110:VAL:HG13 | 1:B:144:PHE:HB3 | 1.87 | 0.57 |
| 1:I:47:VAL:HG11 | 1:I:76:MSE:HE1 | 1.85 | 0.57 |
| 1:F:76:MSE:HA | 1:F:76:MSE:CE | 2.33 | 0.57 |
| 1:B:273:GLY:H | 1:B:274:ARG:HH21 | 1.51 | 0.57 |
| 1:J:152:ASN:C | 1:J:152:ASN:HD22 | 2.07 | 0.57 |
| 1:G:47:VAL:HG11 | 1:G:76:MSE:HE1 | 1.86 | 0.57 |
| 1:I:261:ALA:HA | 1:I:264:LEU:HD22 | 1.86 | 0.57 |
| 1:G:226:VAL:CG1 | 1:G:227:GLU:H | 2.17 | 0.57 |
| 1:F:12:GLU:OE1 | 1:F:16:ARG:NH2 | 2.36 | 0.57 |
| 1:G:114:ASN:HD22 | 1:G:114:ASN:N | 1.98 | 0.57 |
| 1:A:152:ASN:C | 1:A:152:ASN:HD22 | 2.08 | 0.57 |
| 1:D:85:VAL:HG23 | 1:D:85:VAL:O | 2.04 | 0.57 |
| 1:I:274:ARG:H | 1:I:274:ARG:NE | 2.01 | 0.57 |
| 1:H:76:MSE:HA | 1:H:76:MSE:CE | 2.34 | 0.57 |
| 1:D:47:VAL:HG11 | 1:D:76:MSE:HE1 | 1.86 | 0.57 |
| 1:F:261:ALA:HA | 1:F:264:LEU:HD22 | 1.86 | 0.57 |
| 1:E:273:GLY:H | 1:E:274:ARG:HH21 | 1.53 | 0.57 |
| 1:E:273:GLY:N | 1:E:274:ARG:HH21 | 2.02 | 0.57 |
| 1:A:47:VAL:HG11 | 1:A:76:MSE:HE1 | 1.86 | 0.57 |
| 1:J:261:ALA:HA | 1:J:264:LEU:HD22 | 1.86 | 0.57 |
| 1:F:283:ASP:HB3 | 1:F:286:ALA:HB3 | 1.85 | 0.57 |
| 1:I:274:ARG:O | 1:I:277:LEU:O | 2.23 | 0.56 |
| 1:B:226:VAL:CG1 | 1:B:227:GLU:H | 2.17 | 0.56 |
| 1:A:261:ALA:HA | 1:A:264:LEU:HD22 | 1.86 | 0.56 |
| 1:A:85:VAL:HG23 | 1:A:85:VAL:O | 2.04 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:J:273:GLY:N | 1:J:274:ARG:HH21 | 2.02 | 0.56 |
| 1:B:185:MSE:HE3 | 1:B:205:SER:HA | 1.88 | 0.56 |
| 1:D:273:GLY:H | 1:D:274:ARG:HH21 | 1.52 | 0.56 |
| 1:D:152:ASN:C | 1:D:152:ASN:HD22 | 2.07 | 0.56 |
| 1:F:86:ASP:OD2 | 1:F:296:HIS:HE1 | 1.88 | 0.56 |
| 1:G:76:MSE:HA | 1:G:76:MSE:CE | 2.33 | 0.56 |
| 1:I:110:VAL:HG22 | 1:I:144:PHE:HB3 | 1.87 | 0.56 |
| 1:C:110:VAL:HG22 | 1:C:144:PHE:HB3 | 1.87 | 0.56 |
| 1:E:32:ARG:HD2 | 1:E:104:LEU:HB3 | 1.87 | 0.56 |
| 1:A:273:GLY:H | 1:A:274:ARG:HH21 | 1.52 | 0.56 |
| 1:A:274:ARG:H | 1:A:274:ARG:NE | 2.01 | 0.56 |
| 1:H:152:ASN:C | 1:H:152:ASN:HD22 | 2.07 | 0.56 |
| 1:F:278:TYR:N | 1:F:279:PRO:HD3 | 2.21 | 0.56 |
| 1:I:54:ARG:HH21 | 1:I:150:ARG:HH12 | 1.54 | 0.56 |
| 1:J:111:GLY:H | 1:J:137:MSE:HE1 | 1.71 | 0.55 |
| 1:E:76:MSE:CE | 1:E:76:MSE:HA | 2.34 | 0.55 |
| 1:B:185:MSE:HE3 | 1:B:205:SER:CA | 2.36 | 0.55 |
| 1:D:76:MSE:HA | 1:D:76:MSE:CE | 2.34 | 0.55 |
| 1:A:97:ASP:O | 1:A:101:LEU:HD22 | 2.06 | 0.55 |
| 1:G:274:ARG:H | 1:G:274:ARG:NE | 2.02 | 0.55 |
| 1:D:76:MSE:HE2 | 1:D:277:LEU:HD21 | 1.88 | 0.55 |
| 1:H:185:MSE:HE3 | 1:H:205:SER:HA | 1.89 | 0.55 |
| 1:I:273:GLY:H | 1:I:274:ARG:HH21 | 1.53 | 0.55 |
| 1:D:45:PHE:CE2 | 1:D:85:VAL:HG12 | 2.42 | 0.55 |
| 1:J:273:GLY:H | 1:J:274:ARG:HH21 | 1.53 | 0.55 |
| 1:G:273:GLY:N | 1:G:274:ARG:HH21 | 2.05 | 0.55 |
| 1:G:185:MSE:HE3 | 1:G:205:SER:CA | 2.37 | 0.55 |
| 1:F:110:VAL:HG22 | 1:F:144:PHE:CB | 2.37 | 0.55 |
| 1:J:75:ARG:HH21 | 1:J:278:TYR:HA | 1.72 | 0.55 |
| 1:H:105:ASP:O | 1:H:107:LYS:HG2 | 2.07 | 0.55 |
| 1:C:113:MSE:HE3 | 2:C:704:HOH:O | 2.07 | 0.55 |
| 1:B:76:MSE:HA | 1:B:76:MSE:CE | 2.33 | 0.55 |
| 1:C:185:MSE:HE3 | 1:C:205:SER:CA | 2.37 | 0.55 |
| 1:C:185:MSE:HE3 | 1:C:205:SER:HA | 1.88 | 0.55 |
| 1:D:185:MSE:HE3 | 1:D:205:SER:CA | 2.37 | 0.55 |
| 1:J:185:MSE:HE3 | 1:J:205:SER:HA | 1.89 | 0.55 |
| 1:E:45:PHE:CE2 | 1:E:85:VAL:HG12 | 2.42 | 0.55 |
| 1:J:89:LEU:HD12 | 1:J:90:GLY:N | 2.22 | 0.55 |
| 1:B:45:PHE:CE2 | 1:B:85:VAL:HG12 | 2.42 | 0.55 |
| 1:A:45:PHE:CE2 | 1:A:85:VAL:HG12 | 2.42 | 0.55 |
| 1:J:9:GLU:N | 1:J:9:GLU:OE1 | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:185:MSE:HE3 | 1:F:205:SER:CA | 2.38 | 0.54 |
| 1:J:185:MSE:HE3 | 1:J:205:SER:CA | 2.37 | 0.54 |
| 1:G:185:MSE:HE3 | 1:G:205:SER:HA | 1.89 | 0.54 |
| 1:C:45:PHE:CE2 | 1:C:85:VAL:HG12 | 2.42 | 0.54 |
| 1:B:41:ASP:OD2 | 1:B:296:HIS:HD2 | 1.90 | 0.54 |
| 1:I:76:MSE:HA | 1:I:76:MSE:CE | 2.33 | 0.54 |
| 1:E:185:MSE:HE3 | 1:E:205:SER:HA | 1.90 | 0.54 |
| 1:I:185:MSE:HE3 | 1:I:205:SER:HA | 1.88 | 0.54 |
| 1:A:278:TYR:N | 1:A:279:PRO:HD3 | 2.23 | 0.54 |
| 1:H:45:PHE:CE2 | 1:H:85:VAL:HG12 | 2.42 | 0.54 |
| 1:C:76:MSE:HA | 1:C:76:MSE:CE | 2.34 | 0.54 |
| 1:I:185:MSE:HE3 | 1:I:205:SER:CA | 2.37 | 0.54 |
| 1:I:259:GLU:CB | 1:I:294:LEU:HD11 | 2.35 | 0.54 |
| 1:I:14:LEU:HD22 | 1:I:101:LEU:CD1 | 2.37 | 0.54 |
| 1:J:110:VAL:HG22 | 1:J:144:PHE:HB3 | 1.90 | 0.54 |
| 1:C:111:GLY:N | 1:C:137:MSE:HE1 | 2.21 | 0.54 |
| 1:H:185:MSE:HE3 | 1:H:205:SER:CA | 2.37 | 0.54 |
| 1:E:170:ASN:ND2 | 1:E:214:ASN:H | 2.06 | 0.54 |
| 1:F:45:PHE:CE2 | 1:F:85:VAL:HG12 | 2.42 | 0.54 |
| 1:I:45:PHE:CE2 | 1:I:85:VAL:HG12 | 2.42 | 0.54 |
| 1:E:126:ASP:OD2 | 1:E:128:ARG:NH1 | 2.40 | 0.54 |
| 1:E:274:ARG:H | 1:E:274:ARG:NE | 2.02 | 0.54 |
| 1:D:185:MSE:HE3 | 1:D:205:SER:HA | 1.89 | 0.54 |
| 1:F:185:MSE:HE3 | 1:F:205:SER:HA | 1.89 | 0.54 |
| 1:G:45:PHE:CE2 | 1:G:85:VAL:HG12 | 2.43 | 0.53 |
| 1:J:29:PHE:O | 1:J:32:ARG:HB3 | 2.07 | 0.53 |
| 1:D:297:THR:O | 1:D:299:ILE:N | 2.41 | 0.53 |
| 2:C:569:HOH:O | 1:D:55:GLY:HA2 | 2.07 | 0.53 |
| 1:G:273:GLY:H | 1:G:274:ARG:HH21 | 1.56 | 0.53 |
| 1:D:75:ARG:NH2 | 1:D:278:TYR:HA | 2.23 | 0.53 |
| 1:H:33:ARG:NH1 | 1:H:33:ARG:HG3 | 2.23 | 0.53 |
| 1:D:274:ARG:H | 1:D:274:ARG:NE | 2.00 | 0.53 |
| 1:B:54:ARG:HH21 | 1:B:150:ARG:HH12 | 1.54 | 0.53 |
| 1:F:114:ASN:O | 1:F:115:ARG:HD2 | 2.08 | 0.53 |
| 1:J:170:ASN:ND2 | 1:J:214:ASN:H | 2.07 | 0.53 |
| 1:A:110:VAL:HG13 | 1:A:144:PHE:HB3 | 1.91 | 0.53 |
| 1:F:170:ASN:ND2 | 1:F:214:ASN:H | 2.07 | 0.53 |
| 1:H:274:ARG:O | 1:H:277:LEU:O | 2.27 | 0.53 |
| 1:E:185:MSE:HE3 | 1:E:205:SER:CA | 2.38 | 0.53 |
| 1:I:229:MSE:O | 1:I:264:LEU:HD23 | 2.09 | 0.53 |
| 1:H:126:ASP:OD2 | 1:H:128:ARG:NH1 | 2.41 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:278:TYR:N | 1:H:279:PRO:HD3 | 2.24 | 0.53 |
| 1:H:64:THR:O | 1:H:65:ALA:HB3 | 2.09 | 0.53 |
| 1:B:277:LEU:O | 1:B:278:TYR:HB2 | 2.09 | 0.53 |
| 1:B:46:ILE:HD13 | 1:B:110:VAL:HG21 | 1.91 | 0.53 |
| 1:G:170:ASN:ND2 | 1:G:214:ASN:H | 2.07 | 0.53 |
| 1:J:47:VAL:CG1 | 1:J:76:MSE:HE1 | 2.39 | 0.52 |
| 1:G:64:THR:O | 1:G:65:ALA:HB3 | 2.10 | 0.52 |
| 1:F:229:MSE:O | 1:F:264:LEU:HD23 | 2.09 | 0.52 |
| 1:F:12:GLU:OE2 | 1:F:15:ARG:NH2 | 2.42 | 0.52 |
| 1:A:111:GLY:CA | 1:A:137:MSE:CE | 2.86 | 0.52 |
| 1:E:114:ASN:N | 1:E:114:ASN:HD22 | 2.06 | 0.52 |
| 1:A:24:MSE:HG3 | 2:A:316:HOH:O | 2.08 | 0.52 |
| 1:J:274:ARG:NE | 1:J:274:ARG:H | 2.01 | 0.52 |
| 1:E:111:GLY:CA | 1:E:137:MSE:CE | 2.86 | 0.52 |
| 1:I:170:ASN:ND2 | 1:I:214:ASN:H | 2.07 | 0.52 |
