



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:36 am GMT

PDB ID : 1XC1
Title : Oxo Zirconium(IV) Cluster in the Ferric Binding Protein (FBP)
Authors : Zhong, W.; Alexeev, D.; Harvey, I.; Guo, M.; Hunter, D.J.B.; Zhu, H.; Campopiano, D.J.; Sadler, P.J.
Deposited on : 2004-08-31
Resolution : 1.51 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

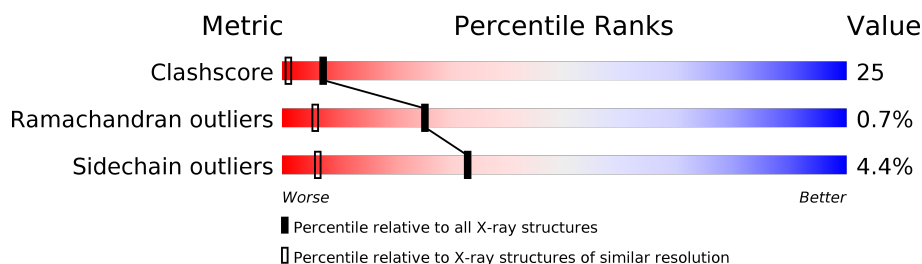
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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)) |
|-----------------------|-----------------------------|---|
| Clashscore | 112137 | 3216 (1.54-1.50) |
| Ramachandran outliers | 110173 | 3145 (1.54-1.50) |
| Sidechain outliers | 110143 | 3143 (1.54-1.50) |



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.

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 309 | |
| 1 | B | 309 | |
| 1 | C | 309 | |
| 1 | D | 309 | |
| 1 | E | 309 | |
| 1 | F | 309 | |
| 1 | G | 309 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | H | 309 |  55% 42% • |
| 1 | I | 309 |  58% 39% • |

2 Entry composition

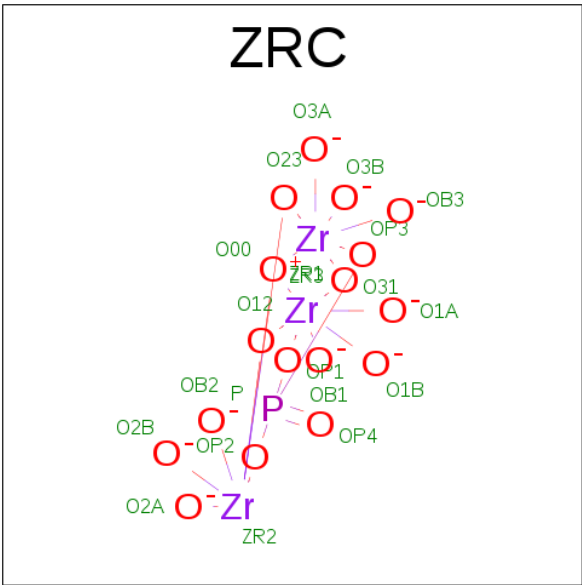
There are 3 unique types of molecules in this entry. The entry contains 22547 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 periplasmic iron-binding protein.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | B | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | C | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | D | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | E | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | F | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | G | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | H | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |
| 1 | I | 309 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2378 | 1508 | 423 | 446 | 1 | | | |

- Molecule 2 is OXO ZIRCONIUM(IV) CLUSTER (three-letter code: ZRC) (formula: O₁₇PZr₃).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---------|---------|
| 2 | A | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | B | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | D | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | G | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | H | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | I | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | C | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | E | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |
| 2 | F | 1 | Total | O | P | Zr | 0 | 0 |
| | | | 19 | 15 | 1 | 3 | | |

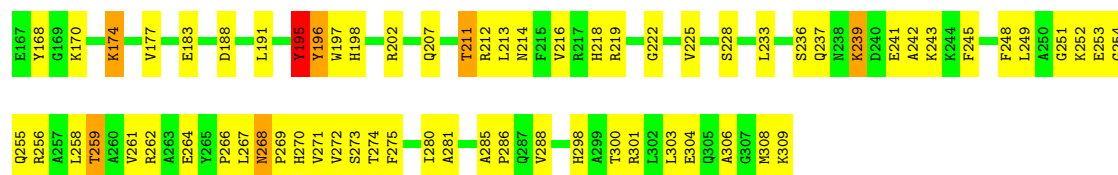
- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 3 | A | 142 | Total | O | 0 | 0 |
| | | | 142 | 142 | | |
| 3 | B | 103 | Total | O | 0 | 0 |
| | | | 103 | 103 | | |
| 3 | C | 111 | Total | O | 0 | 0 |
| | | | 111 | 111 | | |

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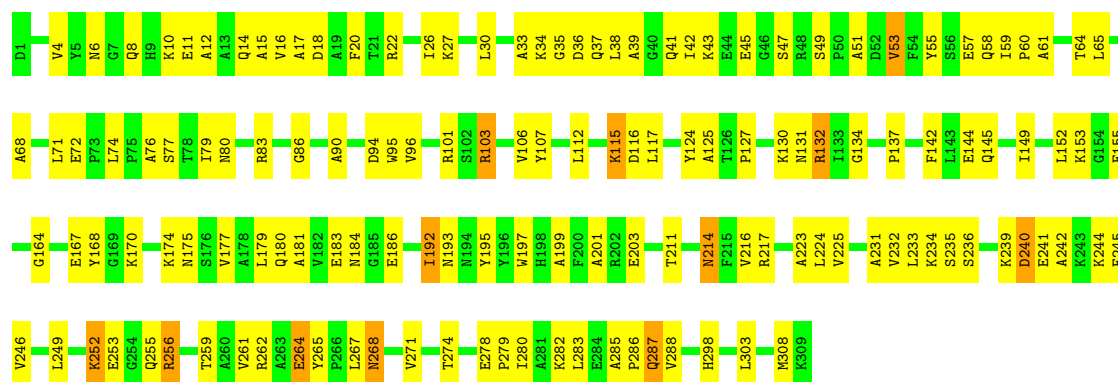
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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3 | D | 113 | Total 113 | O 113 | 0 | 0 |
| 3 | E | 136 | Total 136 | O 136 | 0 | 0 |
| 3 | F | 124 | Total 124 | O 124 | 0 | 0 |
| 3 | G | 79 | Total 79 | O 79 | 0 | 0 |
| 3 | H | 81 | Total 81 | O 81 | 0 | 0 |
| 3 | I | 85 | Total 85 | O 85 | 0 | 0 |



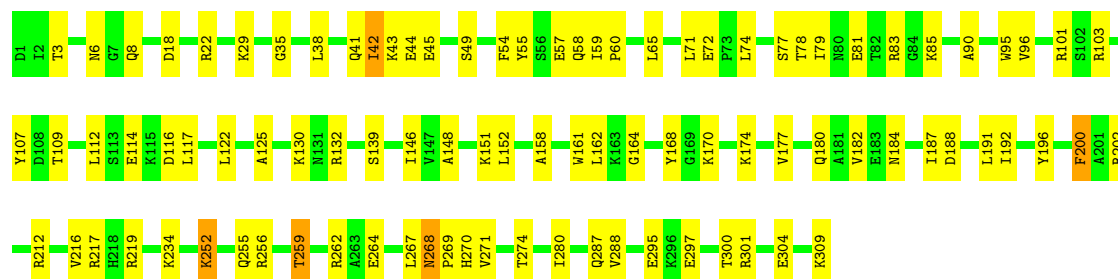
- Molecule 1: periplasmic iron-binding protein

Chain D: 54% 42%



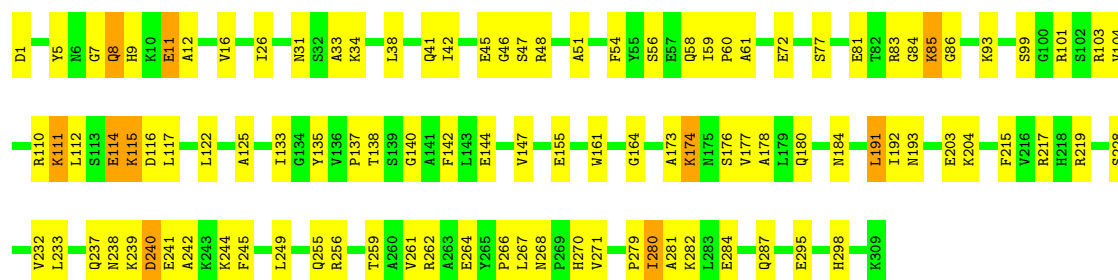
- Molecule 1: periplasmic iron-binding protein

Chain E: 70% 29%



- Molecule 1: periplasmic iron-binding protein

Chain F: 66% 30%



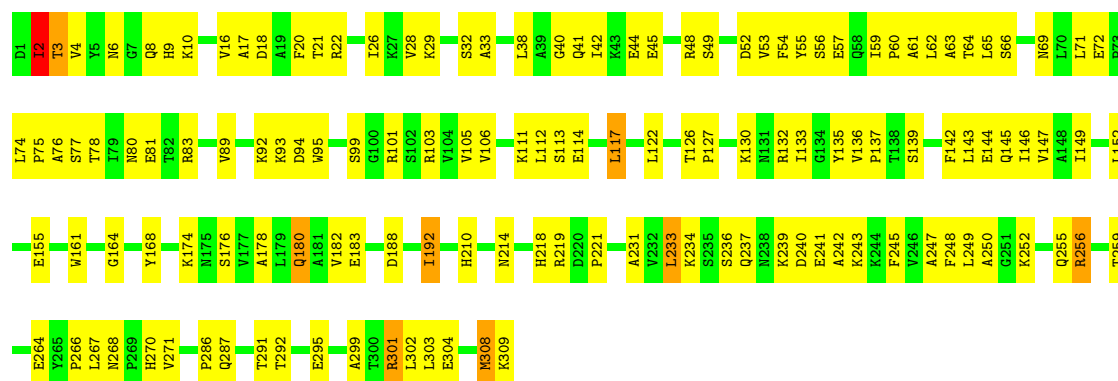
- Molecule 1: periplasmic iron-binding protein

Chain G: 57% 41%



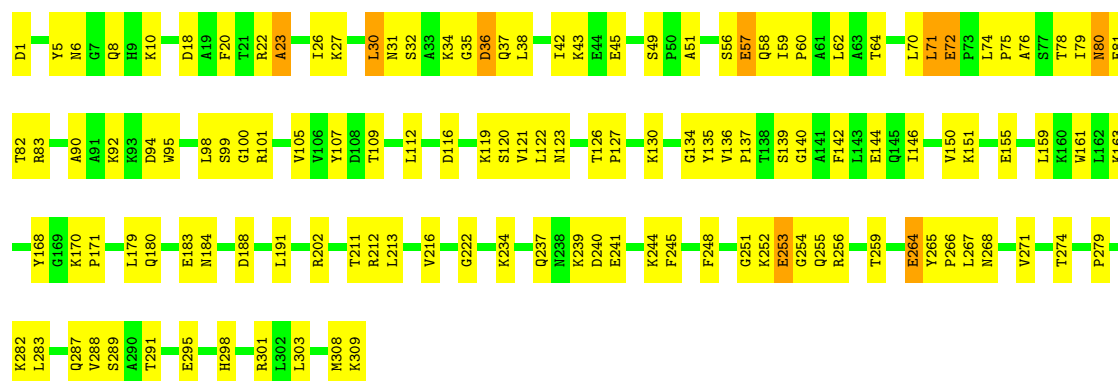
- Molecule 1: periplasmic iron-binding protein

Chain H: 55% 42% .



- Molecule 1: periplasmic iron-binding protein

Chain I: 58% 39% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 32 | Depositor |
| Cell constants a, b, c, α , β , γ | 146.20 Å 146.20 Å 113.56 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 20.00 – 1.51 | Depositor |
| % Data completeness (in resolution range) | 97.3 (20.00-1.51) | Depositor |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | 0.10 | Depositor |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.191 , 0.275 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 22547 | wwPDB-VP |
| Average B, all atoms (Å ²) | 26.0 | wwPDB-VP |

5 Model quality

5.1 Standard geometry

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

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 | 0.39 | 0/2423 | 0.63 | 0/3280 |
| 1 | B | 0.36 | 0/2423 | 0.63 | 1/3280 (0.0%) |
| 1 | C | 0.41 | 0/2423 | 0.65 | 2/3280 (0.1%) |
| 1 | D | 0.37 | 0/2423 | 0.59 | 0/3280 |
| 1 | E | 0.38 | 0/2423 | 0.63 | 0/3280 |
| 1 | F | 0.37 | 0/2423 | 0.63 | 0/3280 |
| 1 | G | 0.34 | 0/2423 | 0.60 | 0/3280 |
| 1 | H | 0.35 | 0/2423 | 0.60 | 0/3280 |
| 1 | I | 0.36 | 0/2423 | 0.61 | 0/3280 |
| All | All | 0.37 | 0/21807 | 0.62 | 3/29520 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | C | 195 | TYR | CB-CG-CD1 | 5.81 | 124.49 | 121.00 |
| 1 | B | 205 | GLY | N-CA-C | -5.34 | 99.75 | 113.10 |
| 1 | C | 196 | TYR | CB-CG-CD2 | 5.22 | 124.13 | 121.00 |

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 | 2378 | 0 | 2424 | 98 | 0 |
| 1 | B | 2378 | 0 | 2424 | 102 | 0 |
| 1 | C | 2378 | 0 | 2424 | 149 | 0 |
| 1 | D | 2378 | 0 | 2424 | 147 | 0 |
| 1 | E | 2378 | 0 | 2424 | 93 | 0 |
| 1 | F | 2378 | 0 | 2424 | 95 | 0 |
| 1 | G | 2378 | 0 | 2424 | 140 | 0 |
| 1 | H | 2378 | 0 | 2424 | 139 | 0 |
| 1 | I | 2378 | 0 | 2424 | 127 | 0 |
| 2 | A | 19 | 0 | 0 | 0 | 0 |
| 2 | B | 19 | 0 | 0 | 1 | 0 |
| 2 | C | 19 | 0 | 0 | 1 | 0 |
| 2 | D | 19 | 0 | 0 | 2 | 0 |
| 2 | E | 19 | 0 | 0 | 0 | 0 |
| 2 | F | 19 | 0 | 0 | 0 | 0 |
| 2 | G | 19 | 0 | 0 | 0 | 0 |
| 2 | H | 19 | 0 | 0 | 1 | 0 |
| 2 | I | 19 | 0 | 0 | 1 | 0 |
| 3 | A | 142 | 0 | 0 | 3 | 0 |
| 3 | B | 103 | 0 | 0 | 4 | 0 |
| 3 | C | 111 | 0 | 0 | 11 | 0 |
| 3 | D | 113 | 0 | 0 | 10 | 0 |
| 3 | E | 136 | 0 | 0 | 5 | 0 |
| 3 | F | 124 | 0 | 0 | 8 | 0 |
| 3 | G | 79 | 0 | 0 | 5 | 0 |
| 3 | H | 81 | 0 | 0 | 6 | 0 |
| 3 | I | 85 | 0 | 0 | 3 | 0 |
| All | All | 22547 | 0 | 21816 | 1086 | 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 (1086) 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:A:259:THR:HG21 | 1:A:266:PRO:HG3 | 1.24 | 1.17 |
| 1:F:259:THR:HG21 | 1:F:266:PRO:HG3 | 1.14 | 1.11 |
| 1:H:80:ASN:HA | 1:H:83:ARG:HG2 | 1.27 | 1.10 |
| 1:H:259:THR:HG21 | 1:H:266:PRO:HG3 | 1.35 | 1.07 |
| 1:G:259:THR:HG21 | 1:G:266:PRO:HG3 | 1.35 | 1.06 |
| 1:C:202:ARG:HH22 | 1:C:274:THR:HG23 | 1.07 | 1.06 |
| 1:E:202:ARG:HH22 | 1:E:274:THR:HG22 | 1.19 | 1.05 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:ARG:NH2 | 1:E:274:THR:HG22 | 1.72 | 1.05 |
| 1:C:162:LEU:HB3 | 1:C:308:MET:HE2 | 1.44 | 0.98 |
| 1:G:119:LYS:HE2 | 1:G:119:LYS:HA | 1.40 | 0.98 |
| 1:I:259:THR:HG21 | 1:I:266:PRO:HG3 | 1.42 | 0.97 |
| 1:I:56:SER:HB3 | 1:I:62:LEU:HD11 | 1.45 | 0.97 |
| 1:B:93:LYS:HE2 | 1:B:93:LYS:H | 1.30 | 0.96 |
| 1:I:80:ASN:HA | 1:I:83:ARG:HG2 | 1.45 | 0.94 |
| 1:I:43:LYS:HD2 | 1:I:70:LEU:HD11 | 1.47 | 0.93 |
| 1:B:170:LYS:HD2 | 1:B:187:ILE:HD12 | 1.51 | 0.92 |
| 1:C:202:ARG:NH2 | 1:C:274:THR:HG23 | 1.84 | 0.91 |
| 1:C:202:ARG:HH22 | 1:C:274:THR:CG2 | 1.84 | 0.91 |
| 1:F:176:SER:O | 1:F:180:GLN:HG2 | 1.72 | 0.90 |
| 1:I:71:LEU:HB3 | 1:I:94:ASP:HB2 | 1.55 | 0.89 |
| 1:D:256:ARG:HH11 | 1:D:256:ARG:HG3 | 1.37 | 0.88 |
| 1:C:162:LEU:HD22 | 1:C:308:MET:HE1 | 1.56 | 0.88 |
| 1:C:262:ARG:HG2 | 1:C:264:GLU:HG3 | 1.53 | 0.88 |
| 1:B:255:GLN:HB2 | 1:B:271:VAL:HG21 | 1.57 | 0.87 |
| 1:C:256:ARG:NH1 | 1:C:272:VAL:H | 1.72 | 0.86 |
| 1:I:202:ARG:NH2 | 1:I:274:THR:HG22 | 1.90 | 0.86 |
| 1:A:159:LEU:HD13 | 1:A:302:LEU:HD22 | 1.56 | 0.86 |
| 1:H:259:THR:CG2 | 1:H:266:PRO:HG3 | 2.06 | 0.86 |
| 1:C:256:ARG:HD3 | 1:C:271:VAL:HG13 | 1.58 | 0.85 |
| 1:E:72:GLU:HG2 | 1:E:234:LYS:HG2 | 1.59 | 0.84 |
| 1:H:268:ASN:HD22 | 1:H:271:VAL:HG23 | 1.42 | 0.84 |
| 1:D:174:LYS:HE3 | 1:D:177:VAL:HG23 | 1.59 | 0.84 |
| 1:D:101:ARG:CZ | 1:D:264:GLU:HG2 | 2.08 | 0.84 |
| 1:A:288:VAL:HB | 3:A:471:HOH:O | 1.77 | 0.83 |
| 1:E:85:LYS:N | 1:E:85:LYS:HD2 | 1.94 | 0.83 |
| 1:H:17:ALA:HB1 | 1:H:28:VAL:HG21 | 1.58 | 0.83 |
| 1:A:304:GLU:HG2 | 1:A:309:LYS:HG2 | 1.58 | 0.83 |
| 1:B:93:LYS:HE2 | 1:B:93:LYS:N | 1.94 | 0.83 |
| 1:B:2:ILE:HG23 | 1:B:241:GLU:OE2 | 1.79 | 0.82 |
| 1:E:85:LYS:H | 1:E:85:LYS:HD2 | 1.44 | 0.82 |
| 1:C:120:SER:HB3 | 1:C:123:ASN:ND2 | 1.95 | 0.82 |
| 1:I:18:ASP:HB3 | 1:I:22:ARG:HH12 | 1.45 | 0.81 |
| 1:C:121:VAL:HB | 3:C:460:HOH:O | 1.78 | 0.81 |
| 1:A:278:GLU:HB2 | 1:A:282:LYS:NZ | 1.96 | 0.81 |
| 1:E:202:ARG:HH22 | 1:E:274:THR:CG2 | 1.93 | 0.80 |
| 1:H:2:ILE:HD11 | 1:H:53:VAL:HG23 | 1.65 | 0.79 |
| 1:D:132:ARG:HH11 | 1:D:132:ARG:HB3 | 1.47 | 0.79 |
| 1:C:252:LYS:O | 1:C:256:ARG:HG2 | 1.83 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:239:LYS:O | 1:G:243:LYS:HG3 | 1.84 | 0.78 |
| 1:I:202:ARG:HH22 | 1:I:274:THR:HG22 | 1.46 | 0.78 |
| 1:G:202:ARG:NH2 | 1:G:274:THR:HG22 | 1.99 | 0.78 |
| 1:C:259:THR:HG23 | 1:C:273:SER:HA | 1.66 | 0.78 |
| 1:I:279:PRO:HD2 | 1:I:282:LYS:HD2 | 1.64 | 0.77 |
| 1:G:72:GLU:HG3 | 1:G:73:PRO:HD2 | 1.66 | 0.77 |
| 1:F:280:ILE:O | 1:F:280:ILE:HD13 | 1.85 | 0.77 |
| 1:H:255:GLN:HB3 | 1:H:271:VAL:HG21 | 1.66 | 0.77 |
| 1:G:90:ALA:HB3 | 1:G:93:LYS:HA | 1.66 | 0.77 |
| 1:H:4:VAL:HG22 | 1:H:53:VAL:HB | 1.65 | 0.77 |
| 1:C:52:ASP:HA | 1:C:236:SER:HB2 | 1.66 | 0.77 |
| 1:I:240:ASP:O | 1:I:244:LYS:HG2 | 1.85 | 0.76 |
| 1:F:11:GLU:HG2 | 1:F:12:ALA:N | 2.00 | 0.76 |
| 1:G:234:LYS:NZ | 1:G:234:LYS:HB3 | 2.01 | 0.76 |
| 1:I:309:LYS:NZ | 1:I:309:LYS:HB3 | 2.00 | 0.76 |
| 1:D:42:ILE:HD13 | 1:D:233:LEU:HD21 | 1.68 | 0.76 |
| 1:G:292:THR:OG1 | 1:G:295:GLU:HG3 | 1.86 | 0.76 |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:HG2 | 1.68 | 0.76 |
| 1:H:255:GLN:CB | 1:H:271:VAL:HG21 | 2.16 | 0.75 |
| 1:C:48:ARG:HE | 1:C:237:GLN:NE2 | 1.84 | 0.75 |
| 1:C:79:ILE:HD12 | 1:C:93:LYS:HG3 | 1.68 | 0.75 |
| 1:A:101:ARG:HH22 | 1:A:228:SER:HB3 | 1.51 | 0.74 |
| 1:C:195:TYR:CE2 | 1:C:196:TYR:CE1 | 2.74 | 0.74 |
| 1:D:132:ARG:NH1 | 1:D:132:ARG:HB3 | 2.00 | 0.74 |
| 1:E:262:ARG:HG2 | 1:E:264:GLU:HG3 | 1.69 | 0.74 |
| 1:I:130:LYS:HG2 | 1:I:168:TYR:HD2 | 1.52 | 0.74 |
| 1:A:130:LYS:HE3 | 1:A:131:ASN:HD22 | 1.52 | 0.74 |
| 1:B:60:PRO:O | 1:B:64:THR:HG23 | 1.88 | 0.74 |
| 1:A:125:ALA:HB1 | 1:A:164:GLY:HA3 | 1.70 | 0.73 |
| 1:B:197:TRP:HE1 | 1:B:211:THR:HG22 | 1.53 | 0.73 |
| 1:I:80:ASN:HB3 | 1:I:83:ARG:NH2 | 2.03 | 0.73 |
| 1:F:9:HIS:CD2 | 1:F:11:GLU:HB3 | 2.23 | 0.73 |
| 1:H:99:SER:HA | 1:H:267:LEU:HG | 1.69 | 0.73 |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:N | 2.03 | 0.73 |
| 1:B:5:TYR:CE1 | 1:B:51:ALA:HB2 | 2.24 | 0.73 |
| 1:D:61:ALA:O | 1:D:65:LEU:HD23 | 1.88 | 0.73 |
| 1:E:158:ALA:O | 1:E:162:LEU:HD13 | 1.89 | 0.73 |
| 1:G:259:THR:CG2 | 1:G:266:PRO:HG3 | 2.15 | 0.72 |
| 1:F:259:THR:CG2 | 1:F:266:PRO:HG3 | 2.06 | 0.72 |
| 1:C:130:LYS:HD3 | 1:C:131:ASN:N | 2.05 | 0.72 |
| 1:D:256:ARG:NH1 | 1:D:256:ARG:HG3 | 1.99 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:130:LYS:CD | 1:G:168:TYR:HB3 | 2.19 | 0.72 |
| 1:A:47:SER:HA | 1:A:235:SER:HB3 | 1.72 | 0.72 |
| 1:F:85:LYS:NZ | 1:F:219:ARG:HH12 | 1.87 | 0.72 |
| 1:A:72:GLU:OE1 | 1:A:73:PRO:HD2 | 1.89 | 0.71 |
| 1:D:39:ALA:HB1 | 1:D:65:LEU:HD21 | 1.72 | 0.71 |
| 1:G:302:LEU:HD23 | 1:G:305:GLN:NE2 | 2.05 | 0.71 |
| 1:B:209:VAL:HG12 | 1:B:211:THR:H | 1.53 | 0.71 |
| 1:B:41:GLN:O | 1:B:45:GLU:HG2 | 1.88 | 0.71 |
| 1:E:3:THR:HG22 | 1:E:29:LYS:HD3 | 1.71 | 0.71 |
| 1:F:85:LYS:HZ1 | 1:F:284:GLU:HA | 1.55 | 0.71 |
| 1:D:174:LYS:HE3 | 1:D:177:VAL:CG2 | 2.19 | 0.71 |
| 1:G:236:SER:HB3 | 1:G:239:LYS:HG2 | 1.73 | 0.71 |
| 1:B:197:TRP:NE1 | 1:B:211:THR:HG22 | 2.05 | 0.71 |
| 1:H:268:ASN:ND2 | 1:H:271:VAL:HG23 | 2.04 | 0.71 |
| 1:H:3:THR:HB | 1:H:29:LYS:HE2 | 1.73 | 0.71 |
| 1:B:252:LYS:HE2 | 1:B:256:ARG:NH2 | 2.06 | 0.70 |
| 1:H:71:LEU:O | 1:H:234:LYS:HE3 | 1.90 | 0.70 |
| 1:H:80:ASN:HA | 1:H:83:ARG:CG | 2.15 | 0.70 |
| 1:C:303:LEU:HG | 1:C:309:LYS:HA | 1.73 | 0.70 |
| 1:B:45:GLU:HB3 | 1:B:49:SER:HB3 | 1.73 | 0.70 |
| 1:C:104:VAL:HG23 | 3:C:511:HOH:O | 1.90 | 0.70 |
| 1:B:45:GLU:CB | 1:B:49:SER:HB3 | 2.21 | 0.70 |
| 1:C:259:THR:O | 1:C:274:THR:HG22 | 1.92 | 0.70 |
| 1:H:8:GLN:HG3 | 1:H:9:HIS:H | 1.54 | 0.70 |
| 1:H:259:THR:HG21 | 1:H:266:PRO:CG | 2.20 | 0.70 |
| 1:D:265:TYR:HB3 | 1:D:280:ILE:HG23 | 1.74 | 0.70 |
| 1:D:259:THR:HG23 | 3:D:411:HOH:O | 1.92 | 0.69 |
| 1:G:4:VAL:HB | 1:G:30:LEU:HD23 | 1.73 | 0.69 |
| 1:A:143:LEU:O | 1:A:146:ILE:HG23 | 1.93 | 0.69 |
| 1:C:255:GLN:HE21 | 1:C:268:ASN:H | 1.39 | 0.69 |
| 1:A:89:VAL:HG12 | 3:A:465:HOH:O | 1.92 | 0.69 |