| 1:J:64:THR:O | 1:J:65:ALA:HB3 | 2.09 | 0.52 |
| 1:F:114:ASN:O | 1:F:115:ARG:CD | 2.58 | 0.52 |
| 1:I:64:THR:O | 1:I:65:ALA:HB3 | 2.09 | 0.52 |
| 1:F:110:VAL:HG13 | 1:F:144:PHE:HB3 | 1.91 | 0.52 |
| 1:B:33:ARG:NH1 | 1:B:33:ARG:HG3 | 2.25 | 0.52 |
| 1:H:47:VAL:HG11 | 1:H:76:MSE:CE | 2.40 | 0.52 |
| 1:D:68:ASN:CG | 1:D:71:GLU:HG3 | 2.30 | 0.52 |
| 1:A:64:THR:O | 1:A:65:ALA:HB3 | 2.09 | 0.52 |
| 1:A:296:HIS:C | 1:A:298:ASP:H | 2.13 | 0.52 |
| 1:A:185:MSE:HE3 | 1:A:205:SER:CA | 2.38 | 0.52 |
| 1:F:64:THR:O | 1:F:65:ALA:HB3 | 2.10 | 0.52 |
| 1:D:64:THR:O | 1:D:65:ALA:HB3 | 2.10 | 0.52 |
| 1:H:229:MSE:O | 1:H:264:LEU:HD23 | 2.10 | 0.52 |
| 1:C:126:ASP:OD2 | 1:C:128:ARG:NH1 | 2.41 | 0.52 |
| 1:A:274:ARG:O | 1:A:277:LEU:O | 2.27 | 0.52 |
| 1:J:45:PHE:HE2 | 1:J:85:VAL:HG12 | 1.73 | 0.52 |
| 1:H:170:ASN:ND2 | 1:H:214:ASN:H | 2.08 | 0.52 |
| 1:J:69:ARG:HH11 | 1:J:72:LEU:HD13 | 1.75 | 0.52 |
| 1:E:68:ASN:CG | 1:E:71:GLU:HG3 | 2.30 | 0.52 |
| 1:D:297:THR:C | 1:D:299:ILE:H | 2.13 | 0.52 |
| 1:F:274:ARG:H | 1:F:274:ARG:NE | 2.00 | 0.51 |
| 1:H:47:VAL:CG1 | 1:H:76:MSE:HE1 | 2.40 | 0.51 |
| 1:B:76:MSE:HE2 | 1:B:277:LEU:HD21 | 1.92 | 0.51 |
| 1:B:64:THR:O | 1:B:65:ALA:HB3 | 2.10 | 0.51 |
| 1:A:185:MSE:HE3 | 1:A:205:SER:HA | 1.90 | 0.51 |
| 1:J:65:ALA:C | 1:J:67:ALA:H | 2.13 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:64:THR:O | 1:C:65:ALA:HB3 | 2.09 | 0.51 |
| 1:A:170:ASN:ND2 | 1:A:214:ASN:H | 2.08 | 0.51 |
| 1:C:297:THR:O | 1:C:298:ASP:HB2 | 2.11 | 0.51 |
| 1:B:170:ASN:ND2 | 1:B:214:ASN:H | 2.08 | 0.51 |
| 1:D:111:GLY:HA3 | 1:D:137:MSE:CE | 2.40 | 0.51 |
| 1:C:229:MSE:O | 1:C:264:LEU:HD23 | 2.11 | 0.51 |
| 1:E:229:MSE:O | 1:E:264:LEU:HD23 | 2.11 | 0.51 |
| 1:B:180:MSE:HE2 | 1:B:241:LEU:HD12 | 1.92 | 0.51 |
| 1:H:111:GLY:N | 1:H:137:MSE:HE1 | 2.25 | 0.51 |
| 1:E:64:THR:O | 1:E:65:ALA:HB3 | 2.09 | 0.51 |
| 1:G:229:MSE:O | 1:G:264:LEU:HD23 | 2.10 | 0.51 |
| 1:I:68:ASN:HD21 | 1:I:70:TYR:HB2 | 1.76 | 0.51 |
| 1:G:68:ASN:CG | 1:G:71:GLU:HG3 | 2.30 | 0.51 |
| 1:B:126:ASP:OD2 | 1:B:128:ARG:NH1 | 2.41 | 0.51 |
| 1:A:111:GLY:N | 1:A:137:MSE:HE1 | 2.26 | 0.51 |
| 1:F:274:ARG:O | 1:F:277:LEU:O | 2.29 | 0.51 |
| 1:C:47:VAL:CG1 | 1:C:76:MSE:HE1 | 2.40 | 0.51 |
| 1:D:114:ASN:N | 1:D:114:ASN:HD22 | 2.04 | 0.51 |
| 1:C:33:ARG:HG3 | 1:C:33:ARG:NH1 | 2.25 | 0.51 |
| 1:B:32:ARG:HD2 | 1:B:104:LEU:HB3 | 1.92 | 0.51 |
| 1:J:129:TYR:OH | 1:J:147:THR:HG21 | 2.11 | 0.51 |
| 1:D:170:ASN:ND2 | 1:D:214:ASN:H | 2.08 | 0.51 |
| 1:G:47:VAL:HG11 | 1:G:76:MSE:CE | 2.41 | 0.51 |
| 1:F:47:VAL:HG11 | 1:F:76:MSE:CE | 2.41 | 0.51 |
| 1:A:75:ARG:HH21 | 1:A:278:TYR:HA | 1.74 | 0.51 |
| 1:B:75:ARG:HH21 | 1:B:278:TYR:HA | 1.75 | 0.51 |
| 1:J:229:MSE:O | 1:J:264:LEU:HD23 | 2.10 | 0.51 |
| 1:C:68:ASN:CG | 1:C:71:GLU:HG3 | 2.31 | 0.51 |
| 1:I:68:ASN:CG | 1:I:71:GLU:HG3 | 2.31 | 0.51 |
| 1:E:297:THR:OG1 | 1:E:299:ILE:HG12 | 2.11 | 0.51 |
| 1:D:180:MSE:HE2 | 1:D:241:LEU:HD12 | 1.93 | 0.51 |
| 1:I:47:VAL:HG11 | 1:I:76:MSE:CE | 2.41 | 0.51 |
| 1:C:47:VAL:HG11 | 1:C:76:MSE:CE | 2.40 | 0.51 |
| 1:C:180:MSE:HE2 | 1:C:241:LEU:HD12 | 1.93 | 0.51 |
| 1:B:68:ASN:CG | 1:B:71:GLU:HG3 | 2.31 | 0.51 |
| 1:D:229:MSE:O | 1:D:264:LEU:HD23 | 2.10 | 0.51 |
| 1:I:33:ARG:NH1 | 1:I:33:ARG:HG3 | 2.24 | 0.51 |
| 1:D:33:ARG:HG3 | 1:D:33:ARG:NH1 | 2.25 | 0.51 |
| 1:A:46:ILE:HD13 | 1:A:110:VAL:HG21 | 1.93 | 0.51 |
| 1:G:275:THR:HG22 | 1:G:276:LEU:HD23 | 1.93 | 0.51 |
| 1:E:129:TYR:OH | 1:E:147:THR:HG21 | 2.11 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:ASN:HD21 | 1:B:70:TYR:HB2 | 1.76 | 0.50 |
| 1:A:229:MSE:O | 1:A:264:LEU:HD23 | 2.10 | 0.50 |
| 1:I:110:VAL:HG22 | 1:I:144:PHE:CB | 2.42 | 0.50 |
| 1:C:170:ASN:ND2 | 1:C:214:ASN:H | 2.08 | 0.50 |
| 1:G:274:ARG:O | 1:G:277:LEU:O | 2.29 | 0.50 |
| 1:E:47:VAL:HG11 | 1:E:76:MSE:CE | 2.41 | 0.50 |
| 1:A:47:VAL:HG11 | 1:A:76:MSE:CE | 2.41 | 0.50 |
| 1:H:57:LEU:O | 1:H:65:ALA:O | 2.30 | 0.50 |
| 1:D:47:VAL:HG11 | 1:D:76:MSE:CE | 2.40 | 0.50 |
| 1:G:129:TYR:OH | 1:G:147:THR:HG21 | 2.11 | 0.50 |
| 1:A:126:ASP:OD2 | 1:A:128:ARG:NH1 | 2.41 | 0.50 |
| 1:I:114:ASN:HD22 | 1:I:114:ASN:N | 1.99 | 0.50 |
| 1:F:68:ASN:HD21 | 1:F:70:TYR:HB2 | 1.77 | 0.50 |
| 1:I:129:TYR:OH | 1:I:147:THR:HG21 | 2.12 | 0.50 |
| 1:G:47:VAL:CG1 | 1:G:76:MSE:HE1 | 2.42 | 0.50 |
| 1:B:47:VAL:CG1 | 1:B:76:MSE:HE1 | 2.42 | 0.50 |
| 1:D:89:LEU:HD13 | 1:D:110:VAL:HG12 | 1.92 | 0.50 |
| 1:G:68:ASN:HD21 | 1:G:70:TYR:HB2 | 1.76 | 0.50 |
| 1:F:126:ASP:OD2 | 1:F:128:ARG:NH1 | 2.41 | 0.50 |
| 1:G:110:VAL:HG22 | 1:G:144:PHE:HB3 | 1.92 | 0.50 |
| 1:B:66:MSE:HG2 | 1:B:278:TYR:CE2 | 2.46 | 0.50 |
| 1:C:278:TYR:N | 1:C:279:PRO:HD3 | 2.27 | 0.50 |
| 1:A:180:MSE:HE2 | 1:A:241:LEU:HD12 | 1.93 | 0.50 |
| 1:E:180:MSE:HE2 | 1:E:241:LEU:HD12 | 1.93 | 0.50 |
| 1:B:111:GLY:N | 1:B:137:MSE:HE1 | 2.25 | 0.50 |
| 1:C:57:LEU:O | 1:C:65:ALA:O | 2.30 | 0.50 |
| 1:A:68:ASN:CG | 1:A:71:GLU:HG3 | 2.31 | 0.50 |
| 1:C:110:VAL:HG22 | 1:C:144:PHE:CB | 2.42 | 0.50 |
| 1:G:126:ASP:OD2 | 1:G:128:ARG:NH1 | 2.41 | 0.50 |
| 1:H:12:GLU:OE1 | 1:H:16:ARG:NH2 | 2.42 | 0.50 |
| 1:J:17:MSE:HE1 | 1:J:28:ARG:HE | 1.75 | 0.50 |
| 1:J:111:GLY:HA3 | 1:J:137:MSE:CE | 2.40 | 0.50 |
| 1:B:47:VAL:HG11 | 1:B:76:MSE:CE | 2.41 | 0.50 |
| 1:F:68:ASN:CG | 1:F:71:GLU:HG3 | 2.32 | 0.50 |
| 1:C:68:ASN:HD21 | 1:C:70:TYR:HB2 | 1.77 | 0.50 |
| 1:F:180:MSE:HE2 | 1:F:241:LEU:HD12 | 1.92 | 0.50 |
| 1:C:111:GLY:CA | 1:C:137:MSE:HE1 | 2.42 | 0.50 |
| 1:H:68:ASN:HD21 | 1:H:70:TYR:HB2 | 1.76 | 0.50 |
| 1:G:12:GLU:OE1 | 1:G:16:ARG:NH2 | 2.45 | 0.50 |
| 1:D:126:ASP:OD2 | 1:D:128:ARG:NH1 | 2.41 | 0.50 |
| 1:F:76:MSE:CE | 1:F:277:LEU:HD21 | 2.42 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:47:VAL:CG1 | 1:A:76:MSE:HE1 | 2.41 | 0.49 |
| 1:D:68:ASN:HD21 | 1:D:70:TYR:HB2 | 1.76 | 0.49 |
| 1:J:68:ASN:HD22 | 1:J:69:ARG:N | 2.10 | 0.49 |
| 1:G:114:ASN:O | 1:G:115:ARG:HD2 | 2.13 | 0.49 |
| 1:B:229:MSE:O | 1:B:264:LEU:HD23 | 2.10 | 0.49 |
| 1:E:33:ARG:HG3 | 1:E:33:ARG:NH1 | 2.25 | 0.49 |
| 1:E:68:ASN:HD21 | 1:E:70:TYR:HB2 | 1.76 | 0.49 |
| 1:H:180:MSE:HE2 | 1:H:241:LEU:HD12 | 1.93 | 0.49 |
| 1:F:129:TYR:OH | 1:F:147:THR:HG21 | 2.12 | 0.49 |
| 1:I:296:HIS:O | 1:I:298:ASP:N | 2.45 | 0.49 |
| 1:D:47:VAL:CG1 | 1:D:76:MSE:HE1 | 2.42 | 0.49 |
| 1:J:180:MSE:HE2 | 1:J:241:LEU:HD12 | 1.93 | 0.49 |
| 1:J:41:ASP:O | 1:J:43:LYS:HD3 | 2.12 | 0.49 |