| 1:I:259:THR:CG2 | 1:I:266:PRO:HG3 | 2.20 | 0.69 |
| 1:I:81:GLU:OE1 | 1:I:251:GLY:HA2 | 1.93 | 0.69 |
| 1:I:30:LEU:C | 1:I:31:ASN:HD22 | 1.96 | 0.69 |
| 1:E:252:LYS:O | 1:E:256:ARG:HG3 | 1.93 | 0.69 |
| 1:H:112:LEU:HD11 | 1:H:188:ASP:HB3 | 1.75 | 0.69 |
| 1:A:60:PRO:O | 1:A:64:THR:HG23 | 1.93 | 0.68 |
| 1:I:126:THR:HB | 1:I:127:PRO:HD2 | 1.75 | 0.68 |
| 1:I:43:LYS:HD2 | 1:I:70:LEU:CD1 | 2.22 | 0.68 |
| 1:A:112:LEU:HD11 | 1:A:188:ASP:HB3 | 1.75 | 0.68 |
| 1:G:300:THR:O | 1:G:304:GLU:HG3 | 1.92 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:174:LYS:NZ | 2:H:400:ZRC:O23 | 2.25 | 0.68 |
| 1:H:192:ILE:N | 1:H:192:ILE:HD13 | 2.09 | 0.68 |
| 1:A:279:PRO:HD2 | 1:A:282:LYS:NZ | 2.09 | 0.68 |
| 1:E:170:LYS:HD2 | 1:E:187:ILE:HD12 | 1.76 | 0.68 |
| 1:H:81:GLU:HB2 | 1:H:250:ALA:HB1 | 1.75 | 0.68 |
| 1:D:77:SER:HA | 1:D:80:ASN:HD22 | 1.56 | 0.67 |
| 1:G:130:LYS:HD2 | 1:G:168:TYR:HB3 | 1.75 | 0.67 |
| 1:B:125:ALA:HB1 | 1:B:164:GLY:HA3 | 1.75 | 0.67 |
| 1:I:56:SER:HB3 | 1:I:62:LEU:CD1 | 2.21 | 0.67 |
| 1:I:127:PRO:O | 1:I:130:LYS:HG3 | 1.94 | 0.67 |
| 1:I:60:PRO:O | 1:I:64:THR:HG23 | 1.93 | 0.67 |
| 1:C:151:LYS:HD2 | 1:C:288:VAL:HG23 | 1.77 | 0.67 |
| 1:D:8:GLN:HE22 | 1:D:101:ARG:HH22 | 1.41 | 0.67 |
| 1:F:5:TYR:CE1 | 1:F:51:ALA:HB2 | 2.30 | 0.67 |
| 1:A:278:GLU:HB2 | 1:A:282:LYS:HZ2 | 1.59 | 0.67 |
| 1:D:255:GLN:O | 1:D:259:THR:HG22 | 1.95 | 0.67 |
| 1:G:125:ALA:HB1 | 1:G:164:GLY:HA3 | 1.77 | 0.67 |
| 1:G:5:TYR:CE1 | 1:G:51:ALA:HB2 | 2.30 | 0.66 |
| 1:F:125:ALA:HB1 | 1:F:164:GLY:HA3 | 1.76 | 0.66 |
| 1:B:255:GLN:CB | 1:B:271:VAL:HG21 | 2.26 | 0.66 |
| 1:C:197:TRP:HE1 | 1:C:211:THR:HG23 | 1.59 | 0.66 |
| 1:B:8:GLN:HA | 1:B:57:GLU:HG3 | 1.77 | 0.66 |
| 1:A:252:LYS:HE3 | 1:A:256:ARG:NH2 | 2.10 | 0.66 |
| 1:B:106:VAL:HG22 | 1:B:211:THR:HG23 | 1.77 | 0.66 |
| 1:C:259:THR:CG2 | 1:C:273:SER:HA | 2.24 | 0.66 |
| 1:D:80:ASN:O | 1:D:83:ARG:HG2 | 1.95 | 0.66 |
| 1:I:59:ILE:N | 1:I:60:PRO:HD2 | 2.11 | 0.66 |
| 1:C:236:SER:H | 1:C:239:LYS:HE2 | 1.59 | 0.66 |
| 1:F:259:THR:HG21 | 1:F:266:PRO:CG | 2.09 | 0.66 |
| 1:D:236:SER:HB3 | 1:D:239:LYS:HG2 | 1.78 | 0.65 |
| 1:I:266:PRO:HD2 | 3:I:417:HOH:O | 1.96 | 0.65 |
| 1:D:240:ASP:HB2 | 3:D:508:HOH:O | 1.95 | 0.65 |
| 1:G:8:GLN:HG3 | 1:G:9:HIS:H | 1.61 | 0.65 |
| 1:G:33:ALA:HB3 | 1:G:38:LEU:CD2 | 2.26 | 0.65 |
| 1:I:119:LYS:O | 1:I:216:VAL:HG23 | 1.97 | 0.65 |
| 1:A:279:PRO:HG2 | 1:A:282:LYS:HG3 | 1.79 | 0.65 |
| 1:F:192:ILE:HG22 | 1:F:193:ASN:H | 1.61 | 0.65 |
| 1:C:121:VAL:HG21 | 1:C:222:GLY:HA3 | 1.79 | 0.65 |
| 1:A:133:ILE:HD11 | 1:A:191:LEU:HD13 | 1.77 | 0.65 |
| 1:D:201:ALA:HB3 | 3:D:512:HOH:O | 1.97 | 0.65 |
| 1:D:15:ALA:CB | 1:D:261:VAL:HG21 | 2.26 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:255:GLN:NE2 | 1:C:268:ASN:H | 1.95 | 0.65 |
| 1:C:48:ARG:HH21 | 1:C:237:GLN:HG3 | 1.61 | 0.64 |
| 1:G:202:ARG:HH22 | 1:G:274:THR:HG22 | 1.59 | 0.64 |
| 1:A:110:ARG:HH21 | 1:A:210:HIS:CD2 | 2.15 | 0.64 |
| 1:A:82:THR:HB | 1:A:267:LEU:HB3 | 1.79 | 0.64 |
| 1:H:78:THR:HG23 | 1:H:247:ALA:HA | 1.77 | 0.64 |
| 1:D:155:GLU:OE2 | 1:D:298:HIS:HE1 | 1.81 | 0.64 |
| 1:H:292:THR:OG1 | 1:H:295:GLU:HG3 | 1.97 | 0.64 |
| 1:A:174:LYS:HB2 | 1:A:177:VAL:HG23 | 1.79 | 0.64 |
| 1:I:72:GLU:HG3 | 1:I:239:LYS:HD2 | 1.78 | 0.64 |
| 1:B:38:LEU:O | 1:B:42:ILE:HG13 | 1.97 | 0.64 |
| 1:D:267:LEU:HD23 | 1:D:280:ILE:HD13 | 1.78 | 0.64 |
| 1:D:45:GLU:HB2 | 1:D:49:SER:HB2 | 1.79 | 0.64 |
| 1:C:119:LYS:O | 1:C:216:VAL:HG13 | 1.97 | 0.64 |
| 1:F:245:PHE:O | 1:F:249:LEU:HG | 1.98 | 0.64 |
| 1:H:38:LEU:O | 1:H:42:ILE:HG13 | 1.97 | 0.63 |
| 1:A:9:HIS:HB3 | 1:A:12:ALA:CB | 2.28 | 0.63 |
| 1:G:162:LEU:HD22 | 1:G:308:MET:HE1 | 1.80 | 0.63 |
| 1:H:126:THR:HB | 1:H:127:PRO:HD2 | 1.81 | 0.63 |
| 1:B:292:THR:OG1 | 1:B:295:GLU:HG3 | 1.98 | 0.63 |
| 1:H:8:GLN:HG3 | 1:H:9:HIS:N | 2.13 | 0.63 |
| 1:B:101:ARG:NH2 | 1:B:226:THR:HG22 | 2.13 | 0.63 |
| 1:B:5:TYR:CD1 | 1:B:51:ALA:HB2 | 2.33 | 0.63 |
| 1:G:140:GLY:O | 1:G:144:GLU:HG2 | 1.98 | 0.63 |
| 1:C:113:SER:C | 1:C:115:LYS:H | 2.02 | 0.63 |
| 1:H:18:ASP:O | 1:H:22:ARG:HG3 | 1.98 | 0.63 |
| 1:H:57:GLU:HB2 | 1:H:101:ARG:NH2 | 2.14 | 0.63 |
| 1:F:192:ILE:CG2 | 1:F:193:ASN:H | 2.12 | 0.63 |
| 1:G:9:HIS:HB3 | 1:G:12:ALA:HB3 | 1.80 | 0.63 |
| 1:B:252:LYS:HE3 | 1:B:270:HIS:O | 1.99 | 0.63 |
| 1:C:2:ILE:HG13 | 1:C:28:VAL:HG13 | 1.81 | 0.62 |
| 1:E:287:GLN:HB3 | 3:E:498:HOH:O | 1.99 | 0.62 |
| 1:I:202:ARG:HH22 | 1:I:274:THR:CG2 | 2.12 | 0.62 |
| 1:C:28:VAL:HG11 | 3:C:462:HOH:O | 1.99 | 0.62 |
| 1:G:130:LYS:HA | 1:G:168:TYR:HB2 | 1.79 | 0.62 |
| 1:C:107:TYR:CD1 | 1:C:117:LEU:HD11 | 2.34 | 0.62 |
| 1:C:162:LEU:HB3 | 1:C:308:MET:CE | 2.25 | 0.62 |
| 1:H:33:ALA:HB3 | 1:H:38:LEU:HG | 1.80 | 0.62 |
| 1:E:268:ASN:HD22 | 1:E:268:ASN:C | 2.03 | 0.62 |
| 1:I:240:ASP:HB3 | 1:I:241:GLU:OE2 | 1.99 | 0.62 |
| 1:C:114:GLU:OE2 | 1:C:214:ASN:HB2 | 1.99 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:34:LYS:O | 1:G:38:LEU:HD23 | 2.00 | 0.62 |
| 1:H:41:GLN:O | 1:H:45:GLU:HG3 | 2.00 | 0.62 |
| 1:D:72:GLU:HG2 | 1:D:234:LYS:HA | 1.82 | 0.62 |
| 1:I:101:ARG:NH1 | 2:I:400:ZRC:O1A | 2.33 | 0.62 |
| 1:G:5:TYR:HB3 | 1:G:38:LEU:HD12 | 1.82 | 0.61 |
| 1:F:115:LYS:O | 1:F:116:ASP:CG | 2.39 | 0.61 |
| 1:F:85:LYS:HD2 | 1:F:281:ALA:HA | 1.82 | 0.61 |
| 1:G:300:THR:O | 1:G:303:LEU:HB3 | 1.99 | 0.61 |
| 1:H:54:PHE:CE2 | 1:H:56:SER:HB2 | 2.35 | 0.61 |
| 1:E:72:GLU:HG2 | 1:E:234:LYS:HA | 1.83 | 0.61 |
| 1:F:122:LEU:HA | 1:F:161:TRP:CD1 | 2.35 | 0.61 |
| 1:C:105:VAL:HG22 | 1:C:191:LEU:HD23 | 1.82 | 0.61 |
| 1:C:268:ASN:C | 1:C:268:ASN:HD22 | 2.04 | 0.61 |
| 1:E:38:LEU:O | 1:E:42:ILE:HG13 | 2.01 | 0.61 |
| 1:G:303:LEU:HD22 | 1:G:308:MET:CE | 2.30 | 0.61 |
| 1:H:16:VAL:HG11 | 1:H:249:LEU:CD2 | 2.30 | 0.61 |
| 1:A:236:SER:HB3 | 1:A:239:LYS:HG2 | 1.83 | 0.61 |
| 1:G:162:LEU:HD22 | 1:G:308:MET:CE | 2.31 | 0.61 |
| 1:C:120:SER:HB3 | 1:C:123:ASN:HD21 | 1.66 | 0.60 |
| 1:H:136:VAL:O | 1:H:139:SER:HB3 | 2.01 | 0.60 |
| 1:B:237:GLN:NE2 | 1:B:237:GLN:H | 1.99 | 0.60 |
| 1:C:17:ALA:O | 1:C:20:PHE:HB3 | 2.00 | 0.60 |
| 1:C:5:TYR:CD1 | 1:C:51:ALA:HB2 | 2.36 | 0.60 |
| 1:F:38:LEU:HD13 | 3:F:494:HOH:O | 2.01 | 0.60 |
| 1:G:2:ILE:HD11 | 1:G:28:VAL:HG22 | 1.81 | 0.60 |
| 1:G:104:VAL:HG12 | 1:G:105:VAL:N | 2.16 | 0.60 |
| 1:G:202:ARG:HH22 | 1:G:274:THR:CG2 | 2.14 | 0.60 |
| 1:A:304:GLU:HA | 1:A:309:LYS:HB3 | 1.84 | 0.60 |
| 1:C:162:LEU:HD22 | 1:C:308:MET:CE | 2.30 | 0.60 |
| 1:H:3:THR:HB | 1:H:29:LYS:HB3 | 1.82 | 0.60 |
| 1:H:95:TRP:HB3 | 1:H:231:ALA:HB2 | 1.82 | 0.60 |
| 1:I:252:LYS:NZ | 1:I:256:ARG:HD2 | 2.17 | 0.60 |
| 1:E:125:ALA:HB1 | 1:E:164:GLY:HA3 | 1.83 | 0.60 |
| 1:F:280:ILE:C | 1:F:280:ILE:HD13 | 2.22 | 0.60 |
| 1:G:162:LEU:HB3 | 1:G:308:MET:HE2 | 1.83 | 0.60 |
| 1:G:1:ASP:OD1 | 1:G:27:LYS:HD3 | 2.01 | 0.60 |
| 1:G:2:ILE:HB | 3:G:443:HOH:O | 2.01 | 0.60 |
| 1:A:45:GLU:HB3 | 1:A:49:SER:HB3 | 1.82 | 0.60 |
| 1:H:59:ILE:N | 1:H:60:PRO:HD2 | 2.16 | 0.60 |
| 1:F:85:LYS:NZ | 1:F:284:GLU:HA | 2.17 | 0.60 |
| 1:A:203:GLU:OE1 | 1:A:204:LYS:HE2 | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:27:LYS:NZ | 1:D:27:LYS:HB3 | 2.16 | 0.60 |
| 1:G:279:PRO:HD2 | 1:G:282:LYS:HG3 | 1.82 | 0.60 |
| 1:H:75:PRO:HB2 | 1:H:77:SER:OG | 2.00 | 0.60 |
| 1:I:10:LYS:HE2 | 1:I:32:SER:HB2 | 1.84 | 0.60 |
| 1:C:121:VAL:CG2 | 1:C:222:GLY:HA3 | 2.32 | 0.60 |
| 1:G:53:VAL:HG22 | 1:G:232:VAL:HG22 | 1.83 | 0.60 |
| 1:B:59:ILE:HD11 | 1:B:227:TYR:HB2 | 1.82 | 0.59 |
| 1:D:279:PRO:HB2 | 1:D:282:LYS:HE2 | 1.84 | 0.59 |
| 1:G:70:LEU:HD22 | 3:G:470:HOH:O | 2.02 | 0.59 |
| 1:A:108:ASP:OD2 | 1:A:110:ARG:HD2 | 2.02 | 0.59 |
| 1:F:77:SER:O | 1:F:81:GLU:HG3 | 2.01 | 0.59 |
| 1:F:101:ARG:NH1 | 1:F:101:ARG:HB2 | 2.18 | 0.59 |
| 1:H:69:ASN:HB3 | 1:H:92:LYS:NZ | 2.16 | 0.59 |
| 1:G:260:ALA:HA | 1:G:274:THR:OG1 | 2.02 | 0.59 |
| 1:G:302:LEU:HD23 | 1:G:305:GLN:HE22 | 1.68 | 0.59 |
| 1:I:109:THR:O | 1:I:109:THR:HG22 | 2.03 | 0.59 |
| 1:I:82:THR:HB | 1:I:267:LEU:HB3 | 1.83 | 0.59 |
| 1:A:146:ILE:CD1 | 1:A:158:ALA:HB1 | 2.32 | 0.59 |
| 1:E:78:THR:HG22 | 1:E:96:VAL:HG21 | 1.84 | 0.59 |
| 1:F:192:ILE:CG2 | 1:F:193:ASN:N | 2.64 | 0.59 |
| 1:G:130:LYS:HD3 | 1:G:168:TYR:HB3 | 1.84 | 0.59 |
| 1:E:148:ALA:O | 1:E:152:LEU:HD23 | 2.03 | 0.59 |
| 1:G:3:THR:CG2 | 1:G:31:ASN:HD21 | 2.15 | 0.59 |
| 1:I:130:LYS:HG2 | 1:I:168:TYR:CD2 | 2.37 | 0.59 |
| 1:I:80:ASN:HD22 | 1:I:80:ASN:N | 2.01 | 0.59 |
| 1:D:4:VAL:HB | 1:D:30:LEU:HD23 | 1.85 | 0.59 |
| 1:F:99:SER:HA | 1:F:267:LEU:HG | 1.84 | 0.59 |
| 1:G:5:TYR:CD1 | 1:G:51:ALA:HB2 | 2.38 | 0.59 |
| 1:I:309:LYS:HB3 | 1:I:309:LYS:HZ3 | 1.68 | 0.59 |
| 1:I:5:TYR:CE1 | 1:I:51:ALA:HB2 | 2.38 | 0.59 |
| 1:B:245:PHE:O | 1:B:248:PHE:HB3 | 2.02 | 0.58 |
| 1:C:266:PRO:HD2 | 3:C:457:HOH:O | 2.03 | 0.58 |
| 1:D:79:ILE:HG12 | 1:D:96:VAL:HG22 | 1.85 | 0.58 |
| 1:C:106:VAL:HB | 3:C:511:HOH:O | 2.02 | 0.58 |
| 1:D:16:VAL:HG11 | 1:D:249:LEU:HD22 | 1.83 | 0.58 |
| 1:B:133:ILE:HD11 | 1:B:191:LEU:CD1 | 2.32 | 0.58 |
| 1:E:255:GLN:HE22 | 1:E:267:LEU:H | 1.51 | 0.58 |
| 1:C:130:LYS:HD2 | 1:C:131:ASN:ND2 | 2.19 | 0.58 |
| 1:E:252:LYS:HE2 | 1:E:252:LYS:H | 1.69 | 0.58 |
| 1:H:146:ILE:HD11 | 1:H:303:LEU:HD21 | 1.86 | 0.58 |
| 1:F:135:TYR:CD2 | 1:F:137:PRO:HD3 | 2.39 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:233:LEU:HD12 | 1:F:233:LEU:N | 2.18 | 0.58 |
| 1:C:252:LYS:HG2 | 1:C:268:ASN:OD1 | 2.03 | 0.58 |
| 1:D:34:LYS:HB3 | 1:D:37:GLN:CD | 2.24 | 0.58 |
| 1:D:96:VAL:HG13 | 3:D:513:HOH:O | 2.03 | 0.58 |
| 1:E:180:GLN:NE2 | 1:E:184:ASN:HD21 | 2.01 | 0.58 |
| 1:I:22:ARG:HG3 | 3:I:426:HOH:O | 2.02 | 0.58 |
| 1:D:4:VAL:HG13 | 1:D:53:VAL:HG22 | 1.85 | 0.58 |
| 1:H:17:ALA:HB1 | 1:H:28:VAL:CG2 | 2.33 | 0.58 |
| 1:B:8:GLN:HA | 1:B:57:GLU:CG | 2.34 | 0.58 |
| 1:C:106:VAL:CG2 | 1:C:211:THR:OG1 | 2.52 | 0.58 |
| 1:G:234:LYS:HB3 | 1:G:234:LYS:HZ2 | 1.68 | 0.58 |
| 1:B:59:ILE:N | 1:B:60:PRO:HD2 | 2.18 | 0.57 |
| 1:H:80:ASN:CA | 1:H:83:ARG:HG2 | 2.18 | 0.57 |
| 1:C:104:VAL:HG21 | 1:C:213:LEU:HD22 | 1.84 | 0.57 |
| 1:E:268:ASN:HD22 | 1:E:270:HIS:H | 1.52 | 0.57 |
| 1:B:197:TRP:CD1 | 1:B:211:THR:HG22 | 2.39 | 0.57 |
| 1:I:31:ASN:HD22 | 1:I:31:ASN:N | 2.00 | 0.57 |
| 1:F:178:ALA:HB3 | 1:F:192:ILE:HD11 | 1.86 | 0.57 |
| 1:G:255:GLN:O | 1:G:259:THR:HG23 | 2.04 | 0.57 |
| 1:A:106:VAL:HG13 | 1:A:213:LEU:HD23 | 1.85 | 0.57 |
| 1:D:184:ASN:HB2 | 1:D:186:GLU:HG3 | 1.87 | 0.57 |
| 1:D:51:ALA:HB3 | 1:D:233:LEU:HD22 | 1.86 | 0.57 |
| 1:F:85:LYS:HB2 | 3:F:514:HOH:O | 2.05 | 0.57 |
| 1:H:152:LEU:HD12 | 3:H:481:HOH:O | 2.05 | 0.57 |
| 1:I:34:LYS:HE3 | 1:I:36:ASP:OD2 | 2.05 | 0.57 |
| 1:E:255:GLN:NE2 | 1:E:268:ASN:H | 2.02 | 0.57 |
| 1:E:268:ASN:ND2 | 1:E:270:HIS:H | 2.02 | 0.57 |
| 1:G:43:LYS:HZ3 | 1:G:65:LEU:HD23 | 1.69 | 0.57 |
| 1:G:90:ALA:CB | 1:G:93:LYS:HA | 2.34 | 0.57 |
| 1:H:83:ARG:NE | 1:H:83:ARG:HA | 2.19 | 0.57 |
| 1:I:179:LEU:O | 1:I:183:GLU:HB2 | 2.05 | 0.57 |
| 1:C:268:ASN:HD22 | 1:C:269:PRO:N | 2.03 | 0.56 |
| 1:B:83:ARG:HB3 | 1:B:83:ARG:HH11 | 1.71 | 0.56 |
| 1:D:101:ARG:HH21 | 1:D:262:ARG:HE | 1.53 | 0.56 |
| 1:D:47:SER:HA | 1:D:235:SER:HB3 | 1.86 | 0.56 |
| 2:D:400:ZRC:O1B | 3:D:407:HOH:O | 2.18 | 0.56 |
| 1:F:147:VAL:HG22 | 1:F:295:GLU:HG3 | 1.86 | 0.56 |
| 1:B:136:VAL:HG21 | 1:B:175:ASN:HD22 | 1.71 | 0.56 |
| 1:D:255:GLN:CB | 1:D:271:VAL:HG21 | 2.35 | 0.56 |
| 1:D:77:SER:HA | 1:D:80:ASN:ND2 | 2.20 | 0.56 |
| 1:F:85:LYS:NZ | 1:F:219:ARG:NH1 | 2.53 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:141:ALA:CB | 1:B:193:ASN:HD21 | 2.18 | 0.56 |
| 1:C:197:TRP:HB3 | 1:C:213:LEU:HD11 | 1.87 | 0.56 |
| 1:C:22:ARG:HD3 | 1:D:184:ASN:HB3 | 1.87 | 0.56 |
| 1:G:20:PHE:C | 1:G:22:ARG:H | 2.09 | 0.56 |
| 1:G:47:SER:HA | 1:G:235:SER:HB3 | 1.86 | 0.56 |
| 1:G:9:HIS:CE1 | 1:G:11:GLU:HB3 | 2.40 | 0.56 |
| 1:B:8:GLN:NE2 | 1:B:57:GLU:HG2 | 2.21 | 0.56 |
| 1:D:252:LYS:HG3 | 1:D:253:GLU:H | 1.70 | 0.56 |
| 1:D:41:GLN:O | 1:D:45:GLU:HG3 | 2.04 | 0.56 |
| 1:H:92:LYS:HB2 | 1:H:94:ASP:OD1 | 2.06 | 0.56 |
| 1:D:57:GLU:N | 1:D:57:GLU:OE2 | 2.36 | 0.56 |
| 1:F:256:ARG:HG2 | 1:F:271:VAL:HG13 | 1.86 | 0.56 |
| 1:A:16:VAL:HG11 | 1:A:249:LEU:CD2 | 2.36 | 0.56 |
| 1:B:43:LYS:NZ | 1:B:64:THR:HB | 2.19 | 0.56 |
| 1:D:11:GLU:CD | 1:D:11:GLU:H | 2.09 | 0.56 |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:ND2 | 2.20 | 0.56 |
| 1:B:18:ASP:O | 1:B:22:ARG:HB2 | 2.06 | 0.56 |
| 1:I:155:GLU:OE1 | 1:I:298:HIS:HE1 | 1.89 | 0.56 |
| 1:D:107:TYR:HB2 | 1:D:112:LEU:HD12 | 1.88 | 0.56 |
| 1:G:303:LEU:HD12 | 1:G:309:LYS:HB2 | 1.88 | 0.56 |
| 1:F:177:VAL:HA | 1:F:180:GLN:CG | 2.36 | 0.56 |
| 1:G:79:ILE:HD11 | 1:G:93:LYS:HB2 | 1.87 | 0.56 |
| 1:I:288:VAL:HG12 | 1:I:289:SER:O | 2.05 | 0.56 |
| 1:D:137:PRO:HB3 | 1:D:308:MET:HE3 | 1.87 | 0.56 |
| 1:I:253:GLU:OE1 | 1:I:254:GLY:N | 2.38 | 0.56 |
| 1:B:159:LEU:O | 1:B:163:LYS:HG3 | 2.06 | 0.55 |
| 1:H:164:GLY:O | 1:H:168:TYR:HD1 | 1.89 | 0.55 |
| 1:G:41:GLN:O | 1:G:45:GLU:HG3 | 2.05 | 0.55 |
| 1:F:203:GLU:HG3 | 1:F:204:LYS:N | 2.20 | 0.55 |
| 1:H:236:SER:HB2 | 1:H:239:LYS:HG2 | 1.86 | 0.55 |
| 1:B:239:LYS:O | 1:B:243:LYS:HG3 | 2.06 | 0.55 |
| 1:E:182:VAL:HG22 | 1:E:187:ILE:HG23 | 1.88 | 0.55 |
| 1:A:47:SER:HA | 1:A:235:SER:CB | 2.34 | 0.55 |
| 1:D:144:GLU:HG3 | 1:D:224:LEU:HD21 | 1.89 | 0.55 |
| 1:H:26:ILE:HD13 | 1:H:241:GLU:HG3 | 1.89 | 0.55 |
| 1:H:57:GLU:N | 1:H:57:GLU:OE2 | 2.25 | 0.55 |
| 1:A:1:ASP:HB2 | 1:A:26:ILE:HG23 | 1.87 | 0.55 |
| 1:D:255:GLN:HB3 | 1:D:271:VAL:HG21 | 1.88 | 0.55 |
| 1:G:233:LEU:HD12 | 1:G:233:LEU:N | 2.22 | 0.55 |
| 1:A:9:HIS:HB3 | 1:A:12:ALA:HB2 | 1.87 | 0.55 |
| 1:A:170:LYS:HG3 | 3:A:450:HOH:O | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:233:LEU:CD1 | 1:B:233:LEU:N | 2.70 | 0.55 |
| 1:C:7:GLY:HA2 | 1:C:33:ALA:O | 2.07 | 0.55 |
| 1:G:71:LEU:O | 1:G:234:LYS:HD3 | 2.07 | 0.55 |
| 1:G:33:ALA:HB3 | 1:G:38:LEU:HD21 | 1.88 | 0.55 |
| 1:H:89:VAL:HG12 | 3:H:456:HOH:O | 2.07 | 0.55 |
| 1:I:58:GLN:O | 1:I:62:LEU:HD13 | 2.07 | 0.55 |
| 1:D:10:LYS:O | 1:D:14:GLN:HG3 | 2.07 | 0.55 |
| 1:H:61:ALA:O | 1:H:64:THR:HG22 | 2.07 | 0.55 |
| 1:I:255:GLN:CB | 1:I:271:VAL:HG21 | 2.36 | 0.55 |
| 1:H:21:THR:HA | 1:H:26:ILE:O | 2.07 | 0.55 |
| 1:H:72:GLU:OE2 | 1:H:239:LYS:HD3 | 2.07 | 0.55 |
| 1:I:98:LEU:O | 1:I:267:LEU:HB2 | 2.07 | 0.55 |
| 1:B:141:ALA:HB1 | 1:B:193:ASN:HD21 | 1.72 | 0.54 |
| 1:E:130:LYS:HD3 | 1:E:168:TYR:HD2 | 1.72 | 0.54 |
| 1:F:85:LYS:HZ3 | 1:F:219:ARG:HH12 | 1.54 | 0.54 |
| 1:A:9:HIS:ND1 | 1:A:262:ARG:HD3 | 2.22 | 0.54 |
| 1:H:40:GLY:O | 1:H:44:GLU:HG3 | 2.06 | 0.54 |
| 1:I:27:LYS:C | 1:I:27:LYS:HD3 | 2.27 | 0.54 |
| 1:B:91:ALA:O | 1:B:93:LYS:HE3 | 2.07 | 0.54 |
| 1:G:71:LEU:CB | 1:G:94:ASP:HB2 | 2.37 | 0.54 |
| 1:G:256:ARG:HG2 | 1:G:271:VAL:HG13 | 1.88 | 0.54 |
| 1:G:72:GLU:OE1 | 1:G:239:LYS:HD3 | 2.07 | 0.54 |
| 1:G:92:LYS:C | 1:G:93:LYS:HG2 | 2.28 | 0.54 |
| 1:H:192:ILE:HD13 | 1:H:192:ILE:H | 1.70 | 0.54 |
| 1:D:39:ALA:O | 1:D:43:LYS:HG2 | 2.08 | 0.54 |
| 1:C:143:LEU:HA | 1:C:146:ILE:HD12 | 1.89 | 0.54 |
| 1:H:245:PHE:O | 1:H:248:PHE:HB3 | 2.07 | 0.54 |
| 1:C:262:ARG:CG | 1:C:264:GLU:HG3 | 2.30 | 0.54 |
| 1:G:146:ILE:HD13 | 1:G:162:LEU:HD11 | 1.89 | 0.54 |