| 1:I:47:VAL:CG1 | 1:I:76:MSE:HE1 | 2.41 | 0.49 |
| 1:F:47:VAL:CG1 | 1:F:76:MSE:HE1 | 2.42 | 0.49 |
| 1:F:76:MSE:HE3 | 1:F:277:LEU:HD11 | 1.94 | 0.49 |
| 1:B:57:LEU:O | 1:B:65:ALA:O | 2.30 | 0.49 |
| 1:B:129:TYR:OH | 1:B:147:THR:HG21 | 2.11 | 0.49 |
| 1:A:129:TYR:OH | 1:A:147:THR:HG21 | 2.12 | 0.49 |
| 1:J:259:GLU:HB2 | 1:J:294:LEU:HD11 | 1.94 | 0.49 |
| 1:C:274:ARG:NE | 1:C:274:ARG:H | 2.01 | 0.49 |
| 1:A:63:GLU:O | 1:A:64:THR:O | 2.31 | 0.49 |
| 1:H:129:TYR:OH | 1:H:147:THR:HG21 | 2.12 | 0.49 |
| 1:J:85:VAL:HG23 | 1:J:85:VAL:O | 2.13 | 0.49 |
| 1:J:92:PRO:HG3 | 1:J:132:TYR:CD2 | 2.47 | 0.49 |
| 1:J:95:ILE:HD12 | 1:J:109:VAL:HG13 | 1.95 | 0.49 |
| 1:F:114:ASN:HD22 | 1:F:114:ASN:N | 2.09 | 0.49 |
| 1:J:91:THR:OG1 | 1:J:93:ASP:OD1 | 2.25 | 0.49 |
| 1:I:110:VAL:HG13 | 1:I:144:PHE:HB3 | 1.95 | 0.49 |
| 1:C:129:TYR:OH | 1:C:147:THR:HG21 | 2.12 | 0.49 |
| 1:A:111:GLY:CA | 1:A:137:MSE:HE1 | 2.43 | 0.49 |
| 1:A:57:LEU:O | 1:A:65:ALA:O | 2.31 | 0.49 |
| 1:G:76:MSE:HE3 | 1:G:277:LEU:HD21 | 1.94 | 0.49 |
| 1:I:57:LEU:O | 1:I:65:ALA:O | 2.31 | 0.49 |
| 1:E:46:ILE:HD13 | 1:E:110:VAL:CG2 | 2.43 | 0.49 |
| 1:C:32:ARG:HD2 | 1:C:104:LEU:HB3 | 1.94 | 0.49 |
| 1:H:68:ASN:CG | 1:H:71:GLU:HG3 | 2.32 | 0.49 |
| 1:F:33:ARG:HG3 | 1:F:33:ARG:NH1 | 2.24 | 0.49 |
| 1:D:129:TYR:OH | 1:D:147:THR:HG21 | 2.11 | 0.49 |
| 1:I:180:MSE:HE2 | 1:I:241:LEU:HD12 | 1.94 | 0.49 |
| 1:B:17:MSE:HE1 | 1:B:28:ARG:NE | 2.27 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:8:PRO:HG2 | 1:G:9:GLU:OE1 | 2.13 | 0.49 |
| 1:A:68:ASN:HD21 | 1:A:70:TYR:HB2 | 1.77 | 0.48 |
| 1:I:296:HIS:C | 1:I:298:ASP:H | 2.16 | 0.48 |
| 1:C:82:ARG:NH2 | 1:C:289:ASP:OD2 | 2.44 | 0.48 |
| 1:E:47:VAL:CG1 | 1:E:76:MSE:HE1 | 2.42 | 0.48 |
| 1:C:274:ARG:O | 1:C:277:LEU:O | 2.30 | 0.48 |
| 1:J:63:GLU:CG | 1:J:64:THR:H | 2.19 | 0.48 |
| 1:J:278:TYR:N | 1:J:279:PRO:HD3 | 2.28 | 0.48 |
| 1:F:57:LEU:O | 1:F:65:ALA:O | 2.31 | 0.48 |
| 1:G:33:ARG:HG3 | 1:G:33:ARG:NH1 | 2.26 | 0.48 |
| 1:C:76:MSE:HE2 | 1:C:277:LEU:HD21 | 1.95 | 0.48 |
| 1:B:63:GLU:O | 1:B:64:THR:O | 2.31 | 0.48 |
| 1:D:214:ASN:HD22 | 1:D:214:ASN:C | 2.17 | 0.48 |
| 1:I:152:ASN:HD22 | 1:I:154:SER:H | 1.62 | 0.48 |
| 1:J:79:ALA:O | 1:J:85:VAL:HG21 | 2.13 | 0.48 |
| 1:J:151:ILE:HB | 1:J:185:MSE:HE1 | 1.96 | 0.48 |
| 1:G:57:LEU:O | 1:G:65:ALA:O | 2.31 | 0.48 |
| 1:C:214:ASN:C | 1:C:214:ASN:HD22 | 2.16 | 0.48 |
| 1:I:103:LEU:O | 1:I:104:LEU:HD12 | 2.14 | 0.48 |
| 1:E:111:GLY:H | 1:E:137:MSE:HE1 | 1.77 | 0.48 |
| 1:D:63:GLU:O | 1:D:64:THR:O | 2.31 | 0.48 |
| 1:A:214:ASN:HD22 | 1:A:214:ASN:C | 2.17 | 0.48 |
| 1:E:63:GLU:O | 1:E:64:THR:O | 2.32 | 0.48 |
| 1:E:57:LEU:O | 1:E:65:ALA:O | 2.31 | 0.48 |
| 1:G:214:ASN:C | 1:G:214:ASN:HD22 | 2.16 | 0.48 |
| 1:H:151:ILE:HB | 1:H:185:MSE:HE1 | 1.96 | 0.48 |
| 1:G:180:MSE:HE2 | 1:G:241:LEU:HD12 | 1.94 | 0.48 |
| 1:H:152:ASN:HD22 | 1:H:154:SER:H | 1.62 | 0.48 |
| 1:D:111:GLY:N | 1:D:137:MSE:HE1 | 2.29 | 0.47 |
| 1:F:115:ARG:HA | 1:F:115:ARG:HD2 | 1.58 | 0.47 |
| 1:I:63:GLU:O | 1:I:64:THR:O | 2.32 | 0.47 |
| 1:I:214:ASN:C | 1:I:214:ASN:HD22 | 2.17 | 0.47 |
| 1:H:214:ASN:C | 1:H:214:ASN:HD22 | 2.17 | 0.47 |
| 1:E:110:VAL:HG13 | 1:E:144:PHE:HB3 | 1.96 | 0.47 |
| 1:E:214:ASN:HD22 | 1:E:214:ASN:C | 2.17 | 0.47 |
| 1:F:214:ASN:C | 1:F:214:ASN:HD22 | 2.16 | 0.47 |
| 1:G:14:LEU:HD13 | 1:G:101:LEU:HD13 | 1.95 | 0.47 |
| 1:I:111:GLY:HA3 | 1:I:137:MSE:CE | 2.42 | 0.47 |
| 1:A:15:ARG:HD3 | 1:A:70:TYR:OH | 2.14 | 0.47 |
| 1:H:17:MSE:HE1 | 1:H:28:ARG:NE | 2.30 | 0.47 |
| 1:H:63:GLU:O | 1:H:64:THR:O | 2.31 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:151:ILE:HB | 1:F:185:MSE:HE1 | 1.97 | 0.47 |
| 1:C:152:ASN:HD22 | 1:C:154:SER:H | 1.63 | 0.47 |
| 1:G:63:GLU:O | 1:G:64:THR:O | 2.31 | 0.47 |
| 1:A:68:ASN:ND2 | 1:A:68:ASN:C | 2.67 | 0.47 |
| 1:F:273:GLY:H | 1:F:274:ARG:NH2 | 2.12 | 0.47 |
| 1:H:273:GLY:H | 1:H:274:ARG:NH2 | 2.13 | 0.47 |
| 1:J:214:ASN:HD22 | 1:J:214:ASN:C | 2.17 | 0.47 |
| 1:J:126:ASP:OD2 | 1:J:128:ARG:NH1 | 2.40 | 0.47 |
| 1:A:273:GLY:H | 1:A:274:ARG:NH2 | 2.13 | 0.47 |
| 1:D:151:ILE:HB | 1:D:185:MSE:HE1 | 1.97 | 0.47 |
| 1:C:63:GLU:O | 1:C:64:THR:O | 2.32 | 0.47 |
| 1:A:54:ARG:HH21 | 1:A:150:ARG:HH12 | 1.62 | 0.47 |
| 1:D:273:GLY:H | 1:D:274:ARG:NH2 | 2.12 | 0.47 |
| 1:F:63:GLU:O | 1:F:64:THR:O | 2.31 | 0.47 |
| 1:F:85:VAL:HG23 | 1:F:107:LYS:HE3 | 1.96 | 0.47 |
| 1:A:86:ASP:OD2 | 1:A:296:HIS:HE1 | 1.97 | 0.47 |
| 1:J:273:GLY:H | 1:J:274:ARG:NH2 | 2.13 | 0.47 |
| 1:G:152:ASN:HD22 | 1:G:154:SER:H | 1.63 | 0.47 |
| 1:J:32:ARG:NH1 | 1:J:109:VAL:HG23 | 2.30 | 0.47 |
| 1:I:40:GLU:N | 1:I:40:GLU:OE2 | 2.45 | 0.47 |
| 1:J:47:VAL:CB | 1:J:76:MSE:HE1 | 2.44 | 0.47 |
| 1:B:227:GLU:HB2 | 2:B:578:HOH:O | 2.15 | 0.47 |
| 1:D:284:VAL:O | 1:D:288:VAL:HG23 | 2.14 | 0.47 |
| 1:G:111:GLY:N | 1:G:137:MSE:HE1 | 2.27 | 0.46 |
| 1:I:273:GLY:H | 1:I:274:ARG:NH2 | 2.13 | 0.46 |
| 1:D:57:LEU:O | 1:D:65:ALA:O | 2.31 | 0.46 |
| 1:A:14:LEU:HD22 | 1:A:101:LEU:HD11 | 1.97 | 0.46 |
| 1:A:23:THR:OG1 | 1:A:24:MSE:HE2 | 2.15 | 0.46 |
| 1:I:46:ILE:O | 1:I:271:THR:HA | 2.15 | 0.46 |
| 1:A:152:ASN:HD22 | 1:A:154:SER:H | 1.62 | 0.46 |
| 1:B:152:ASN:HD22 | 1:B:154:SER:H | 1.63 | 0.46 |
| 1:E:152:ASN:HD22 | 1:E:154:SER:H | 1.62 | 0.46 |
| 1:G:54:ARG:NH2 | 1:G:150:ARG:HH12 | 2.12 | 0.46 |
| 1:I:115:ARG:HD2 | 1:I:115:ARG:HA | 1.56 | 0.46 |
| 1:C:273:GLY:H | 1:C:274:ARG:NH2 | 2.13 | 0.46 |
| 1:H:54:ARG:HH21 | 1:H:150:ARG:HH12 | 1.62 | 0.46 |
| 1:A:115:ARG:HA | 1:A:115:ARG:HD2 | 1.58 | 0.46 |
| 1:E:273:GLY:H | 1:E:274:ARG:NH2 | 2.14 | 0.46 |
| 1:D:15:ARG:HD3 | 1:D:70:TYR:OH | 2.15 | 0.46 |
| 1:E:68:ASN:C | 1:E:68:ASN:ND2 | 2.67 | 0.46 |
| 1:B:214:ASN:C | 1:B:214:ASN:HD22 | 2.18 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:111:GLY:CA | 1:E:137:MSE:HE1 | 2.45 | 0.46 |
| 1:J:63:GLU:O | 1:J:67:ALA:HB2 | 2.16 | 0.46 |
| 1:D:115:ARG:HD2 | 1:D:115:ARG:HA | 1.57 | 0.46 |
| 1:D:68:ASN:C | 1:D:68:ASN:ND2 | 2.67 | 0.46 |
| 1:B:273:GLY:H | 1:B:274:ARG:NH2 | 2.12 | 0.46 |
| 1:G:151:ILE:HB | 1:G:185:MSE:HE1 | 1.96 | 0.46 |
| 1:J:152:ASN:HD22 | 1:J:154:SER:H | 1.63 | 0.46 |
| 1:B:111:GLY:CA | 1:B:137:MSE:CE | 2.93 | 0.46 |
| 1:H:111:GLY:CA | 1:H:137:MSE:CE | 2.93 | 0.46 |
| 1:E:75:ARG:NH2 | 1:E:278:TYR:HA | 2.29 | 0.46 |
| 1:E:89:LEU:HA | 1:E:110:VAL:HB | 1.97 | 0.46 |
| 1:I:126:ASP:OD2 | 1:I:128:ARG:NH1 | 2.41 | 0.46 |
| 1:G:111:GLY:CA | 1:G:137:MSE:CE | 2.93 | 0.46 |
| 1:D:152:ASN:HD22 | 1:D:154:SER:H | 1.63 | 0.46 |
| 1:F:111:GLY:CA | 1:F:137:MSE:CE | 2.93 | 0.45 |
| 1:H:68:ASN:C | 1:H:68:ASN:ND2 | 2.67 | 0.45 |
| 1:E:151:ILE:HB | 1:E:185:MSE:HE1 | 1.97 | 0.45 |
| 1:B:46:ILE:O | 1:B:271:THR:HA | 2.16 | 0.45 |
| 1:J:296:HIS:C | 1:J:298:ASP:H | 2.20 | 0.45 |
| 1:I:151:ILE:HB | 1:I:185:MSE:HE1 | 1.96 | 0.45 |
| 1:G:297:THR:OG1 | 1:G:299:ILE:HG13 | 2.16 | 0.45 |
| 1:F:146:LYS:HE3 | 2:F:308:HOH:O | 2.16 | 0.45 |
| 1:I:24:MSE:HE1 | 1:I:27:GLU:OE1 | 2.15 | 0.45 |
| 1:F:111:GLY:N | 1:F:137:MSE:HE1 | 2.30 | 0.45 |
| 1:G:273:GLY:H | 1:G:274:ARG:NH2 | 2.15 | 0.45 |
| 1:G:115:ARG:HD2 | 1:G:115:ARG:HA | 1.58 | 0.45 |
| 1:F:152:ASN:HD22 | 1:F:154:SER:H | 1.63 | 0.45 |
| 1:C:151:ILE:HB | 1:C:185:MSE:HE1 | 1.97 | 0.45 |
| 1:C:76:MSE:HE3 | 1:C:277:LEU:HD21 | 1.98 | 0.45 |
| 1:I:68:ASN:ND2 | 1:I:68:ASN:C | 2.67 | 0.45 |
| 1:G:68:ASN:ND2 | 1:G:71:GLU:H | 2.15 | 0.45 |
| 1:H:296:HIS:C | 1:H:298:ASP:H | 2.19 | 0.45 |
| 1:I:284:VAL:O | 1:I:288:VAL:HG23 | 2.17 | 0.45 |
| 1:E:115:ARG:HD2 | 1:E:115:ARG:HA | 1.56 | 0.45 |
| 1:E:283:ASP:HB3 | 1:E:286:ALA:HB3 | 1.99 | 0.45 |
| 1:H:115:ARG:HA | 1:H:115:ARG:HD2 | 1.55 | 0.45 |
| 1:H:68:ASN:ND2 | 1:H:71:GLU:H | 2.15 | 0.45 |
| 1:A:33:ARG:HG3 | 1:A:33:ARG:NH1 | 2.24 | 0.45 |
| 1:G:75:ARG:HH21 | 1:G:278:TYR:HA | 1.81 | 0.45 |
| 1:I:68:ASN:ND2 | 1:I:71:GLU:H | 2.15 | 0.45 |
| 1:C:41:ASP:OD2 | 1:C:296:HIS:HD2 | 2.00 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:76:MSE:CE | 1:G:277:LEU:HD21 | 2.47 | 0.44 |
| 1:H:76:MSE:HE2 | 1:H:277:LEU:HD21 | 1.97 | 0.44 |
| 1:G:114:ASN:O | 1:G:115:ARG:CD | 2.65 | 0.44 |
| 1:F:41:ASP:OD2 | 1:F:296:HIS:CD2 | 2.61 | 0.44 |
| 1:G:16:ARG:HD2 | 2:G:489:HOH:O | 2.16 | 0.44 |
| 1:D:68:ASN:ND2 | 1:D:71:GLU:H | 2.15 | 0.44 |
| 1:B:151:ILE:HB | 1:B:185:MSE:HE1 | 1.96 | 0.44 |
| 1:J:8:PRO:HG2 | 1:J:9:GLU:OE1 | 2.18 | 0.44 |
| 1:G:110:VAL:HG22 | 1:G:144:PHE:CB | 2.48 | 0.44 |
| 1:A:98:LEU:HB3 | 1:A:104:LEU:HD11 | 1.99 | 0.44 |
| 1:D:85:VAL:HG23 | 1:D:107:LYS:NZ | 2.32 | 0.44 |
| 1:C:46:ILE:O | 1:C:271:THR:HA | 2.17 | 0.44 |
| 1:I:111:GLY:N | 1:I:137:MSE:HE1 | 2.33 | 0.44 |
| 1:A:68:ASN:ND2 | 1:A:71:GLU:H | 2.16 | 0.44 |
| 1:J:85:VAL:HG23 | 1:J:107:LYS:NZ | 2.33 | 0.44 |
| 1:B:40:GLU:N | 1:B:40:GLU:OE2 | 2.46 | 0.44 |
| 1:C:103:LEU:HD22 | 2:C:522:HOH:O | 2.16 | 0.44 |
| 1:D:247:GLY:HA3 | 2:D:361:HOH:O | 2.18 | 0.44 |
| 1:B:114:ASN:HD22 | 1:B:114:ASN:N | 1.97 | 0.44 |
| 1:A:63:GLU:HB3 | 2:H:637:HOH:O | 2.16 | 0.44 |
| 1:A:246:GLU:HG2 | 1:A:247:GLY:N | 2.33 | 0.44 |
| 1:B:159:ALA:HB3 | 1:B:160:PRO:CD | 2.48 | 0.44 |
| 1:F:40:GLU:N | 1:F:40:GLU:OE2 | 2.45 | 0.44 |
| 1:J:159:ALA:HB3 | 1:J:160:PRO:CD | 2.48 | 0.43 |
| 1:A:61:ASP:OD1 | 1:A:61:ASP:C | 2.56 | 0.43 |
| 1:C:115:ARG:HD2 | 1:C:115:ARG:HA | 1.57 | 0.43 |
| 1:G:246:GLU:HG2 | 1:G:247:GLY:N | 2.33 | 0.43 |
| 1:A:159:ALA:HB3 | 1:A:160:PRO:CD | 2.49 | 0.43 |
| 1:C:44:LEU:O | 1:C:269:GLY:HA3 | 2.17 | 0.43 |
| 1:B:44:LEU:O | 1:B:269:GLY:HA3 | 2.18 | 0.43 |
| 1:H:61:ASP:OD1 | 1:H:61:ASP:C | 2.57 | 0.43 |
| 1:C:12:GLU:OE1 | 1:C:12:GLU:HA | 2.18 | 0.43 |
| 1:F:75:ARG:NH2 | 1:F:278:TYR:HA | 2.33 | 0.43 |
| 1:D:65:ALA:O | 1:D:66:MSE:HB2 | 2.18 | 0.43 |
| 1:G:68:ASN:C | 1:G:68:ASN:ND2 | 2.67 | 0.43 |
| 1:G:98:LEU:HB3 | 1:G:104:LEU:CD1 | 2.49 | 0.43 |
| 1:J:110:VAL:HG22 | 1:J:144:PHE:CB | 2.48 | 0.43 |
| 1:E:274:ARG:O | 1:E:277:LEU:O | 2.37 | 0.43 |
| 1:B:68:ASN:ND2 | 1:B:71:GLU:H | 2.15 | 0.43 |
| 1:A:151:ILE:HB | 1:A:185:MSE:HE1 | 1.97 | 0.43 |
| 1:B:114:ASN:O | 1:B:115:ARG:HD2 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:114:ASN:O | 1:D:115:ARG:HD2 | 2.17 | 0.43 |
| 1:F:68:ASN:ND2 | 1:F:71:GLU:H | 2.16 | 0.43 |
| 1:I:85:VAL:HG23 | 1:I:107:LYS:NZ | 2.34 | 0.43 |
| 1:C:89:LEU:HD11 | 1:C:146:LYS:HG2 | 2.00 | 0.43 |
| 1:G:46:ILE:O | 1:G:271:THR:HA | 2.19 | 0.43 |
| 1:J:68:ASN:ND2 | 1:J:70:TYR:N | 2.67 | 0.43 |
| 1:C:65:ALA:O | 1:C:66:MSE:HB2 | 2.19 | 0.43 |
| 1:G:40:GLU:N | 1:G:40:GLU:OE2 | 2.46 | 0.43 |
| 1:I:277:LEU:O | 1:I:278:TYR:HB2 | 2.17 | 0.43 |
| 1:F:184:PHE:O | 1:F:185:MSE:HE2 | 2.19 | 0.43 |
| 1:G:65:ALA:O | 1:G:66:MSE:HB2 | 2.19 | 0.43 |
| 1:I:65:ALA:O | 1:I:66:MSE:HB2 | 2.19 | 0.43 |
| 1:C:214:ASN:HD22 | 1:C:215:ASP:N | 2.17 | 0.43 |
| 1:C:158:THR:HB | 1:D:123:PHE:CE2 | 2.54 | 0.43 |
| 1:I:159:ALA:HB3 | 1:I:160:PRO:CD | 2.49 | 0.43 |
| 1:B:61:ASP:OD1 | 1:B:61:ASP:C | 2.57 | 0.43 |
| 1:D:277:LEU:O | 1:D:278:TYR:CB | 2.62 | 0.43 |
| 1:B:246:GLU:HG2 | 1:B:247:GLY:N | 2.34 | 0.43 |
| 1:A:46:ILE:HD13 | 1:A:110:VAL:CG2 | 2.49 | 0.43 |
| 1:E:61:ASP:C | 1:E:61:ASP:OD1 | 2.57 | 0.43 |
| 1:F:61:ASP:C | 1:F:61:ASP:OD1 | 2.57 | 0.43 |
| 1:H:40:GLU:N | 1:H:40:GLU:OE2 | 2.46 | 0.43 |
| 1:H:65:ALA:O | 1:H:66:MSE:HB2 | 2.19 | 0.43 |
| 1:C:125:MSE:CE | 1:C:152:ASN:HB2 | 2.44 | 0.43 |
| 1:E:65:ALA:O | 1:E:66:MSE:HB2 | 2.19 | 0.43 |
| 1:F:206:VAL:CG1 | 1:F:236:THR:HG23 | 2.49 | 0.43 |
| 1:F:236:THR:HG22 | 2:G:520:HOH:O | 2.17 | 0.43 |
| 1:C:61:ASP:C | 1:C:61:ASP:OD1 | 2.57 | 0.43 |
| 1:J:184:PHE:O | 1:J:185:MSE:HE2 | 2.19 | 0.43 |
| 1:J:223:LEU:CD1 | 1:J:233:MSE:HE1 | 2.43 | 0.43 |
| 1:E:214:ASN:HD22 | 1:E:215:ASP:N | 2.17 | 0.43 |
| 1:E:159:ALA:HB3 | 1:E:160:PRO:CD | 2.49 | 0.43 |
| 1:F:159:ALA:HB3 | 1:F:160:PRO:CD | 2.49 | 0.43 |
| 1:D:44:LEU:O | 1:D:269:GLY:HA3 | 2.19 | 0.43 |
| 1:C:68:ASN:ND2 | 1:C:71:GLU:H | 2.16 | 0.43 |
| 1:E:68:ASN:ND2 | 1:E:71:GLU:H | 2.16 | 0.43 |
| 1:C:246:GLU:HG2 | 1:C:247:GLY:N | 2.33 | 0.43 |
| 1:C:214:ASN:C | 1:C:214:ASN:ND2 | 2.73 | 0.43 |
| 1:A:40:GLU:OE2 | 1:A:40:GLU:N | 2.45 | 0.43 |
| 1:J:274:ARG:O | 1:J:277:LEU:O | 2.37 | 0.42 |
| 1:C:115:ARG:HB2 | 2:C:313:HOH:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:86:ASP:OD2 | 1:H:296:HIS:HE1 | 2.02 | 0.42 |
| 1:C:159:ALA:HB3 | 1:C:160:PRO:CD | 2.49 | 0.42 |
| 1:E:281:ASP:OD2 | 1:E:281:ASP:C | 2.58 | 0.42 |
| 1:E:111:GLY:N | 1:E:137:MSE:HE1 | 2.34 | 0.42 |
| 1:H:184:PHE:O | 1:H:185:MSE:HE2 | 2.19 | 0.42 |
| 1:A:65:ALA:O | 1:A:66:MSE:HB2 | 2.19 | 0.42 |
| 1:J:214:ASN:HD22 | 1:J:215:ASP:N | 2.17 | 0.42 |
| 1:I:214:ASN:HD22 | 1:I:215:ASP:N | 2.17 | 0.42 |
| 1:F:214:ASN:HD22 | 1:F:215:ASP:N | 2.16 | 0.42 |
| 1:I:44:LEU:O | 1:I:269:GLY:HA3 | 2.19 | 0.42 |
| 1:D:61:ASP:OD1 | 1:D:61:ASP:C | 2.57 | 0.42 |
| 1:G:194:VAL:O | 1:G:194:VAL:HG23 | 2.20 | 0.42 |
| 1:G:272:VAL:HA | 2:G:549:HOH:O | 2.19 | 0.42 |