| 1:G:303:LEU:HD22 | 1:G:308:MET:HE1 | 1.89 | 0.54 |
| 1:I:151:LYS:HD2 | 1:I:288:VAL:HG13 | 1.88 | 0.54 |
| 1:C:51:ALA:HB3 | 1:C:233:LEU:CD2 | 2.38 | 0.54 |
| 1:I:183:GLU:OE1 | 1:I:211:THR:HG23 | 2.08 | 0.54 |
| 1:I:34:LYS:HE2 | 1:I:37:GLN:HG3 | 1.89 | 0.54 |
| 1:A:252:LYS:NZ | 1:H:237:GLN:HB3 | 2.23 | 0.54 |
| 1:C:236:SER:O | 1:C:237:GLN:HB2 | 2.08 | 0.54 |
| 1:D:34:LYS:HE3 | 1:D:36:ASP:H | 1.73 | 0.54 |
| 1:F:147:VAL:HG13 | 1:F:295:GLU:CG | 2.37 | 0.54 |
| 1:G:183:GLU:HA | 1:G:211:THR:HG23 | 1.90 | 0.54 |
| 1:I:146:ILE:O | 1:I:150:VAL:HG23 | 2.08 | 0.54 |
| 1:C:303:LEU:CG | 1:C:309:LYS:HA | 2.38 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:202:ARG:NH2 | 1:E:274:THR:CG2 | 2.57 | 0.54 |
| 1:H:255:GLN:HB2 | 1:H:271:VAL:HG21 | 1.88 | 0.54 |
| 1:C:130:LYS:HD3 | 1:C:130:LYS:C | 2.29 | 0.53 |
| 1:I:137:PRO:HA | 1:I:142:PHE:CD2 | 2.43 | 0.53 |
| 1:I:57:GLU:HG2 | 1:I:58:GLN:HG3 | 1.89 | 0.53 |
| 1:C:51:ALA:HB3 | 1:C:233:LEU:HD21 | 1.90 | 0.53 |
| 1:E:216:VAL:HG13 | 3:E:436:HOH:O | 2.08 | 0.53 |
| 1:F:173:ALA:HB3 | 1:F:174:LYS:CE | 2.38 | 0.53 |
| 1:C:166:LYS:HD2 | 3:C:417:HOH:O | 2.07 | 0.53 |
| 1:G:303:LEU:CD1 | 1:G:309:LYS:HB2 | 2.38 | 0.53 |
| 1:A:75:PRO:HD3 | 1:A:243:LYS:HZ2 | 1.73 | 0.53 |
| 1:C:125:ALA:HB1 | 1:C:164:GLY:HA3 | 1.90 | 0.53 |
| 1:G:242:ALA:O | 1:G:246:VAL:HG23 | 2.09 | 0.53 |
| 1:G:255:GLN:HB2 | 1:G:271:VAL:HG21 | 1.89 | 0.53 |
| 1:D:262:ARG:HG2 | 1:D:264:GLU:HG3 | 1.90 | 0.53 |
| 1:G:104:VAL:HG12 | 1:G:105:VAL:H | 1.72 | 0.53 |
| 1:E:196:TYR:O | 1:E:200:PHE:CD1 | 2.62 | 0.53 |
| 1:E:268:ASN:HD22 | 1:E:269:PRO:N | 2.06 | 0.53 |
| 1:F:41:GLN:O | 1:F:45:GLU:HG3 | 2.09 | 0.53 |
| 1:B:9:HIS:NE2 | 1:B:11:GLU:HG2 | 2.23 | 0.53 |
| 1:C:51:ALA:O | 1:C:233:LEU:HD22 | 2.09 | 0.53 |
| 1:E:43:LYS:HA | 3:E:527:HOH:O | 2.08 | 0.53 |
| 1:F:8:GLN:OE1 | 1:F:12:ALA:HB3 | 2.08 | 0.53 |
| 1:I:252:LYS:CD | 1:I:256:ARG:HD2 | 2.39 | 0.53 |
| 1:B:22:ARG:O | 1:F:110:ARG:NH1 | 2.39 | 0.53 |
| 1:G:255:GLN:CB | 1:G:271:VAL:HG21 | 2.39 | 0.53 |
| 1:B:233:LEU:HD12 | 1:B:233:LEU:N | 2.24 | 0.53 |
| 1:G:67:ALA:HA | 1:G:92:LYS:NZ | 2.24 | 0.53 |
| 1:H:114:GLU:HA | 1:H:117:LEU:HD22 | 1.90 | 0.53 |
| 1:E:252:LYS:CD | 1:E:252:LYS:H | 2.22 | 0.53 |
| 1:F:255:GLN:HB2 | 1:F:271:VAL:HG21 | 1.90 | 0.53 |
| 1:G:256:ARG:NH1 | 1:G:256:ARG:HB3 | 2.23 | 0.53 |
| 1:G:33:ALA:HB3 | 1:G:38:LEU:HD22 | 1.89 | 0.53 |
| 1:A:297:GLU:HA | 1:A:297:GLU:OE2 | 2.09 | 0.52 |
| 1:G:21:THR:HG22 | 1:G:21:THR:O | 2.09 | 0.52 |
| 1:E:79:ILE:HG12 | 1:E:96:VAL:HG22 | 1.90 | 0.52 |
| 1:B:22:ARG:HG2 | 1:F:184:ASN:O | 2.09 | 0.52 |
| 1:B:291:THR:CG2 | 1:B:296:LYS:HE2 | 2.39 | 0.52 |
| 1:D:145:GLN:O | 1:D:149:ILE:HG13 | 2.10 | 0.52 |
| 1:D:233:LEU:N | 1:D:233:LEU:HD12 | 2.24 | 0.52 |
| 1:G:121:VAL:CG1 | 1:G:222:GLY:HA3 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:259:THR:OG1 | 1:C:266:PRO:HG3 | 2.09 | 0.52 |
| 1:I:253:GLU:CD | 1:I:254:GLY:H | 2.12 | 0.52 |
| 1:B:36:ASP:HB2 | 3:B:489:HOH:O | 2.09 | 0.52 |
| 1:C:48:ARG:HE | 1:C:237:GLN:HE21 | 1.54 | 0.52 |
| 1:E:252:LYS:CE | 1:E:252:LYS:H | 2.23 | 0.52 |
| 1:I:122:LEU:HA | 1:I:161:TRP:CD1 | 2.44 | 0.52 |
| 1:E:161:TRP:CE3 | 1:E:162:LEU:HD12 | 2.45 | 0.52 |
| 1:H:105:VAL:HG23 | 3:H:480:HOH:O | 2.09 | 0.52 |
| 1:H:16:VAL:HG11 | 1:H:249:LEU:HD23 | 1.91 | 0.52 |
| 1:C:33:ALA:HB3 | 1:C:38:LEU:HD21 | 1.92 | 0.52 |
| 1:D:6:ASN:OD1 | 1:D:55:TYR:HD2 | 1.93 | 0.52 |
| 1:H:268:ASN:HD22 | 1:H:271:VAL:CG2 | 2.18 | 0.52 |
| 1:B:216:VAL:HG23 | 3:B:437:HOH:O | 2.10 | 0.52 |
| 1:G:59:ILE:N | 1:G:60:PRO:CD | 2.73 | 0.52 |
| 1:H:240:ASP:HA | 1:H:243:LYS:HD2 | 1.91 | 0.52 |
| 1:H:304:GLU:HA | 1:H:309:LYS:O | 2.09 | 0.52 |
| 1:H:66:SER:O | 1:H:92:LYS:HE2 | 2.10 | 0.52 |
| 1:I:34:LYS:HE2 | 1:I:37:GLN:CG | 2.40 | 0.52 |
| 1:I:34:LYS:HG2 | 1:I:37:GLN:CD | 2.30 | 0.52 |
| 1:I:59:ILE:N | 1:I:60:PRO:CD | 2.73 | 0.52 |
| 1:D:33:ALA:HB1 | 1:D:37:GLN:OE1 | 2.10 | 0.52 |
| 1:G:80:ASN:OD1 | 1:G:83:ARG:NH2 | 2.41 | 0.52 |
| 1:A:8:GLN:CG | 1:A:9:HIS:H | 2.23 | 0.51 |
| 1:C:121:VAL:HG23 | 1:C:216:VAL:HG21 | 1.92 | 0.51 |
| 1:C:300:THR:O | 1:C:304:GLU:HG3 | 2.10 | 0.51 |
| 1:C:304:GLU:HG2 | 1:C:309:LYS:HG3 | 1.91 | 0.51 |
| 1:C:4:VAL:HG22 | 1:C:53:VAL:HB | 1.92 | 0.51 |
| 1:D:103:ARG:HD2 | 1:D:145:GLN:HB2 | 1.92 | 0.51 |
| 1:F:5:TYR:CD1 | 1:F:51:ALA:HB2 | 2.44 | 0.51 |
| 1:H:152:LEU:HD11 | 1:H:286:PRO:HB2 | 1.92 | 0.51 |
| 1:I:245:PHE:O | 1:I:248:PHE:HB3 | 2.09 | 0.51 |
| 1:F:262:ARG:HH11 | 1:F:264:GLU:HG3 | 1.74 | 0.51 |
| 1:G:2:ILE:O | 1:G:2:ILE:HG13 | 2.09 | 0.51 |
| 1:I:140:GLY:O | 1:I:144:GLU:HG2 | 2.10 | 0.51 |
| 1:D:26:ILE:HD13 | 1:D:241:GLU:HB3 | 1.91 | 0.51 |
| 1:G:104:VAL:HG11 | 1:G:213:LEU:HB3 | 1.93 | 0.51 |
| 1:H:6:ASN:OD1 | 1:H:8:GLN:HB3 | 2.11 | 0.51 |
| 1:I:259:THR:HG21 | 1:I:266:PRO:CG | 2.29 | 0.51 |
| 1:I:34:LYS:HG2 | 1:I:37:GLN:OE1 | 2.09 | 0.51 |
| 1:B:202:ARG:NH2 | 1:B:274:THR:O | 2.43 | 0.51 |
| 1:G:252:LYS:O | 1:G:256:ARG:HG3 | 2.10 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:110:ARG:NH2 | 1:A:183:GLU:O | 2.32 | 0.51 |
| 1:I:20:PHE:CZ | 1:I:26:ILE:HD12 | 2.45 | 0.51 |
| 1:A:9:HIS:HB3 | 1:A:12:ALA:HB3 | 1.92 | 0.51 |
| 1:C:1:ASP:OD1 | 1:C:27:LYS:HG2 | 2.11 | 0.51 |
| 1:D:10:LYS:HD2 | 1:D:14:GLN:NE2 | 2.25 | 0.51 |
| 1:F:114:GLU:O | 1:F:117:LEU:HB2 | 2.10 | 0.51 |
| 1:I:18:ASP:HB3 | 1:I:22:ARG:NH1 | 2.21 | 0.51 |
| 1:E:45:GLU:HG3 | 1:E:49:SER:HB2 | 1.91 | 0.51 |
| 1:F:137:PRO:HA | 1:F:142:PHE:CD2 | 2.46 | 0.51 |
| 1:I:121:VAL:HB | 1:I:222:GLY:HA3 | 1.92 | 0.51 |
| 1:A:245:PHE:O | 1:A:249:LEU:HG | 2.10 | 0.51 |
| 1:C:174:LYS:HG3 | 1:C:177:VAL:HG23 | 1.93 | 0.51 |
| 1:D:106:VAL:HG22 | 1:D:211:THR:OG1 | 2.11 | 0.51 |
| 1:E:146:ILE:HG12 | 1:E:162:LEU:HD11 | 1.93 | 0.51 |
| 1:G:136:VAL:HG21 | 1:G:175:ASN:HD22 | 1.76 | 0.51 |
| 1:I:234:LYS:O | 1:I:239:LYS:NZ | 2.44 | 0.51 |
| 1:I:252:LYS:HZ3 | 1:I:256:ARG:HD2 | 1.76 | 0.51 |
| 1:C:109:THR:HG21 | 1:C:212:ARG:NE | 2.26 | 0.51 |
| 1:C:43:LYS:HE3 | 1:C:64:THR:HG22 | 1.93 | 0.51 |
| 1:F:191:LEU:O | 1:F:192:ILE:HG13 | 2.11 | 0.51 |
| 1:H:239:LYS:O | 1:H:243:LYS:HG3 | 2.11 | 0.51 |
| 1:I:34:LYS:CE | 1:I:37:GLN:HG3 | 2.40 | 0.51 |
| 1:C:255:GLN:CB | 1:C:271:VAL:HG21 | 2.41 | 0.51 |
| 1:E:255:GLN:O | 1:E:259:THR:HB | 2.11 | 0.51 |
| 1:F:51:ALA:O | 1:F:233:LEU:HD22 | 2.11 | 0.51 |
| 1:G:137:PRO:HA | 1:G:142:PHE:CD2 | 2.46 | 0.51 |
| 1:I:1:ASP:OD1 | 1:I:27:LYS:HB3 | 2.12 | 0.51 |
| 1:D:236:SER:O | 1:D:239:LYS:HG3 | 2.11 | 0.50 |
| 1:E:256:ARG:HD3 | 3:E:504:HOH:O | 2.11 | 0.50 |
| 1:F:54:PHE:CE2 | 1:F:56:SER:HB2 | 2.46 | 0.50 |
| 1:I:79:ILE:HG22 | 1:I:83:ARG:NH1 | 2.26 | 0.50 |
| 1:B:174:LYS:NZ | 2:B:400:ZRC:O23 | 2.45 | 0.50 |
| 1:C:109:THR:HG21 | 1:C:212:ARG:CD | 2.41 | 0.50 |
| 1:C:15:ALA:HB2 | 1:C:261:VAL:HG11 | 1.93 | 0.50 |
| 1:D:76:ALA:O | 1:D:80:ASN:ND2 | 2.44 | 0.50 |
| 1:E:77:SER:O | 1:E:81:GLU:HG3 | 2.11 | 0.50 |
| 1:H:234:LYS:HE2 | 3:H:450:HOH:O | 2.11 | 0.50 |
| 1:H:252:LYS:HE2 | 1:H:270:HIS:CB | 2.41 | 0.50 |
| 1:I:248:PHE:CD1 | 1:I:253:GLU:OE1 | 2.63 | 0.50 |
| 1:F:58:GLN:HG3 | 1:F:61:ALA:H | 1.76 | 0.50 |
| 1:H:38:LEU:HB3 | 1:H:54:PHE:HE1 | 1.75 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:80:ASN:HA | 1:I:83:ARG:CG | 2.30 | 0.50 |
| 1:D:34:LYS:HD2 | 1:D:35:GLY:N | 2.26 | 0.50 |
| 1:E:255:GLN:CB | 1:E:271:VAL:HG21 | 2.41 | 0.50 |
| 1:G:51:ALA:O | 1:G:233:LEU:HD22 | 2.11 | 0.50 |
| 1:G:258:LEU:HD11 | 1:G:264:GLU:OE1 | 2.11 | 0.50 |
| 1:C:130:LYS:HE2 | 1:C:168:TYR:HA | 1.94 | 0.50 |
| 1:E:74:LEU:CD1 | 1:E:96:VAL:HG23 | 2.42 | 0.50 |
| 1:B:111:LYS:HA | 1:B:111:LYS:HE2 | 1.94 | 0.50 |