| 1:C:184:PHE:O | 1:C:185:MSE:HE2 | 2.19 | 0.42 |
| 1:J:45:PHE:HD2 | 1:J:85:VAL:HA | 1.82 | 0.42 |
| 1:H:214:ASN:HD22 | 1:H:215:ASP:N | 2.18 | 0.42 |
| 1:H:159:ALA:HB3 | 1:H:160:PRO:CD | 2.49 | 0.42 |
| 1:F:54:ARG:HH21 | 1:F:150:ARG:HH12 | 1.66 | 0.42 |
| 1:C:40:GLU:OE2 | 1:C:40:GLU:N | 2.46 | 0.42 |
| 1:B:76:MSE:HE3 | 1:B:277:LEU:HD21 | 2.00 | 0.42 |
| 1:F:125:MSE:CE | 1:F:152:ASN:HB2 | 2.45 | 0.42 |
| 1:H:214:ASN:ND2 | 1:H:214:ASN:C | 2.73 | 0.42 |
| 1:A:214:ASN:HD22 | 1:A:215:ASP:N | 2.17 | 0.42 |
| 1:J:28:ARG:HD3 | 1:J:100:ALA:HA | 2.01 | 0.42 |
| 1:D:159:ALA:HB3 | 1:D:160:PRO:CD | 2.50 | 0.42 |
| 1:E:262:LEU:HD12 | 1:E:262:LEU:HA | 1.93 | 0.42 |
| 1:I:61:ASP:OD1 | 1:I:61:ASP:C | 2.57 | 0.42 |
| 1:C:114:ASN:O | 1:C:115:ARG:HD2 | 2.20 | 0.42 |
| 1:D:89:LEU:HD12 | 1:D:90:GLY:N | 2.35 | 0.42 |
| 1:C:33:ARG:HH11 | 1:C:33:ARG:CG | 2.29 | 0.42 |
| 1:H:246:GLU:HG2 | 1:H:247:GLY:N | 2.33 | 0.42 |
| 1:E:214:ASN:ND2 | 1:E:214:ASN:C | 2.73 | 0.42 |
| 1:G:214:ASN:HD22 | 1:G:215:ASP:N | 2.17 | 0.42 |
| 1:E:206:VAL:CG1 | 1:E:236:THR:HG23 | 2.50 | 0.42 |
| 1:D:194:VAL:HG23 | 1:D:194:VAL:O | 2.20 | 0.42 |
| 1:G:61:ASP:OD1 | 1:G:61:ASP:C | 2.57 | 0.42 |
| 1:B:206:VAL:CG1 | 1:B:236:THR:HG23 | 2.50 | 0.42 |
| 1:H:89:LEU:HD12 | 1:H:90:GLY:N | 2.35 | 0.42 |
| 1:I:184:PHE:O | 1:I:185:MSE:HE2 | 2.20 | 0.42 |
| 1:D:115:ARG:HB2 | 2:D:356:HOH:O | 2.19 | 0.42 |
| 1:J:45:PHE:CD2 | 1:J:85:VAL:HA | 2.55 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:46:ILE:O | 1:E:271:THR:HA | 2.20 | 0.42 |
| 1:D:214:ASN:HD22 | 1:D:215:ASP:N | 2.17 | 0.42 |
| 1:J:206:VAL:CG1 | 1:J:236:THR:HG23 | 2.50 | 0.42 |
| 1:J:57:LEU:N | 1:J:57:LEU:HD22 | 2.35 | 0.42 |
| 1:D:46:ILE:O | 1:D:271:THR:HA | 2.19 | 0.42 |
| 1:D:246:GLU:HG2 | 1:D:247:GLY:N | 2.33 | 0.42 |
| 1:A:32:ARG:HD2 | 1:A:104:LEU:HB3 | 2.01 | 0.42 |
| 1:F:44:LEU:O | 1:F:269:GLY:HA3 | 2.19 | 0.42 |
| 1:I:194:VAL:O | 1:I:194:VAL:HG23 | 2.20 | 0.42 |
| 1:C:194:VAL:HG23 | 1:C:194:VAL:O | 2.20 | 0.42 |
| 1:A:92:PRO:HB2 | 2:H:468:HOH:O | 2.19 | 0.42 |
| 1:A:112:SER:HA | 1:A:146:LYS:HG3 | 2.01 | 0.42 |
| 1:J:47:VAL:HG11 | 1:J:76:MSE:HE1 | 2.02 | 0.42 |
| 1:B:65:ALA:O | 1:B:66:MSE:HB2 | 2.19 | 0.42 |
| 1:D:223:LEU:CD1 | 1:D:233:MSE:HE1 | 2.43 | 0.42 |
| 1:F:296:HIS:C | 1:F:298:ASP:H | 2.23 | 0.42 |
| 1:C:258:TRP:O | 1:C:262:LEU:HB2 | 2.20 | 0.42 |
| 1:C:10:SER:O | 1:C:13:ALA:HB3 | 2.20 | 0.42 |
| 1:J:194:VAL:HG23 | 1:J:194:VAL:O | 2.20 | 0.42 |
| 1:E:40:GLU:OE2 | 1:E:40:GLU:N | 2.46 | 0.42 |
| 1:F:91:THR:HG23 | 1:F:94:ILE:HG12 | 2.01 | 0.42 |
| 1:A:223:LEU:CD1 | 1:A:233:MSE:HE1 | 2.43 | 0.42 |
| 1:G:184:PHE:O | 1:G:185:MSE:HE2 | 2.20 | 0.42 |
| 1:J:258:TRP:O | 1:J:262:LEU:HB2 | 2.20 | 0.42 |
| 1:I:206:VAL:CG1 | 1:I:236:THR:HG23 | 2.50 | 0.42 |
| 1:B:114:ASN:ND2 | 1:B:114:ASN:N | 2.68 | 0.41 |
| 1:F:66:MSE:HG2 | 1:F:278:TYR:CE2 | 2.55 | 0.41 |
| 1:E:246:GLU:HG2 | 1:E:247:GLY:N | 2.33 | 0.41 |
| 1:J:214:ASN:ND2 | 1:J:214:ASN:C | 2.73 | 0.41 |
| 1:G:159:ALA:HB3 | 1:G:160:PRO:CD | 2.50 | 0.41 |
| 1:I:12:GLU:HG3 | 1:I:16:ARG:NH1 | 2.21 | 0.41 |
| 1:J:125:MSE:CE | 1:J:152:ASN:HB2 | 2.44 | 0.41 |
| 1:E:89:LEU:HD12 | 1:E:90:GLY:N | 2.36 | 0.41 |
| 1:E:258:TRP:O | 1:E:262:LEU:HB2 | 2.20 | 0.41 |
| 1:G:206:VAL:CG1 | 1:G:236:THR:HG23 | 2.50 | 0.41 |
| 1:H:194:VAL:O | 1:H:194:VAL:HG23 | 2.19 | 0.41 |
| 1:B:194:VAL:O | 1:B:194:VAL:HG23 | 2.20 | 0.41 |
| 1:D:184:PHE:O | 1:D:185:MSE:HE2 | 2.20 | 0.41 |
| 1:H:125:MSE:CE | 1:H:152:ASN:HB2 | 2.44 | 0.41 |
| 1:H:91:THR:HG23 | 1:H:94:ILE:HG12 | 2.03 | 0.41 |
| 1:H:206:VAL:CG1 | 1:H:236:THR:HG23 | 2.50 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:206:VAL:CG1 | 1:C:236:THR:HG23 | 2.50 | 0.41 |
| 1:I:3:PRO:HA | 2:I:486:HOH:O | 2.20 | 0.41 |
| 1:E:44:LEU:O | 1:E:269:GLY:HA3 | 2.20 | 0.41 |
| 1:D:296:HIS:C | 1:D:298:ASP:H | 2.21 | 0.41 |
| 1:I:152:ASN:ND2 | 1:I:154:SER:H | 2.18 | 0.41 |
| 1:A:46:ILE:O | 1:A:271:THR:HA | 2.20 | 0.41 |
| 1:F:214:ASN:ND2 | 1:F:214:ASN:C | 2.72 | 0.41 |
| 1:D:214:ASN:C | 1:D:214:ASN:ND2 | 2.73 | 0.41 |
| 1:B:89:LEU:HD11 | 1:B:146:LYS:HG2 | 2.02 | 0.41 |
| 1:D:40:GLU:OE2 | 1:D:40:GLU:N | 2.45 | 0.41 |
| 1:A:89:LEU:HD12 | 1:A:90:GLY:N | 2.35 | 0.41 |
| 1:E:184:PHE:O | 1:E:185:MSE:HE2 | 2.20 | 0.41 |
| 2:F:548:HOH:O | 1:G:115:ARG:HB2 | 2.20 | 0.41 |
| 1:E:125:MSE:CE | 1:E:152:ASN:HB2 | 2.43 | 0.41 |
| 1:H:33:ARG:CG | 1:H:33:ARG:NH1 | 2.83 | 0.41 |
| 1:B:214:ASN:HD22 | 1:B:215:ASP:N | 2.18 | 0.41 |
| 1:A:98:LEU:HB3 | 1:A:104:LEU:CD1 | 2.51 | 0.41 |
| 1:F:89:LEU:HD12 | 1:F:90:GLY:N | 2.35 | 0.41 |
| 1:H:66:MSE:HG2 | 1:H:278:TYR:CE2 | 2.56 | 0.41 |
| 1:A:184:PHE:O | 1:A:185:MSE:HE2 | 2.20 | 0.41 |
| 1:G:223:LEU:CD1 | 1:G:233:MSE:HE1 | 2.43 | 0.41 |
| 1:F:65:ALA:O | 1:F:66:MSE:HB2 | 2.19 | 0.41 |
| 1:G:214:ASN:ND2 | 1:G:214:ASN:C | 2.73 | 0.41 |
| 1:C:297:THR:OG1 | 1:C:299:ILE:HG13 | 2.20 | 0.41 |
| 1:J:37:LEU:HD13 | 1:J:38:LEU:HG | 2.02 | 0.41 |
| 1:A:194:VAL:HG23 | 1:A:194:VAL:O | 2.21 | 0.41 |
| 1:C:47:VAL:CB | 1:C:76:MSE:HE1 | 2.50 | 0.41 |
| 1:C:89:LEU:HD12 | 1:C:90:GLY:N | 2.35 | 0.41 |
| 1:I:258:TRP:O | 1:I:262:LEU:HB2 | 2.20 | 0.41 |
| 1:F:194:VAL:O | 1:F:194:VAL:HG23 | 2.21 | 0.41 |
| 1:J:63:GLU:CG | 1:J:64:THR:N | 2.80 | 0.41 |
| 1:G:152:ASN:ND2 | 1:G:154:SER:H | 2.19 | 0.41 |
| 1:D:114:ASN:O | 1:D:115:ARG:CD | 2.69 | 0.41 |
| 1:B:125:MSE:CE | 1:B:152:ASN:HB2 | 2.44 | 0.41 |
| 1:B:214:ASN:C | 1:B:214:ASN:ND2 | 2.73 | 0.41 |
| 1:E:223:LEU:CD1 | 1:E:233:MSE:HE1 | 2.43 | 0.41 |
| 1:J:229:MSE:O | 1:J:233:MSE:HG2 | 2.21 | 0.41 |
| 1:B:54:ARG:NH2 | 1:B:150:ARG:HH12 | 2.18 | 0.41 |
| 1:A:214:ASN:ND2 | 1:A:214:ASN:C | 2.73 | 0.41 |
| 1:G:110:VAL:HG13 | 1:G:144:PHE:HB3 | 2.03 | 0.41 |
| 1:F:158:THR:HB | 1:G:123:PHE:CE2 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:46:ILE:O | 1:F:271:THR:HA | 2.20 | 0.41 |
| 1:B:258:TRP:O | 1:B:262:LEU:HB2 | 2.20 | 0.41 |
| 1:D:206:VAL:CG1 | 1:D:236:THR:HG23 | 2.50 | 0.41 |
| 1:A:206:VAL:CG1 | 1:A:236:THR:HG23 | 2.50 | 0.41 |
| 1:G:89:LEU:HD12 | 1:G:90:GLY:N | 2.36 | 0.41 |
| 1:B:220:TRP:CE3 | 1:B:239:PRO:HB2 | 2.56 | 0.41 |
| 1:E:119:ARG:HD3 | 2:E:324:HOH:O | 2.21 | 0.41 |
| 1:H:47:VAL:CB | 1:H:76:MSE:HE1 | 2.51 | 0.41 |
| 1:D:125:MSE:CE | 1:D:152:ASN:HB2 | 2.44 | 0.41 |
| 1:I:214:ASN:ND2 | 1:I:214:ASN:C | 2.74 | 0.41 |
| 1:A:258:TRP:O | 1:A:262:LEU:HB2 | 2.21 | 0.41 |
| 1:I:232:VAL:O | 1:I:235:SER:HB2 | 2.21 | 0.41 |
| 1:A:47:VAL:CB | 1:A:76:MSE:HE1 | 2.51 | 0.40 |
| 1:D:47:VAL:CB | 1:D:76:MSE:HE1 | 2.51 | 0.40 |
| 1:B:184:PHE:O | 1:B:185:MSE:HE2 | 2.20 | 0.40 |
| 1:F:152:ASN:ND2 | 1:F:154:SER:H | 2.19 | 0.40 |
| 1:F:68:ASN:ND2 | 1:F:68:ASN:C | 2.67 | 0.40 |
| 1:I:33:ARG:NH1 | 1:I:33:ARG:CG | 2.84 | 0.40 |
| 1:I:89:LEU:HD11 | 1:I:146:LYS:HG2 | 2.03 | 0.40 |
| 1:G:258:TRP:O | 1:G:262:LEU:HB2 | 2.20 | 0.40 |
| 1:I:12:GLU:OE1 | 1:I:16:ARG:NH2 | 2.55 | 0.40 |
| 1:B:47:VAL:CB | 1:B:76:MSE:HE1 | 2.51 | 0.40 |
| 1:J:65:ALA:C | 1:J:67:ALA:N | 2.74 | 0.40 |
| 1:H:114:ASN:ND2 | 1:H:147:THR:HG23 | 2.37 | 0.40 |
| 1:J:105:ASP:O | 1:J:107:LYS:HG2 | 2.20 | 0.40 |
| 1:G:101:LEU:HA | 1:G:101:LEU:HD12 | 1.91 | 0.40 |
| 1:H:220:TRP:CE3 | 1:H:239:PRO:HB2 | 2.57 | 0.40 |
| 1:C:220:TRP:CE3 | 1:C:239:PRO:HB2 | 2.56 | 0.40 |
| 1:A:220:TRP:CE3 | 1:A:239:PRO:HB2 | 2.56 | 0.40 |
| 1:B:115:ARG:HD2 | 1:B:115:ARG:HA | 1.57 | 0.40 |
| 1:G:33:ARG:CG | 1:G:33:ARG:HH11 | 2.29 | 0.40 |
| 1:G:98:LEU:HB3 | 1:G:104:LEU:HD11 | 2.03 | 0.40 |
| 1:C:110:VAL:HG13 | 1:C:144:PHE:HB3 | 2.02 | 0.40 |
| 1:E:194:VAL:O | 1:E:194:VAL:HG23 | 2.20 | 0.40 |
| 1:A:83:PRO:HG2 | 2:A:319:HOH:O | 2.22 | 0.40 |
| 1:A:75:ARG:NH2 | 1:A:278:TYR:HA | 2.37 | 0.40 |
| 1:I:85:VAL:HG23 | 1:I:107:LYS:HZ2 | 1.86 | 0.40 |
| 1:J:129:TYR:OH | 1:J:147:THR:CG2 | 2.70 | 0.40 |
| 1:I:296:HIS:C | 1:I:298:ASP:N | 2.74 | 0.40 |
| 1:I:281:ASP:O | 1:I:283:ASP:N | 2.54 | 0.40 |
| 1:B:47:VAL:HB | 1:B:76:MSE:HE1 | 2.03 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:229:MSE:O | 1:C:233:MSE:HG2 | 2.22 | 0.40 |
| 1:J:246:GLU:HG2 | 1:J:247:GLY:N | 2.33 | 0.40 |
| 1:I:103:LEU:C | 1:I:104:LEU:HD12 | 2.42 | 0.40 |
| 1:B:89:LEU:HD12 | 1:B:90:GLY:N | 2.36 | 0.40 |
| 1:E:95:ILE:HD12 | 1:E:109:VAL:HG13 | 2.03 | 0.40 |
| 1:H:258:TRP:O | 1:H:262:LEU:HB2 | 2.21 | 0.40 |
| 1:E:220:TRP:CE3 | 1:E:239:PRO:HB2 | 2.57 | 0.40 |
| 1:D:258:TRP:O | 1:D:262:LEU:HB2 | 2.21 | 0.40 |
| 1:J:115:ARG:HD2 | 1:J:115:ARG:HA | 1.56 | 0.40 |
| 1:J:94:ILE:HD13 | 1:J:94:ILE:HA | 1.98 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 291/307 (95%) | 266 (91%) | 19 (6%) | 6 (2%) | 9 | 14 |
| 1 | B | 291/307 (95%) | 269 (92%) | 17 (6%) | 5 (2%) | 11 | 19 |
| 1 | C | 291/307 (95%) | 269 (92%) | 17 (6%) | 5 (2%) | 11 | 19 |
| 1 | D | 291/307 (95%) | 266 (91%) | 18 (6%) | 7 (2%) | 7 | 11 |
| 1 | E | 291/307 (95%) | 267 (92%) | 19 (6%) | 5 (2%) | 11 | 19 |
| 1 | F | 291/307 (95%) | 266 (91%) | 19 (6%) | 6 (2%) | 9 | 14 |
| 1 | G | 291/307 (95%) | 268 (92%) | 18 (6%) | 5 (2%) | 11 | 19 |
| 1 | H | 291/307 (95%) | 266 (91%) | 19 (6%) | 6 (2%) | 9 | 14 |
| 1 | I | 291/307 (95%) | 268 (92%) | 16 (6%) | 7 (2%) | 7 | 11 |
| 1 | J | 291/307 (95%) | 265 (91%) | 19 (6%) | 7 (2%) | 7 | 11 |
| All | All | 2910/3070 (95%) | 2670 (92%) | 181 (6%) | 59 (2%) | 9 | 15 |

All (59) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 64 | THR |
| 1 | B | 64 | THR |
| 1 | C | 64 | THR |
| 1 | D | 64 | THR |
| 1 | D | 298 | ASP |
| 1 | E | 64 | THR |
| 1 | F | 64 | THR |
| 1 | G | 64 | THR |
| 1 | H | 64 | THR |
| 1 | I | 64 | THR |
| 1 | J | 62 | ASN |
| 1 | A | 62 | ASN |
| 1 | A | 63 | GLU |
| 1 | A | 245 | GLY |
| 1 | B | 62 | ASN |
| 1 | B | 63 | GLU |
| 1 | B | 245 | GLY |
| 1 | C | 62 | ASN |
| 1 | C | 63 | GLU |
| 1 | C | 245 | GLY |
| 1 | D | 62 | ASN |
| 1 | D | 63 | GLU |
| 1 | D | 245 | GLY |
| 1 | E | 62 | ASN |
| 1 | E | 63 | GLU |
| 1 | E | 245 | GLY |
| 1 | F | 62 | ASN |
| 1 | F | 63 | GLU |
| 1 | F | 245 | GLY |
| 1 | G | 62 | ASN |
| 1 | G | 63 | GLU |
| 1 | G | 245 | GLY |
| 1 | H | 62 | ASN |
| 1 | H | 63 | GLU |
| 1 | H | 245 | GLY |
| 1 | I | 62 | ASN |
| 1 | I | 63 | GLU |
| 1 | I | 245 | GLY |
| 1 | I | 282 | GLY |
| 1 | I | 297 | THR |
| 1 | J | 245 | GLY |
| 1 | A | 297 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 297 | THR |
| 1 | F | 297 | THR |
| 1 | J | 59 | VAL |
| 1 | J | 297 | THR |
| 1 | A | 60 | GLY |
| 1 | B | 60 | GLY |
| 1 | C | 60 | GLY |
| 1 | D | 60 | GLY |
| 1 | E | 60 | GLY |
| 1 | F | 60 | GLY |
| 1 | G | 60 | GLY |
| 1 | H | 60 | GLY |
| 1 | H | 297 | THR |
| 1 | I | 60 | GLY |
| 1 | J | 63 | GLU |
| 1 | J | 65 | ALA |
| 1 | J | 60 | GLY |

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 | 230/229 (100%) | 207 (90%) | 23 (10%) | 9 | 18 |
| 1 | B | 230/229 (100%) | 206 (90%) | 24 (10%) | 9 | 16 |
| 1 | C | 230/229 (100%) | 205 (89%) | 25 (11%) | 8 | 15 |
| 1 | D | 230/229 (100%) | 206 (90%) | 24 (10%) | 9 | 16 |
| 1 | E | 230/229 (100%) | 206 (90%) | 24 (10%) | 9 | 16 |
| 1 | F | 230/229 (100%) | 206 (90%) | 24 (10%) | 9 | 16 |
| 1 | G | 230/229 (100%) | 207 (90%) | 23 (10%) | 9 | 18 |
| 1 | H | 230/229 (100%) | 206 (90%) | 24 (10%) | 9 | 16 |
| 1 | I | 230/229 (100%) | 208 (90%) | 22 (10%) | 10 | 19 |
| 1 | J | 230/229 (100%) | 208 (90%) | 22 (10%) | 10 | 19 |
| All | All | 2300/2290 (100%) | 2065 (90%) | 235 (10%) | 9 | 17 |

All (235) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 29 | PHE |
| 1 | A | 37 | LEU |
| 1 | A | 61 | ASP |
| 1 | A | 68 | ASN |
| 1 | A | 69 | ARG |
| 1 | A | 72 | LEU |
| 1 | A | 76 | MSE |
| 1 | A | 91 | THR |
| 1 | A | 101 | LEU |
| 1 | A | 114 | ASN |
| 1 | A | 115 | ARG |
| 1 | A | 140 | ARG |
| 1 | A | 144 | PHE |
| 1 | A | 146 | LYS |
| 1 | A | 148 | LEU |
| 1 | A | 152 | ASN |
| 1 | A | 214 | ASN |
| 1 | A | 216 | SER |
| 1 | A | 219 | THR |
| 1 | A | 262 | LEU |
| 1 | A | 264 | LEU |
| 1 | A | 274 | ARG |
| 1 | A | 299 | ILE |
| 1 | B | 29 | PHE |
| 1 | B | 37 | LEU |
| 1 | B | 61 | ASP |
| 1 | B | 68 | ASN |
| 1 | B | 69 | ARG |
| 1 | B | 72 | LEU |
| 1 | B | 76 | MSE |
| 1 | B | 91 | THR |
| 1 | B | 101 | LEU |
| 1 | B | 104 | LEU |
| 1 | B | 114 | ASN |
| 1 | B | 115 | ARG |
| 1 | B | 140 | ARG |
| 1 | B | 144 | PHE |
| 1 | B | 146 | LYS |
| 1 | B | 148 | LEU |
| 1 | B | 152 | ASN |
| 1 | B | 214 | ASN |
| 1 | B | 216 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 219 | THR |
| 1 | B | 262 | LEU |
| 1 | B | 264 | LEU |
| 1 | B | 274 | ARG |
| 1 | B | 294 | LEU |
| 1 | C | 29 | PHE |
| 1 | C | 37 | LEU |
| 1 | C | 61 | ASP |
| 1 | C | 68 | ASN |
| 1 | C | 69 | ARG |
| 1 | C | 72 | LEU |
| 1 | C | 76 | MSE |
| 1 | C | 91 | THR |
| 1 | C | 101 | LEU |
| 1 | C | 104 | LEU |
| 1 | C | 114 | ASN |
| 1 | C | 115 | ARG |
| 1 | C | 140 | ARG |
| 1 | C | 144 | PHE |
| 1 | C | 146 | LYS |