| 1:C:52:ASP:HA | 1:C:236:SER:CB | 2.37 | 0.50 |
| 1:C:252:LYS:HE2 | 1:C:270:HIS:CD2 | 2.46 | 0.50 |
| 1:D:34:LYS:O | 1:D:37:GLN:HG2 | 2.11 | 0.50 |
| 1:F:133:ILE:HD11 | 1:F:191:LEU:HD13 | 1.93 | 0.50 |
| 1:D:217:ARG:NH1 | 1:D:278:GLU:OE2 | 2.45 | 0.50 |
| 1:G:3:THR:HG23 | 1:G:31:ASN:HD21 | 1.77 | 0.50 |
| 1:C:195:TYR:HE2 | 1:C:196:TYR:CE1 | 2.29 | 0.50 |
| 1:E:6:ASN:HD21 | 1:E:8:GLN:HB2 | 1.75 | 0.50 |
| 1:H:236:SER:HB2 | 1:H:239:LYS:CG | 2.42 | 0.50 |
| 1:E:252:LYS:HE2 | 1:E:252:LYS:N | 2.27 | 0.49 |
| 1:G:12:ALA:O | 1:G:16:VAL:HG22 | 2.12 | 0.49 |
| 1:E:304:GLU:HG3 | 1:E:309:LYS:HD3 | 1.92 | 0.49 |
| 1:E:8:GLN:NE2 | 1:E:55:TYR:CE1 | 2.79 | 0.49 |
| 1:A:269:PRO:HG3 | 1:H:48:ARG:CZ | 2.41 | 0.49 |
| 1:H:53:VAL:CG2 | 1:H:242:ALA:HB1 | 2.42 | 0.49 |
| 1:A:37:GLN:O | 1:A:41:GLN:HB2 | 2.12 | 0.49 |
| 1:D:42:ILE:CD1 | 1:D:233:LEU:HD21 | 2.39 | 0.49 |
| 1:D:287:GLN:OE1 | 1:D:288:VAL:N | 2.46 | 0.49 |
| 1:I:80:ASN:HB3 | 1:I:83:ARG:CZ | 2.42 | 0.49 |
| 1:A:146:ILE:HD11 | 1:A:302:LEU:CD1 | 2.42 | 0.49 |
| 1:A:51:ALA:O | 1:A:233:LEU:HD22 | 2.13 | 0.49 |
| 1:B:89:VAL:HG22 | 3:B:408:HOH:O | 2.11 | 0.49 |
| 1:D:71:LEU:HD13 | 1:D:231:ALA:CB | 2.43 | 0.49 |
| 1:E:297:GLU:O | 1:E:301:ARG:HG2 | 2.12 | 0.49 |
| 1:H:122:LEU:HD21 | 1:H:149:ILE:HD13 | 1.94 | 0.49 |
| 1:D:217:ARG:HA | 1:D:283:LEU:O | 2.12 | 0.49 |
| 1:D:4:VAL:HG13 | 1:D:53:VAL:CG2 | 2.42 | 0.49 |
| 1:G:121:VAL:HG11 | 1:G:222:GLY:HA3 | 1.93 | 0.49 |
| 1:A:142:PHE:O | 1:A:146:ILE:HG22 | 2.13 | 0.49 |
| 1:A:4:VAL:HB | 1:A:30:LEU:HD23 | 1.93 | 0.49 |
| 1:C:90:ALA:HB2 | 1:C:95:TRP:CE2 | 2.46 | 0.49 |
| 1:D:117:LEU:HD12 | 1:D:117:LEU:N | 2.27 | 0.49 |
| 1:D:268:ASN:HD22 | 1:D:268:ASN:C | 2.15 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:148:ALA:O | 1:E:152:LEU:CD2 | 2.61 | 0.49 |
| 1:G:66:SER:OG | 1:G:92:LYS:HE3 | 2.13 | 0.49 |
| 1:I:38:LEU:O | 1:I:42:ILE:HG13 | 2.13 | 0.49 |
| 1:C:301:ARG:HA | 1:C:304:GLU:OE1 | 2.13 | 0.49 |
| 1:E:41:GLN:O | 1:E:45:GLU:HG2 | 2.11 | 0.49 |
| 1:H:106:VAL:HB | 1:H:192:ILE:HD11 | 1.94 | 0.49 |
| 1:H:54:PHE:HD2 | 1:H:62:LEU:HD23 | 1.78 | 0.49 |
| 1:A:248:PHE:O | 1:A:254:GLY:HA3 | 2.13 | 0.49 |
| 1:C:40:GLY:O | 1:C:44:GLU:HG3 | 2.12 | 0.49 |
| 1:E:191:LEU:HD22 | 1:E:191:LEU:N | 2.27 | 0.49 |
| 1:G:234:LYS:HB3 | 1:G:234:LYS:HZ3 | 1.78 | 0.49 |
| 1:A:110:ARG:HE | 1:A:210:HIS:CG | 2.31 | 0.49 |
| 1:C:48:ARG:NH2 | 1:C:237:GLN:HG3 | 2.26 | 0.49 |
| 1:D:101:ARG:NH2 | 1:D:262:ARG:HE | 2.11 | 0.49 |
| 1:F:155:GLU:OE2 | 1:F:298:HIS:HE1 | 1.96 | 0.49 |
| 1:H:2:ILE:HG23 | 1:H:2:ILE:O | 2.13 | 0.49 |
| 1:I:268:ASN:HB3 | 1:I:271:VAL:HG23 | 1.95 | 0.49 |
| 1:C:122:LEU:HA | 1:C:161:TRP:CD1 | 2.48 | 0.49 |
| 1:D:256:ARG:NH2 | 1:D:274:THR:HG22 | 2.27 | 0.49 |
| 1:D:37:GLN:HG3 | 3:D:494:HOH:O | 2.13 | 0.49 |
| 1:F:140:GLY:O | 1:F:144:GLU:HG2 | 2.13 | 0.49 |
| 1:H:81:GLU:HB3 | 1:H:250:ALA:O | 2.13 | 0.49 |
| 1:D:8:GLN:NE2 | 1:D:101:ARG:HH22 | 2.11 | 0.48 |
| 1:D:232:VAL:HG23 | 1:D:246:VAL:HG21 | 1.95 | 0.48 |
| 1:I:105:VAL:HG22 | 1:I:191:LEU:HD23 | 1.94 | 0.48 |
| 1:D:101:ARG:NH1 | 1:D:264:GLU:HG2 | 2.28 | 0.48 |
| 1:E:255:GLN:HB2 | 1:E:271:VAL:HG21 | 1.95 | 0.48 |
| 1:A:304:GLU:HG2 | 1:A:309:LYS:CG | 2.39 | 0.48 |
| 1:D:17:ALA:O | 1:D:20:PHE:HB3 | 2.13 | 0.48 |
| 1:F:111:LYS:HD2 | 1:F:111:LYS:N | 2.28 | 0.48 |
| 1:F:237:GLN:O | 1:F:238:ASN:ND2 | 2.46 | 0.48 |
| 1:H:2:ILE:C | 1:H:2:ILE:HD13 | 2.34 | 0.48 |
| 1:H:99:SER:OG | 1:H:264:GLU:HG2 | 2.13 | 0.48 |
| 1:I:76:ALA:O | 1:I:80:ASN:ND2 | 2.46 | 0.48 |
| 1:B:256:ARG:HA | 1:B:259:THR:HG22 | 1.94 | 0.48 |
| 1:C:255:GLN:HB2 | 1:C:271:VAL:HG21 | 1.95 | 0.48 |
| 1:C:53:VAL:HG23 | 1:C:242:ALA:HB1 | 1.96 | 0.48 |
| 1:E:256:ARG:O | 1:E:259:THR:HG22 | 2.13 | 0.48 |
| 1:F:191:LEU:C | 1:F:192:ILE:HG13 | 2.34 | 0.48 |
| 1:G:245:PHE:O | 1:G:249:LEU:HG | 2.13 | 0.48 |
| 1:I:100:GLY:O | 1:I:264:GLU:HG3 | 2.12 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:107:TYR:O | 1:I:211:THR:HA | 2.14 | 0.48 |
| 1:I:309:LYS:HZ2 | 1:I:309:LYS:HB3 | 1.78 | 0.48 |
| 1:B:8:GLN:HG3 | 1:B:9:HIS:N | 2.28 | 0.48 |
| 1:C:46:GLY:O | 1:C:47:SER:C | 2.51 | 0.48 |
| 1:C:72:GLU:OE1 | 1:C:73:PRO:HD2 | 2.13 | 0.48 |
| 1:D:197:TRP:CD1 | 1:D:211:THR:HG23 | 2.47 | 0.48 |
| 1:D:74:LEU:HD12 | 1:D:96:VAL:HG23 | 1.95 | 0.48 |
| 1:E:200:PHE:CD1 | 1:E:200:PHE:N | 2.81 | 0.48 |
| 1:E:200:PHE:HD1 | 1:E:200:PHE:N | 2.11 | 0.48 |
| 1:G:303:LEU:O | 1:G:303:LEU:HD13 | 2.13 | 0.48 |
| 1:D:90:ALA:HB2 | 1:D:95:TRP:CD2 | 2.49 | 0.48 |
| 1:F:72:GLU:OE2 | 1:F:239:LYS:HD3 | 2.14 | 0.48 |
| 1:A:111:LYS:HE2 | 1:A:111:LYS:HB3 | 1.74 | 0.48 |
| 1:C:22:ARG:HG2 | 3:C:433:HOH:O | 2.13 | 0.48 |
| 1:G:220:ASP:OD1 | 1:G:221:PRO:HD2 | 2.14 | 0.48 |
| 1:G:47:SER:HA | 1:G:235:SER:CB | 2.43 | 0.48 |
| 1:I:119:LYS:O | 1:I:216:VAL:CG2 | 2.60 | 0.48 |
| 1:B:255:GLN:O | 1:B:259:THR:HG22 | 2.14 | 0.48 |
| 1:C:59:ILE:N | 1:C:60:PRO:HD2 | 2.29 | 0.48 |
| 1:D:43:LYS:HZ3 | 1:D:68:ALA:CB | 2.26 | 0.48 |
| 1:F:58:GLN:HB2 | 3:F:508:HOH:O | 2.13 | 0.48 |
| 1:G:71:LEU:HB3 | 1:G:94:ASP:HB2 | 1.96 | 0.48 |
| 1:H:256:ARG:HH11 | 1:H:256:ARG:CB | 2.26 | 0.48 |
| 1:B:117:LEU:HD22 | 1:B:214:ASN:HB2 | 1.95 | 0.47 |
| 1:C:183:GLU:HG2 | 1:C:211:THR:CG2 | 2.44 | 0.47 |
| 1:F:240:ASP:OD1 | 1:F:241:GLU:HG3 | 2.14 | 0.47 |
| 1:G:256:ARG:HH11 | 1:G:256:ARG:CB | 2.27 | 0.47 |
| 1:G:282:LYS:HA | 1:G:282:LYS:HE2 | 1.95 | 0.47 |
| 1:H:143:LEU:O | 1:H:147:VAL:HG23 | 2.13 | 0.47 |
| 1:H:76:ALA:O | 1:H:80:ASN:ND2 | 2.46 | 0.47 |
| 1:B:9:HIS:CE1 | 1:B:11:GLU:HG2 | 2.49 | 0.47 |
| 1:D:180:GLN:NE2 | 1:D:184:ASN:OD1 | 2.46 | 0.47 |
| 1:E:41:GLN:O | 1:E:42:ILE:C | 2.51 | 0.47 |
| 1:G:2:ILE:HG21 | 1:G:241:GLU:O | 2.14 | 0.47 |
| 1:G:5:TYR:CB | 1:G:38:LEU:HD12 | 2.44 | 0.47 |
| 1:I:80:ASN:ND2 | 1:I:80:ASN:N | 2.61 | 0.47 |
| 1:C:113:SER:C | 1:C:115:LYS:N | 2.67 | 0.47 |
| 1:D:197:TRP:NE1 | 1:D:211:THR:HG23 | 2.30 | 0.47 |
| 1:D:34:LYS:HD2 | 1:D:35:GLY:H | 1.79 | 0.47 |
| 1:G:237:GLN:NE2 | 1:G:237:GLN:HA | 2.29 | 0.47 |
| 1:B:117:LEU:HD12 | 1:B:117:LEU:N | 2.29 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:59:ILE:N | 1:E:60:PRO:CD | 2.78 | 0.47 |
| 1:G:233:LEU:HD12 | 1:G:233:LEU:H | 1.80 | 0.47 |
| 1:I:134:GLY:HA2 | 1:I:170:LYS:O | 2.15 | 0.47 |
| 1:I:252:LYS:HD2 | 1:I:256:ARG:HD2 | 1.96 | 0.47 |
| 1:C:170:LYS:HB2 | 1:C:170:LYS:HE3 | 1.67 | 0.47 |
| 1:D:267:LEU:CD2 | 1:D:280:ILE:HD13 | 2.44 | 0.47 |
| 1:D:279:PRO:HD2 | 1:D:282:LYS:HG3 | 1.96 | 0.47 |
| 1:E:151:LYS:HE3 | 1:E:295:GLU:OE1 | 2.13 | 0.47 |
| 1:I:72:GLU:HG2 | 1:I:234:LYS:HA | 1.97 | 0.47 |
| 1:I:252:LYS:O | 1:I:256:ARG:HG3 | 2.15 | 0.47 |
| 1:A:279:PRO:CG | 1:A:282:LYS:HE3 | 2.44 | 0.47 |
| 1:C:239:LYS:O | 1:C:243:LYS:HG3 | 2.15 | 0.47 |
| 1:D:43:LYS:HZ1 | 1:D:64:THR:C | 2.18 | 0.47 |
| 1:F:101:ARG:HB2 | 1:F:101:ARG:HH11 | 1.79 | 0.47 |
| 1:H:133:ILE:HG23 | 1:H:133:ILE:O | 2.14 | 0.47 |
| 1:I:135:TYR:O | 1:I:171:PRO:HA | 2.15 | 0.47 |
| 1:I:98:LEU:C | 1:I:267:LEU:HD22 | 2.34 | 0.47 |
| 1:D:142:PHE:HE2 | 1:D:308:MET:HE1 | 1.80 | 0.47 |
| 1:E:74:LEU:HD13 | 1:E:96:VAL:HG23 | 1.97 | 0.47 |
| 1:F:138:THR:HG23 | 3:F:441:HOH:O | 2.13 | 0.47 |
| 1:G:21:THR:O | 1:G:25:GLY:HA2 | 2.15 | 0.47 |
| 1:I:127:PRO:HA | 1:I:168:TYR:CD2 | 2.50 | 0.47 |
| 1:F:59:ILE:N | 1:F:60:PRO:CD | 2.77 | 0.47 |
| 1:H:59:ILE:N | 1:H:60:PRO:CD | 2.77 | 0.47 |
| 1:A:57:GLU:HG2 | 1:A:101:ARG:NH1 | 2.29 | 0.47 |
| 1:A:217:ARG:HG2 | 1:A:217:ARG:HH11 | 1.80 | 0.47 |
| 1:C:147:VAL:O | 1:C:151:LYS:HG3 | 2.14 | 0.47 |
| 1:D:197:TRP:HE1 | 1:D:211:THR:HG23 | 1.80 | 0.47 |
| 1:D:240:ASP:O | 1:D:244:LYS:HG3 | 2.15 | 0.47 |