| 1 | C | 148 | LEU |
| 1 | C | 152 | ASN |
| 1 | C | 214 | ASN |
| 1 | C | 216 | SER |
| 1 | C | 219 | THR |
| 1 | C | 262 | LEU |
| 1 | C | 264 | LEU |
| 1 | C | 274 | ARG |
| 1 | C | 280 | GLN |
| 1 | C | 294 | LEU |
| 1 | D | 29 | PHE |
| 1 | D | 37 | LEU |
| 1 | D | 61 | ASP |
| 1 | D | 68 | ASN |
| 1 | D | 69 | ARG |
| 1 | D | 72 | LEU |
| 1 | D | 76 | MSE |
| 1 | D | 91 | THR |
| 1 | D | 101 | LEU |
| 1 | D | 104 | LEU |
| 1 | D | 114 | ASN |
| 1 | D | 115 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 140 | ARG |
| 1 | D | 144 | PHE |
| 1 | D | 146 | LYS |
| 1 | D | 148 | LEU |
| 1 | D | 152 | ASN |
| 1 | D | 214 | ASN |
| 1 | D | 216 | SER |
| 1 | D | 219 | THR |
| 1 | D | 262 | LEU |
| 1 | D | 264 | LEU |
| 1 | D | 274 | ARG |
| 1 | D | 280 | GLN |
| 1 | E | 29 | PHE |
| 1 | E | 37 | LEU |
| 1 | E | 61 | ASP |
| 1 | E | 68 | ASN |
| 1 | E | 69 | ARG |
| 1 | E | 72 | LEU |
| 1 | E | 76 | MSE |
| 1 | E | 91 | THR |
| 1 | E | 101 | LEU |
| 1 | E | 104 | LEU |
| 1 | E | 114 | ASN |
| 1 | E | 115 | ARG |
| 1 | E | 140 | ARG |
| 1 | E | 144 | PHE |
| 1 | E | 146 | LYS |
| 1 | E | 148 | LEU |
| 1 | E | 152 | ASN |
| 1 | E | 214 | ASN |
| 1 | E | 216 | SER |
| 1 | E | 219 | THR |
| 1 | E | 262 | LEU |
| 1 | E | 264 | LEU |
| 1 | E | 274 | ARG |
| 1 | E | 299 | ILE |
| 1 | F | 29 | PHE |
| 1 | F | 37 | LEU |
| 1 | F | 61 | ASP |
| 1 | F | 68 | ASN |
| 1 | F | 69 | ARG |
| 1 | F | 72 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 76 | MSE |
| 1 | F | 91 | THR |
| 1 | F | 101 | LEU |
| 1 | F | 104 | LEU |
| 1 | F | 114 | ASN |
| 1 | F | 115 | ARG |
| 1 | F | 140 | ARG |
| 1 | F | 144 | PHE |
| 1 | F | 146 | LYS |
| 1 | F | 148 | LEU |
| 1 | F | 152 | ASN |
| 1 | F | 214 | ASN |
| 1 | F | 216 | SER |
| 1 | F | 219 | THR |
| 1 | F | 262 | LEU |
| 1 | F | 264 | LEU |
| 1 | F | 274 | ARG |
| 1 | F | 283 | ASP |
| 1 | G | 29 | PHE |
| 1 | G | 37 | LEU |
| 1 | G | 61 | ASP |
| 1 | G | 68 | ASN |
| 1 | G | 69 | ARG |
| 1 | G | 72 | LEU |
| 1 | G | 76 | MSE |
| 1 | G | 91 | THR |
| 1 | G | 101 | LEU |
| 1 | G | 114 | ASN |
| 1 | G | 115 | ARG |
| 1 | G | 140 | ARG |
| 1 | G | 144 | PHE |
| 1 | G | 146 | LYS |
| 1 | G | 148 | LEU |
| 1 | G | 152 | ASN |
| 1 | G | 214 | ASN |
| 1 | G | 216 | SER |
| 1 | G | 219 | THR |
| 1 | G | 262 | LEU |
| 1 | G | 264 | LEU |
| 1 | G | 274 | ARG |
| 1 | G | 276 | LEU |
| 1 | H | 9 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 29 | PHE |
| 1 | H | 37 | LEU |
| 1 | H | 61 | ASP |
| 1 | H | 68 | ASN |
| 1 | H | 69 | ARG |
| 1 | H | 72 | LEU |
| 1 | H | 76 | MSE |
| 1 | H | 91 | THR |
| 1 | H | 101 | LEU |
| 1 | H | 104 | LEU |
| 1 | H | 114 | ASN |
| 1 | H | 115 | ARG |
| 1 | H | 140 | ARG |
| 1 | H | 144 | PHE |
| 1 | H | 146 | LYS |
| 1 | H | 148 | LEU |
| 1 | H | 152 | ASN |
| 1 | H | 214 | ASN |
| 1 | H | 216 | SER |
| 1 | H | 219 | THR |
| 1 | H | 262 | LEU |
| 1 | H | 264 | LEU |
| 1 | H | 274 | ARG |
| 1 | I | 29 | PHE |
| 1 | I | 37 | LEU |
| 1 | I | 61 | ASP |
| 1 | I | 68 | ASN |
| 1 | I | 69 | ARG |
| 1 | I | 72 | LEU |
| 1 | I | 76 | MSE |
| 1 | I | 91 | THR |
| 1 | I | 114 | ASN |
| 1 | I | 115 | ARG |
| 1 | I | 140 | ARG |
| 1 | I | 144 | PHE |
| 1 | I | 146 | LYS |
| 1 | I | 148 | LEU |
| 1 | I | 152 | ASN |
| 1 | I | 214 | ASN |
| 1 | I | 216 | SER |
| 1 | I | 219 | THR |
| 1 | I | 262 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 264 | LEU |
| 1 | I | 274 | ARG |
| 1 | I | 281 | ASP |
| 1 | J | 29 | PHE |
| 1 | J | 33 | ARG |
| 1 | J | 37 | LEU |
| 1 | J | 54 | ARG |
| 1 | J | 57 | LEU |
| 1 | J | 68 | ASN |
| 1 | J | 74 | GLU |
| 1 | J | 76 | MSE |
| 1 | J | 91 | THR |
| 1 | J | 114 | ASN |
| 1 | J | 115 | ARG |
| 1 | J | 140 | ARG |
| 1 | J | 144 | PHE |
| 1 | J | 146 | LYS |
| 1 | J | 148 | LEU |
| 1 | J | 152 | ASN |
| 1 | J | 214 | ASN |
| 1 | J | 216 | SER |
| 1 | J | 219 | THR |
| 1 | J | 262 | LEU |
| 1 | J | 264 | LEU |
| 1 | J | 274 | ARG |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 31 | GLN |
| 1 | A | 68 | ASN |
| 1 | A | 114 | ASN |
| 1 | A | 152 | ASN |
| 1 | A | 167 | HIS |
| 1 | A | 170 | ASN |
| 1 | A | 176 | GLN |
| 1 | A | 204 | GLN |
| 1 | A | 214 | ASN |
| 1 | A | 280 | GLN |
| 1 | A | 296 | HIS |
| 1 | B | 31 | GLN |
| 1 | B | 68 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 114 | ASN |
| 1 | B | 152 | ASN |
| 1 | B | 167 | HIS |
| 1 | B | 170 | ASN |
| 1 | B | 176 | GLN |
| 1 | B | 204 | GLN |
| 1 | B | 214 | ASN |
| 1 | B | 280 | GLN |
| 1 | B | 296 | HIS |
| 1 | C | 68 | ASN |
| 1 | C | 114 | ASN |
| 1 | C | 152 | ASN |
| 1 | C | 167 | HIS |
| 1 | C | 170 | ASN |
| 1 | C | 176 | GLN |
| 1 | C | 204 | GLN |
| 1 | C | 214 | ASN |
| 1 | C | 280 | GLN |
| 1 | C | 296 | HIS |
| 1 | D | 68 | ASN |
| 1 | D | 114 | ASN |
| 1 | D | 152 | ASN |
| 1 | D | 167 | HIS |
| 1 | D | 170 | ASN |
| 1 | D | 176 | GLN |
| 1 | D | 190 | ASN |
| 1 | D | 204 | GLN |
| 1 | D | 214 | ASN |
| 1 | D | 296 | HIS |
| 1 | E | 31 | GLN |
| 1 | E | 68 | ASN |
| 1 | E | 114 | ASN |
| 1 | E | 152 | ASN |
| 1 | E | 170 | ASN |
| 1 | E | 176 | GLN |
| 1 | E | 190 | ASN |
| 1 | E | 204 | GLN |
| 1 | E | 214 | ASN |
| 1 | E | 260 | HIS |
| 1 | E | 280 | GLN |
| 1 | E | 296 | HIS |
| 1 | F | 31 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 68 | ASN |
| 1 | F | 114 | ASN |
| 1 | F | 152 | ASN |
| 1 | F | 167 | HIS |
| 1 | F | 170 | ASN |
| 1 | F | 176 | GLN |
| 1 | F | 190 | ASN |
| 1 | F | 204 | GLN |
| 1 | F | 214 | ASN |
| 1 | F | 260 | HIS |
| 1 | F | 280 | GLN |
| 1 | F | 296 | HIS |
| 1 | G | 31 | GLN |
| 1 | G | 68 | ASN |
| 1 | G | 114 | ASN |
| 1 | G | 152 | ASN |
| 1 | G | 167 | HIS |
| 1 | G | 170 | ASN |
| 1 | G | 176 | GLN |
| 1 | G | 204 | GLN |
| 1 | G | 214 | ASN |
| 1 | G | 280 | GLN |
| 1 | G | 296 | HIS |
| 1 | H | 31 | GLN |
| 1 | H | 68 | ASN |
| 1 | H | 114 | ASN |
| 1 | H | 152 | ASN |
| 1 | H | 167 | HIS |
| 1 | H | 170 | ASN |
| 1 | H | 176 | GLN |
| 1 | H | 204 | GLN |
| 1 | H | 214 | ASN |
| 1 | H | 280 | GLN |
| 1 | H | 296 | HIS |
| 1 | I | 68 | ASN |
| 1 | I | 114 | ASN |
| 1 | I | 152 | ASN |
| 1 | I | 167 | HIS |
| 1 | I | 170 | ASN |
| 1 | I | 176 | GLN |
| 1 | I | 204 | GLN |
| 1 | I | 214 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | I | 280 | GLN |
| 1 | I | 296 | HIS |
| 1 | J | 31 | GLN |
| 1 | J | 68 | ASN |