| 1:F:262:ARG:HH11 | 1:F:262:ARG:HG2 | 1.79 | 0.47 |
| 1:G:303:LEU:HD22 | 1:G:308:MET:HE3 | 1.97 | 0.47 |
| 1:A:10:LYS:HE2 | 1:I:81:GLU:OE2 | 2.15 | 0.46 |
| 1:A:135:TYR:CD2 | 1:A:137:PRO:HD3 | 2.50 | 0.46 |
| 1:B:6:ASN:HD22 | 1:B:32:SER:HB3 | 1.79 | 0.46 |
| 1:E:122:LEU:HA | 1:E:161:TRP:CD1 | 2.49 | 0.46 |
| 1:G:71:LEU:HB2 | 1:G:94:ASP:HB2 | 1.96 | 0.46 |
| 1:H:71:LEU:HD23 | 1:H:233:LEU:HD12 | 1.97 | 0.46 |
| 1:H:55:TYR:CE1 | 1:H:249:LEU:HD13 | 2.51 | 0.46 |
| 1:D:256:ARG:NH2 | 1:D:274:THR:CG2 | 2.78 | 0.46 |
| 1:F:103:ARG:NH1 | 3:F:411:HOH:O | 2.48 | 0.46 |
| 1:H:183:GLU:OE2 | 1:H:210:HIS:HB2 | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:H:99:SER:HB2 | 1:H:264:GLU:HG2 | 1.98 | 0.46 |
| 1:H:252:LYS:HE2 | 1:H:270:HIS:HB3 | 1.97 | 0.46 |
| 1:H:146:ILE:CD1 | 1:H:303:LEU:HD21 | 2.44 | 0.46 |
| 1:A:106:VAL:HG13 | 1:A:213:LEU:CD2 | 2.45 | 0.46 |
| 1:D:33:ALA:HB3 | 1:D:38:LEU:HG | 1.97 | 0.46 |
| 1:D:65:LEU:N | 1:D:65:LEU:HD22 | 2.30 | 0.46 |
| 1:F:228:SER:HB3 | 3:F:500:HOH:O | 2.15 | 0.46 |
| 1:D:43:LYS:NZ | 1:D:68:ALA:HB2 | 2.30 | 0.46 |
| 1:E:112:LEU:N | 1:E:112:LEU:HD22 | 2.31 | 0.46 |
| 1:E:109:THR:HG21 | 1:E:212:ARG:HG2 | 1.96 | 0.46 |
| 1:G:112:LEU:HD21 | 1:G:132:ARG:HH12 | 1.79 | 0.46 |
| 1:G:301:ARG:O | 1:G:305:GLN:HG3 | 2.15 | 0.46 |
| 1:G:3:THR:CG2 | 1:G:31:ASN:ND2 | 2.79 | 0.46 |
| 1:H:122:LEU:HA | 1:H:161:TRP:CD1 | 2.51 | 0.46 |
| 1:H:69:ASN:HB3 | 1:H:92:LYS:HZ2 | 1.80 | 0.46 |
| 1:I:18:ASP:O | 1:I:22:ARG:NH1 | 2.49 | 0.46 |
| 1:B:258:LEU:C | 1:B:260:ALA:H | 2.19 | 0.46 |
| 1:H:135:TYR:CE2 | 1:H:308:MET:HE3 | 2.50 | 0.46 |
| 1:H:99:SER:CB | 1:H:264:GLU:HG2 | 2.46 | 0.46 |
| 1:I:101:ARG:HG2 | 1:I:264:GLU:CD | 2.36 | 0.46 |
| 1:A:279:PRO:HD2 | 1:A:282:LYS:HZ2 | 1.79 | 0.46 |
| 1:A:146:ILE:HD11 | 1:A:302:LEU:HD12 | 1.97 | 0.46 |
| 1:B:117:LEU:HD12 | 1:B:117:LEU:H | 1.79 | 0.46 |
| 1:B:117:LEU:HD22 | 1:B:214:ASN:CB | 2.45 | 0.46 |
| 1:B:7:GLY:HA2 | 1:B:33:ALA:O | 2.16 | 0.46 |
| 1:B:41:GLN:O | 1:B:45:GLU:CG | 2.61 | 0.46 |
| 1:A:159:LEU:HD12 | 1:A:159:LEU:HA | 1.81 | 0.46 |
| 1:B:245:PHE:CE2 | 1:B:249:LEU:HD11 | 2.51 | 0.46 |
| 1:B:28:VAL:HG12 | 1:B:30:LEU:CD1 | 2.46 | 0.46 |
| 1:B:83:ARG:NH1 | 1:B:83:ARG:HB3 | 2.31 | 0.46 |
| 1:D:125:ALA:HB1 | 1:D:164:GLY:HA3 | 1.98 | 0.46 |
| 1:D:15:ALA:HB3 | 1:D:261:VAL:HG21 | 1.97 | 0.46 |
| 1:G:2:ILE:O | 1:G:4:VAL:HG23 | 2.15 | 0.46 |
| 1:C:82:THR:HB | 1:C:267:LEU:HB3 | 1.97 | 0.46 |
| 1:F:112:LEU:HD13 | 1:F:117:LEU:HD11 | 1.97 | 0.46 |
| 1:H:192:ILE:N | 1:H:192:ILE:CD1 | 2.78 | 0.46 |
| 1:A:151:LYS:HD2 | 1:A:288:VAL:CG2 | 2.46 | 0.46 |
| 1:B:71:LEU:O | 1:B:234:LYS:HE3 | 2.15 | 0.46 |
| 1:C:245:PHE:O | 1:C:248:PHE:HB3 | 2.15 | 0.46 |
| 1:C:280:ILE:HG23 | 1:C:281:ALA:N | 2.31 | 0.46 |
| 1:D:242:ALA:O | 1:D:246:VAL:HG23 | 2.16 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:11:GLU:HG3 | 1:F:261:VAL:HG12 | 1.96 | 0.46 |
| 1:F:34:LYS:O | 1:F:38:LEU:HD22 | 2.16 | 0.46 |
| 1:I:120:SER:HB3 | 1:I:123:ASN:ND2 | 2.30 | 0.46 |
| 1:A:137:PRO:HA | 1:A:142:PHE:CD2 | 2.50 | 0.45 |
| 1:C:26:ILE:HD13 | 1:C:26:ILE:HA | 1.85 | 0.45 |
| 1:C:92:LYS:O | 1:C:93:LYS:HB3 | 2.15 | 0.45 |
| 1:D:279:PRO:O | 1:D:282:LYS:HG2 | 2.16 | 0.45 |
| 1:H:219:ARG:O | 1:H:286:PRO:HB3 | 2.17 | 0.45 |
| 1:I:112:LEU:HB2 | 1:I:116:ASP:HB2 | 1.98 | 0.45 |
| 1:I:159:LEU:O | 1:I:163:LYS:HG3 | 2.16 | 0.45 |
| 1:B:106:VAL:HG22 | 1:B:211:THR:CG2 | 2.45 | 0.45 |
| 1:C:113:SER:O | 1:C:115:LYS:N | 2.44 | 0.45 |
| 1:C:255:GLN:O | 1:C:259:THR:HB | 2.16 | 0.45 |
| 1:F:174:LYS:HG3 | 1:F:176:SER:OG | 2.16 | 0.45 |
| 1:A:130:LYS:HA | 1:A:168:TYR:HB3 | 1.97 | 0.45 |
| 1:A:300:THR:O | 1:A:304:GLU:HG3 | 2.16 | 0.45 |
| 1:B:119:LYS:O | 1:B:216:VAL:HG13 | 2.17 | 0.45 |
| 1:C:268:ASN:ND2 | 1:C:268:ASN:C | 2.68 | 0.45 |
| 1:I:31:ASN:N | 1:I:31:ASN:ND2 | 2.65 | 0.45 |
| 1:C:219:ARG:O | 1:C:286:PRO:HB3 | 2.16 | 0.45 |
| 1:D:74:LEU:CD1 | 1:D:96:VAL:HG23 | 2.47 | 0.45 |
| 1:E:72:GLU:CG | 1:E:234:LYS:HA | 2.45 | 0.45 |
| 1:G:10:LYS:HE2 | 1:G:32:SER:HB3 | 1.99 | 0.45 |
| 1:G:243:LYS:HG2 | 3:G:471:HOH:O | 2.15 | 0.45 |
| 1:H:155:GLU:HG3 | 1:H:302:LEU:HD11 | 1.98 | 0.45 |
| 1:B:245:PHE:O | 1:B:249:LEU:HG | 2.16 | 0.45 |
| 1:F:85:LYS:CE | 1:F:219:ARG:HH22 | 2.29 | 0.45 |
| 1:H:52:ASP:HA | 1:H:236:SER:OG | 2.17 | 0.45 |
| 1:F:270:HIS:CG | 1:I:237:GLN:HG3 | 2.51 | 0.45 |
| 1:A:256:ARG:HG3 | 1:A:271:VAL:HG13 | 1.98 | 0.45 |
| 1:B:291:THR:HG21 | 1:B:296:LYS:HE2 | 1.99 | 0.45 |
| 1:C:106:VAL:HG23 | 1:C:211:THR:OG1 | 2.16 | 0.45 |
| 1:D:4:VAL:HG22 | 1:D:53:VAL:HG22 | 1.98 | 0.45 |
| 1:E:54:PHE:CD2 | 1:E:65:LEU:HD12 | 2.52 | 0.45 |
| 1:G:20:PHE:C | 1:G:22:ARG:N | 2.70 | 0.45 |
| 1:A:212:ARG:HG2 | 1:A:212:ARG:HH11 | 1.81 | 0.45 |
| 1:B:106:VAL:HB | 1:B:192:ILE:HD11 | 1.97 | 0.45 |
| 1:D:117:LEU:HD22 | 1:D:214:ASN:HB2 | 1.99 | 0.45 |
| 1:D:137:PRO:HB3 | 1:D:308:MET:CE | 2.47 | 0.45 |
| 1:A:57:GLU:CG | 1:A:101:ARG:NH1 | 2.79 | 0.45 |
| 1:A:181:ALA:O | 1:A:186:GLU:HG2 | 2.17 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:105:VAL:HB | 1:B:214:ASN:HB3 | 1.98 | 0.45 |
| 1:D:245:PHE:CE1 | 1:D:249:LEU:HD21 | 2.52 | 0.45 |
| 1:E:192:ILE:HB | 3:E:536:HOH:O | 2.17 | 0.45 |
| 1:F:233:LEU:CD1 | 1:F:233:LEU:N | 2.80 | 0.45 |
| 1:I:22:ARG:O | 1:I:23:ALA:HB2 | 2.17 | 0.45 |
| 1:A:252:LYS:HE3 | 1:A:256:ARG:HH22 | 1.78 | 0.45 |
| 1:B:193:ASN:HB3 | 1:B:195:TYR:CE1 | 2.52 | 0.45 |
| 1:E:90:ALA:HB2 | 1:E:95:TRP:CE2 | 2.52 | 0.45 |
| 1:G:239:LYS:HB3 | 1:G:243:LYS:HE3 | 1.99 | 0.45 |
| 1:G:279:PRO:HB2 | 1:G:282:LYS:HG2 | 1.98 | 0.45 |
| 1:B:140:GLY:O | 1:B:144:GLU:HG2 | 2.16 | 0.45 |
| 1:D:27:LYS:HZ3 | 1:D:27:LYS:HB3 | 1.81 | 0.45 |
| 1:F:31:ASN:HB2 | 3:G:476:HOH:O | 2.17 | 0.45 |
| 1:F:93:LYS:HD3 | 3:F:511:HOH:O | 2.17 | 0.45 |
| 1:H:76:ALA:HB1 | 1:H:80:ASN:HD21 | 1.81 | 0.45 |
| 1:B:151:LYS:HE2 | 1:B:295:GLU:OE2 | 2.17 | 0.44 |
| 1:D:43:LYS:HZ3 | 1:D:68:ALA:HB3 | 1.82 | 0.44 |
| 1:F:255:GLN:HE22 | 1:F:267:LEU:H | 1.64 | 0.44 |
| 1:I:265:TYR:CE2 | 1:I:283:LEU:HD11 | 2.51 | 0.44 |
| 1:A:252:LYS:HE3 | 1:A:256:ARG:CZ | 2.46 | 0.44 |
| 1:E:59:ILE:HB | 1:E:60:PRO:HD3 | 1.98 | 0.44 |
| 1:G:120:SER:HB3 | 1:G:123:ASN:ND2 | 2.33 | 0.44 |
| 1:G:80:ASN:HA | 1:G:83:ARG:HB2 | 1.99 | 0.44 |
| 1:H:62:LEU:HD13 | 1:H:95:TRP:HB2 | 1.98 | 0.44 |
| 1:A:159:LEU:HG | 1:A:163:LYS:HE3 | 1.99 | 0.44 |
| 1:C:218:HIS:HB3 | 3:C:500:HOH:O | 2.18 | 0.44 |
| 1:C:54:PHE:CE2 | 1:C:56:SER:HB3 | 2.52 | 0.44 |
| 1:E:262:ARG:CG | 1:E:264:GLU:HG3 | 2.44 | 0.44 |
| 1:H:122:LEU:CD2 | 1:H:149:ILE:HD13 | 2.47 | 0.44 |
| 1:H:21:THR:HG22 | 1:H:21:THR:O | 2.17 | 0.44 |
| 1:A:146:ILE:HD12 | 1:A:158:ALA:HB1 | 1.99 | 0.44 |
| 1:B:30:LEU:N | 1:B:30:LEU:HD12 | 2.33 | 0.44 |
| 1:C:54:PHE:CZ | 1:C:56:SER:HB3 | 2.52 | 0.44 |
| 1:D:94:ASP:OD1 | 1:D:94:ASP:N | 2.49 | 0.44 |
| 1:E:41:GLN:O | 1:E:44:GLU:N | 2.49 | 0.44 |
| 1:H:57:GLU:HB2 | 1:H:101:ARG:HH22 | 1.80 | 0.44 |
| 1:I:256:ARG:HG2 | 1:I:271:VAL:HG13 | 1.99 | 0.44 |
| 1:B:51:ALA:HB3 | 1:B:233:LEU:CD2 | 2.47 | 0.44 |
| 1:F:85:LYS:CE | 1:F:219:ARG:HH12 | 2.30 | 0.44 |
| 1:H:76:ALA:HB1 | 1:H:80:ASN:ND2 | 2.32 | 0.44 |
| 1:A:8:GLN:CG | 1:A:9:HIS:N | 2.80 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:225:VAL:HG23 | 1:B:285:ALA:HB2 | 2.00 | 0.44 |
| 1:D:256:ARG:HD2 | 1:D:256:ARG:HA | 1.71 | 0.44 |
| 1:E:161:TRP:HE3 | 1:E:162:LEU:HD12 | 1.82 | 0.44 |
| 1:E:300:THR:HG23 | 1:E:309:LYS:HE2 | 2.00 | 0.44 |
| 1:H:142:PHE:O | 1:H:145:GLN:HB3 | 2.17 | 0.44 |
| 1:A:162:LEU:HB3 | 1:A:306:ALA:CB | 2.48 | 0.44 |
| 1:C:119:LYS:HE3 | 3:C:489:HOH:O | 2.17 | 0.44 |
| 1:C:303:LEU:HG | 1:C:309:LYS:CA | 2.46 | 0.44 |