| 1 | J | 114 | ASN |
| 1 | J | 152 | ASN |
| 1 | J | 167 | HIS |
| 1 | J | 170 | ASN |
| 1 | J | 176 | GLN |
| 1 | J | 204 | GLN |
| 1 | J | 214 | ASN |
| 1 | J | 260 | HIS |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 | 282/307 (91%) | 0.41 | 16 (5%) | 27 | 31 | 10, 23, 47, 62 | 0 |
| 1 | B | 282/307 (91%) | 0.28 | 15 (5%) | 30 | 34 | 12, 22, 43, 65 | 0 |
| 1 | C | 282/307 (91%) | 0.24 | 12 (4%) | 39 | 44 | 10, 23, 43, 61 | 0 |
| 1 | D | 282/307 (91%) | 0.36 | 18 (6%) | 23 | 25 | 12, 23, 45, 67 | 0 |
| 1 | E | 282/307 (91%) | 0.30 | 17 (6%) | 25 | 28 | 11, 24, 48, 65 | 0 |
| 1 | F | 282/307 (91%) | 0.27 | 12 (4%) | 39 | 44 | 12, 25, 48, 66 | 0 |
| 1 | G | 282/307 (91%) | 0.31 | 14 (4%) | 32 | 37 | 13, 26, 45, 67 | 0 |
| 1 | H | 282/307 (91%) | 0.50 | 24 (8%) | 13 | 14 | 11, 24, 45, 70 | 0 |
| 1 | I | 282/307 (91%) | 0.53 | 26 (9%) | 11 | 12 | 13, 27, 51, 73 | 0 |
| 1 | J | 282/307 (91%) | 0.40 | 23 (8%) | 14 | 15 | 12, 29, 51, 68 | 0 |
| All | All | 2820/3070 (91%) | 0.36 | 177 (6%) | 23 | 26 | 10, 24, 49, 73 | 0 |

All (177) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 299 | ILE | 16.7 |
| 1 | E | 299 | ILE | 12.5 |
| 1 | I | 299 | ILE | 11.1 |
| 1 | H | 299 | ILE | 10.9 |
| 1 | C | 299 | ILE | 9.4 |
| 1 | F | 299 | ILE | 9.1 |
| 1 | H | 282 | GLY | 8.2 |
| 1 | D | 299 | ILE | 8.1 |
| 1 | A | 299 | ILE | 8.0 |
| 1 | A | 282 | GLY | 7.8 |
| 1 | G | 299 | ILE | 7.5 |
| 1 | J | 282 | GLY | 7.0 |
| 1 | D | 282 | GLY | 6.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 64 | THR | 6.1 |
| 1 | B | 247 | GLY | 6.0 |
| 1 | J | 299 | ILE | 5.7 |
| 1 | D | 247 | GLY | 5.5 |
| 1 | C | 247 | GLY | 5.5 |
| 1 | F | 282 | GLY | 5.5 |
| 1 | D | 64 | THR | 5.4 |
| 1 | H | 63 | GLU | 5.1 |
| 1 | I | 247 | GLY | 5.1 |
| 1 | B | 282 | GLY | 5.0 |
| 1 | D | 246 | GLU | 4.9 |
| 1 | B | 64 | THR | 4.8 |
| 1 | C | 64 | THR | 4.7 |
| 1 | I | 63 | GLU | 4.7 |
| 1 | F | 63 | GLU | 4.6 |
| 1 | A | 64 | THR | 4.6 |
| 1 | B | 63 | GLU | 4.5 |
| 1 | H | 64 | THR | 4.4 |
| 1 | F | 247 | GLY | 4.4 |
| 1 | I | 248 | GLY | 4.2 |
| 1 | A | 298 | ASP | 4.0 |
| 1 | B | 216 | SER | 4.0 |
| 1 | C | 63 | GLU | 3.9 |
| 1 | G | 64 | THR | 3.9 |
| 1 | I | 298 | ASP | 3.8 |
| 1 | A | 246 | GLU | 3.8 |
| 1 | I | 252 | ASP | 3.8 |
| 1 | H | 251 | PRO | 3.8 |
| 1 | E | 282 | GLY | 3.8 |
| 1 | D | 65 | ALA | 3.8 |
| 1 | A | 63 | GLU | 3.8 |
| 1 | F | 64 | THR | 3.7 |
| 1 | G | 298 | ASP | 3.7 |
| 1 | H | 298 | ASP | 3.7 |
| 1 | J | 247 | GLY | 3.7 |
| 1 | F | 246 | GLU | 3.6 |
| 1 | E | 216 | SER | 3.6 |
| 1 | J | 64 | THR | 3.6 |
| 1 | A | 280 | GLN | 3.6 |
| 1 | H | 255 | PHE | 3.6 |
| 1 | I | 255 | PHE | 3.5 |
| 1 | I | 288 | VAL | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | G | 63 | GLU | 3.5 |
| 1 | C | 248 | GLY | 3.5 |
| 1 | G | 247 | GLY | 3.5 |
| 1 | H | 247 | GLY | 3.5 |
| 1 | F | 216 | SER | 3.4 |
| 1 | I | 216 | SER | 3.4 |
| 1 | D | 63 | GLU | 3.4 |
| 1 | H | 216 | SER | 3.4 |
| 1 | B | 248 | GLY | 3.4 |
| 1 | E | 63 | GLU | 3.3 |
| 1 | A | 216 | SER | 3.3 |
| 1 | J | 3 | PRO | 3.3 |
| 1 | H | 33 | ARG | 3.2 |
| 1 | E | 280 | GLN | 3.2 |
| 1 | J | 246 | GLU | 3.2 |
| 1 | J | 63 | GLU | 3.2 |
| 1 | C | 3 | PRO | 3.2 |
| 1 | E | 40 | GLU | 3.1 |
| 1 | C | 65 | ALA | 3.1 |
| 1 | D | 29 | PHE | 3.1 |
| 1 | A | 247 | GLY | 3.1 |
| 1 | D | 60 | GLY | 3.1 |
| 1 | B | 40 | GLU | 3.1 |
| 1 | E | 60 | GLY | 3.1 |
| 1 | E | 3 | PRO | 3.0 |
| 1 | A | 40 | GLU | 3.0 |
| 1 | I | 253 | ALA | 3.0 |
| 1 | H | 60 | GLY | 3.0 |
| 1 | F | 230 | GLU | 2.9 |
| 1 | D | 252 | ASP | 2.9 |
| 1 | I | 282 | GLY | 2.9 |
| 1 | B | 65 | ALA | 2.9 |
| 1 | A | 293 | ARG | 2.9 |
| 1 | D | 230 | GLU | 2.9 |
| 1 | H | 246 | GLU | 2.9 |
| 1 | C | 216 | SER | 2.8 |
| 1 | J | 276 | LEU | 2.8 |
| 1 | J | 216 | SER | 2.8 |
| 1 | A | 230 | GLU | 2.8 |
| 1 | I | 230 | GLU | 2.8 |
| 1 | D | 28 | ARG | 2.8 |
| 1 | F | 65 | ALA | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | I | 3 | PRO | 2.8 |
| 1 | H | 254 | THR | 2.8 |
| 1 | I | 251 | PRO | 2.7 |
| 1 | H | 297 | THR | 2.7 |
| 1 | C | 246 | GLU | 2.7 |
| 1 | E | 246 | GLU | 2.7 |
| 1 | D | 216 | SER | 2.7 |
| 1 | G | 297 | THR | 2.7 |
| 1 | B | 246 | GLU | 2.7 |
| 1 | C | 59 | VAL | 2.6 |
| 1 | H | 65 | ALA | 2.6 |
| 1 | J | 293 | ARG | 2.6 |
| 1 | H | 252 | ASP | 2.6 |
| 1 | I | 281 | ASP | 2.6 |
| 1 | E | 64 | THR | 2.6 |
| 1 | J | 281 | ASP | 2.6 |
| 1 | D | 3 | PRO | 2.6 |
| 1 | I | 246 | GLU | 2.6 |
| 1 | G | 40 | GLU | 2.5 |
| 1 | H | 280 | GLN | 2.5 |
| 1 | H | 29 | PHE | 2.5 |
| 1 | B | 60 | GLY | 2.5 |
| 1 | J | 252 | ASP | 2.5 |
| 1 | E | 230 | GLU | 2.5 |
| 1 | H | 85 | VAL | 2.5 |
| 1 | I | 85 | VAL | 2.5 |
| 1 | J | 287 | ALA | 2.5 |
| 1 | G | 5 | ILE | 2.4 |
| 1 | G | 65 | ALA | 2.4 |
| 1 | G | 216 | SER | 2.4 |
| 1 | I | 65 | ALA | 2.4 |
| 1 | I | 280 | GLN | 2.4 |
| 1 | H | 34 | LYS | 2.4 |
| 1 | J | 294 | LEU | 2.4 |
| 1 | G | 246 | GLU | 2.4 |
| 1 | H | 230 | GLU | 2.4 |
| 1 | B | 298 | ASP | 2.4 |
| 1 | A | 252 | ASP | 2.4 |
| 1 | H | 62 | ASN | 2.4 |
| 1 | H | 248 | GLY | 2.4 |
| 1 | I | 284 | VAL | 2.4 |
| 1 | D | 62 | ASN | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | J | 65 | ALA | 2.3 |
| 1 | D | 30 | LYS | 2.3 |
| 1 | E | 298 | ASP | 2.3 |
| 1 | A | 60 | GLY | 2.3 |
| 1 | J | 248 | GLY | 2.3 |
| 1 | I | 259 | GLU | 2.3 |
| 1 | J | 255 | PHE | 2.3 |
| 1 | E | 61 | ASP | 2.3 |
| 1 | J | 230 | GLU | 2.3 |
| 1 | I | 276 | LEU | 2.3 |
| 1 | F | 248 | GLY | 2.3 |
| 1 | J | 82 | ARG | 2.3 |
| 1 | I | 295 | VAL | 2.2 |
| 1 | D | 253 | ALA | 2.2 |
| 1 | G | 283 | ASP | 2.2 |
| 1 | D | 248 | GLY | 2.2 |
| 1 | J | 285 | ALA | 2.2 |
| 1 | E | 252 | ASP | 2.2 |
| 1 | J | 280 | GLN | 2.2 |
| 1 | G | 226 | VAL | 2.2 |
| 1 | B | 244 | GLY | 2.2 |
| 1 | B | 62 | ASN | 2.2 |
| 1 | J | 256 | ALA | 2.2 |
| 1 | C | 230 | GLU | 2.2 |
| 1 | G | 230 | GLU | 2.1 |
| 1 | A | 59 | VAL | 2.1 |
| 1 | I | 39 | GLY | 2.1 |
| 1 | A | 254 | THR | 2.1 |
| 1 | E | 4 | PRO | 2.1 |
| 1 | F | 59 | VAL | 2.1 |
| 1 | J | 4 | PRO | 2.1 |
| 1 | F | 40 | GLU | 2.1 |
| 1 | H | 40 | GLU | 2.1 |
| 1 | E | 65 | ALA | 2.1 |
| 1 | E | 59 | VAL | 2.1 |
| 1 | I | 40 | GLU | 2.0 |
| 1 | B | 190 | ASN | 2.0 |
| 1 | C | 62 | ASN | 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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.