| 1:D:174:LYS:HE2 | 3:D:466:HOH:O | 2.16 | 0.44 |
| 1:E:107:TYR:CD1 | 1:E:117:LEU:HD11 | 2.52 | 0.44 |
| 1:E:71:LEU:O | 1:E:234:LYS:HE3 | 2.18 | 0.44 |
| 1:E:90:ALA:HB2 | 1:E:95:TRP:CD2 | 2.53 | 0.44 |
| 1:H:2:ILE:HD11 | 1:H:53:VAL:CG2 | 2.43 | 0.44 |
| 1:I:78:THR:O | 1:I:81:GLU:HB2 | 2.18 | 0.44 |
| 1:B:90:ALA:O | 1:B:93:LYS:HE2 | 2.18 | 0.44 |
| 1:F:279:PRO:O | 1:F:282:LYS:HB2 | 2.17 | 0.44 |
| 1:G:5:TYR:CD2 | 1:G:38:LEU:HD12 | 2.53 | 0.44 |
| 1:H:266:PRO:HA | 3:H:479:HOH:O | 2.17 | 0.44 |
| 1:I:81:GLU:OE1 | 1:I:268:ASN:ND2 | 2.51 | 0.44 |
| 1:B:13:ALA:HA | 1:B:16:VAL:HG12 | 2.00 | 0.44 |
| 1:E:174:LYS:HB2 | 1:E:177:VAL:HG23 | 1.99 | 0.44 |
| 1:E:151:LYS:NZ | 1:E:295:GLU:OE1 | 2.47 | 0.44 |
| 1:G:205:GLY:O | 1:G:207:GLN:N | 2.51 | 0.44 |
| 1:G:223:ALA:HB3 | 1:G:286:PRO:HD3 | 2.00 | 0.44 |
| 1:H:2:ILE:HG13 | 1:H:242:ALA:HA | 2.00 | 0.44 |
| 1:I:45:GLU:HB2 | 1:I:49:SER:HB2 | 1.99 | 0.43 |
| 1:A:9:HIS:NE2 | 1:A:11:GLU:HB3 | 2.33 | 0.43 |
| 1:C:140:GLY:O | 1:C:144:GLU:HG2 | 2.19 | 0.43 |
| 1:D:117:LEU:HD22 | 1:D:214:ASN:CB | 2.48 | 0.43 |
| 1:I:255:GLN:HB2 | 1:I:271:VAL:HG21 | 1.99 | 0.43 |
| 1:C:256:ARG:HH12 | 1:C:272:VAL:HB | 1.82 | 0.43 |
| 1:C:6:ASN:HB2 | 1:C:30:LEU:HD22 | 2.00 | 0.43 |
| 1:D:72:GLU:OE2 | 1:D:234:LYS:HG2 | 2.18 | 0.43 |
| 1:G:145:GLN:O | 1:G:149:ILE:HG13 | 2.18 | 0.43 |
| 1:G:298:HIS:O | 1:G:302:LEU:HG | 2.18 | 0.43 |
| 1:G:9:HIS:HB3 | 1:G:12:ALA:CB | 2.46 | 0.43 |
| 1:H:252:LYS:O | 1:H:256:ARG:HG3 | 2.18 | 0.43 |
| 1:C:155:GLU:OE2 | 1:C:298:HIS:HE1 | 2.00 | 0.43 |
| 1:C:5:TYR:CE1 | 1:C:51:ALA:HB2 | 2.53 | 0.43 |
| 1:D:217:ARG:HH11 | 1:D:217:ARG:HG2 | 1.84 | 0.43 |
| 1:E:130:LYS:O | 1:E:132:ARG:HG3 | 2.19 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:130:LYS:HE3 | 1:D:131:ASN:ND2 | 2.34 | 0.43 |
| 1:E:255:GLN:HE22 | 1:E:267:LEU:N | 2.14 | 0.43 |
| 1:A:101:ARG:HG2 | 1:A:101:ARG:O | 2.19 | 0.43 |
| 1:B:101:ARG:HG3 | 1:B:264:GLU:HG2 | 2.01 | 0.43 |
| 1:B:292:THR:O | 1:B:296:LYS:HG3 | 2.18 | 0.43 |
| 1:C:108:ASP:OD2 | 1:C:110:ARG:HB2 | 2.18 | 0.43 |
| 1:C:248:PHE:CE2 | 1:C:254:GLY:HA2 | 2.54 | 0.43 |
| 1:D:223:ALA:HB3 | 1:D:286:PRO:HD3 | 2.01 | 0.43 |
| 1:C:12:ALA:HB1 | 1:C:258:LEU:CD1 | 2.49 | 0.43 |
| 1:E:57:GLU:HG2 | 1:E:58:GLN:HG2 | 2.00 | 0.43 |
| 1:F:1:ASP:HA | 1:F:26:ILE:HG23 | 2.00 | 0.43 |
| 1:D:183:GLU:OE1 | 1:D:211:THR:HG22 | 2.19 | 0.43 |
| 1:E:42:ILE:HD12 | 1:E:65:LEU:HD11 | 2.01 | 0.43 |
| 1:F:144:GLU:OE1 | 1:F:144:GLU:HA | 2.19 | 0.43 |
| 1:F:232:VAL:HG13 | 1:F:242:ALA:HB1 | 2.01 | 0.43 |
| 1:G:130:LYS:HA | 1:G:168:TYR:CB | 2.46 | 0.43 |
| 1:H:9:HIS:CD2 | 1:H:10:LYS:N | 2.87 | 0.43 |
| 1:I:255:GLN:HG3 | 1:I:268:ASN:HB2 | 2.01 | 0.43 |
| 1:I:6:ASN:ND2 | 1:I:8:GLN:H | 2.17 | 0.43 |
| 1:A:106:VAL:CG2 | 1:A:192:ILE:HG12 | 2.48 | 0.43 |
| 1:D:265:TYR:CD1 | 1:D:265:TYR:N | 2.86 | 0.43 |
| 1:E:45:GLU:H | 1:E:45:GLU:HG2 | 1.66 | 0.43 |
| 1:H:20:PHE:CE2 | 1:H:26:ILE:HB | 2.54 | 0.43 |
| 1:I:22:ARG:HG3 | 1:I:22:ARG:HH11 | 1.84 | 0.43 |
| 1:I:34:LYS:CG | 1:I:37:GLN:HG3 | 2.48 | 0.43 |
| 1:A:182:VAL:HG12 | 1:A:211:THR:HG22 | 2.01 | 0.43 |
| 1:D:55:TYR:CE1 | 1:D:249:LEU:HD13 | 2.54 | 0.43 |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:HB2 | 2.01 | 0.43 |
| 1:G:267:LEU:HD23 | 1:G:267:LEU:HA | 1.86 | 0.43 |
| 1:I:180:GLN:O | 1:I:184:ASN:ND2 | 2.51 | 0.43 |
| 1:I:20:PHE:CE2 | 1:I:26:ILE:HB | 2.54 | 0.43 |
| 1:A:103:ARG:HD2 | 1:A:145:GLN:HB2 | 2.01 | 0.42 |
| 1:A:38:LEU:O | 1:A:41:GLN:HB3 | 2.19 | 0.42 |
| 1:B:40:GLY:O | 1:B:44:GLU:HG2 | 2.19 | 0.42 |
| 1:B:43:LYS:HZ1 | 1:B:64:THR:HB | 1.84 | 0.42 |
| 1:D:115:LYS:HD2 | 1:D:116:ASP:OD1 | 2.18 | 0.42 |
| 1:D:255:GLN:HB2 | 1:D:271:VAL:HG21 | 2.00 | 0.42 |
| 1:D:80:ASN:HA | 1:D:83:ARG:HD3 | 1.99 | 0.42 |
| 1:F:11:GLU:HG3 | 1:F:261:VAL:CG1 | 2.49 | 0.42 |
| 1:F:7:GLY:HA2 | 1:F:33:ALA:O | 2.19 | 0.42 |
| 1:H:117:LEU:CD1 | 1:H:117:LEU:N | 2.82 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:303:LEU:HD23 | 1:I:308:MET:SD | 2.59 | 0.42 |
| 1:I:99:SER:HA | 1:I:267:LEU:HD13 | 2.01 | 0.42 |
| 1:A:217:ARG:NH1 | 1:A:278:GLU:OE1 | 2.52 | 0.42 |
| 1:A:59:ILE:N | 1:A:60:PRO:CD | 2.82 | 0.42 |
| 1:C:26:ILE:HG13 | 1:C:241:GLU:OE1 | 2.19 | 0.42 |
| 1:F:16:VAL:HG11 | 1:F:249:LEU:CD2 | 2.49 | 0.42 |
| 1:H:113:SER:O | 1:H:117:LEU:HD13 | 2.20 | 0.42 |
| 1:A:203:GLU:HG3 | 1:A:204:LYS:N | 2.34 | 0.42 |
| 1:A:309:LYS:HG3 | 1:A:309:LYS:O | 2.19 | 0.42 |
| 1:C:3:THR:O | 1:C:51:ALA:HA | 2.19 | 0.42 |
| 1:D:152:LEU:O | 1:D:153:LYS:HD3 | 2.19 | 0.42 |
| 1:D:256:ARG:NE | 3:D:411:HOH:O | 2.51 | 0.42 |
| 1:I:234:LYS:HD2 | 1:I:234:LYS:C | 2.39 | 0.42 |
| 1:C:228:SER:HB3 | 3:C:476:HOH:O | 2.18 | 0.42 |
| 1:C:256:ARG:HH12 | 1:C:272:VAL:H | 1.58 | 0.42 |
| 1:C:27:LYS:HD3 | 1:C:27:LYS:N | 2.35 | 0.42 |
| 1:C:306:ALA:HB3 | 1:C:308:MET:HE3 | 2.01 | 0.42 |
| 1:F:104:VAL:HG12 | 1:F:215:PHE:CE2 | 2.55 | 0.42 |
| 1:G:67:ALA:HA | 1:G:92:LYS:HZ2 | 1.84 | 0.42 |
| 1:B:90:ALA:HB2 | 1:B:95:TRP:CE2 | 2.55 | 0.42 |
| 1:D:193:ASN:HB3 | 1:D:195:TYR:CE1 | 2.54 | 0.42 |
| 1:D:252:LYS:HG3 | 1:D:253:GLU:N | 2.34 | 0.42 |
| 1:D:303:LEU:CD2 | 1:D:308:MET:HE1 | 2.50 | 0.42 |
| 1:D:58:GLN:HG3 | 1:D:60:PRO:HD2 | 2.00 | 0.42 |
| 1:E:18:ASP:O | 1:E:22:ARG:HG3 | 2.19 | 0.42 |
| 1:G:69:ASN:O | 1:G:234:LYS:HG3 | 2.20 | 0.42 |
| 1:H:180:GLN:HA | 1:H:183:GLU:HB3 | 2.00 | 0.42 |
| 1:H:93:LYS:HE3 | 3:H:466:HOH:O | 2.19 | 0.42 |
| 1:A:267:LEU:HD23 | 1:A:267:LEU:HA | 1.91 | 0.42 |
| 1:B:24:THR:HB | 1:B:26:ILE:HG13 | 2.02 | 0.42 |
| 1:D:12:ALA:O | 1:D:16:VAL:HG23 | 2.19 | 0.42 |
| 1:D:245:PHE:O | 1:D:249:LEU:HG | 2.20 | 0.42 |
| 1:E:6:ASN:ND2 | 1:E:8:GLN:H | 2.17 | 0.42 |
| 1:F:83:ARG:HD3 | 3:F:457:HOH:O | 2.20 | 0.42 |
| 1:F:84:GLY:O | 1:F:85:LYS:C | 2.57 | 0.42 |
| 1:G:146:ILE:O | 1:G:150:VAL:HG23 | 2.20 | 0.42 |
| 1:G:2:ILE:CG1 | 1:G:28:VAL:HG22 | 2.50 | 0.42 |
| 1:H:45:GLU:HB2 | 1:H:49:SER:HB2 | 2.02 | 0.42 |
| 1:I:8:GLN:HE21 | 1:I:8:GLN:HB2 | 1.67 | 0.42 |
| 1:A:75:PRO:CD | 1:A:243:LYS:HZ2 | 2.32 | 0.42 |
| 1:B:106:VAL:CG2 | 1:B:211:THR:HG23 | 2.45 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:52:ASP:HA | 1:B:236:SER:HB2 | 2.01 | 0.42 |
| 1:D:199:ALA:O | 1:D:203:GLU:OE1 | 2.37 | 0.42 |
| 1:D:144:GLU:CG | 1:D:224:LEU:HD21 | 2.49 | 0.42 |
| 2:D:400:ZRC:O3A | 2:D:400:ZRC:O31 | 2.38 | 0.42 |
| 1:D:86:GLY:HA2 | 1:D:287:GLN:HG2 | 2.00 | 0.42 |
| 1:E:57:GLU:O | 1:E:101:ARG:NH2 | 2.52 | 0.42 |
| 1:H:174:LYS:HD3 | 1:H:174:LYS:HA | 1.83 | 0.42 |
| 1:H:301:ARG:HA | 1:H:304:GLU:OE1 | 2.19 | 0.42 |
| 1:I:291:THR:HA | 1:I:295:GLU:OE1 | 2.20 | 0.42 |
| 1:B:17:ALA:O | 1:B:20:PHE:HB3 | 2.20 | 0.42 |
| 1:E:112:LEU:HD12 | 1:E:116:ASP:CB | 2.50 | 0.42 |
| 1:H:176:SER:O | 1:H:180:GLN:NE2 | 2.53 | 0.42 |
| 1:C:198:HIS:HB3 | 1:C:275:PHE:CD2 | 2.54 | 0.41 |
| 1:D:265:TYR:CZ | 1:D:283:LEU:HD11 | 2.56 | 0.41 |
| 1:H:130:LYS:O | 1:H:132:ARG:HG3 | 2.20 | 0.41 |
| 1:H:42:ILE:HD12 | 1:H:65:LEU:HD11 | 2.02 | 0.41 |
| 1:A:206:VAL:HA | 1:A:209:VAL:HG22 | 2.01 | 0.41 |
| 1:A:279:PRO:HD2 | 1:A:282:LYS:HZ1 | 1.83 | 0.41 |
| 1:A:76:ALA:O | 1:A:80:ASN:HB2 | 2.20 | 0.41 |
| 1:E:71:LEU:C | 1:E:234:LYS:HG3 | 2.40 | 0.41 |
| 1:F:173:ALA:HB3 | 1:F:174:LYS:HE3 | 2.01 | 0.41 |
| 1:G:143:LEU:O | 1:G:147:VAL:HG23 | 2.19 | 0.41 |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:HB2 | 2.02 | 0.41 |
| 1:B:106:VAL:CG2 | 1:B:211:THR:CG2 | 2.98 | 0.41 |
| 1:C:130:LYS:O | 1:C:132:ARG:HG3 | 2.19 | 0.41 |
| 1:C:121:VAL:CG2 | 1:C:216:VAL:HG21 | 2.50 | 0.41 |
| 1:C:233:LEU:N | 1:C:233:LEU:HD12 | 2.35 | 0.41 |
| 1:I:109:THR:O | 1:I:109:THR:CG2 | 2.68 | 0.41 |
| 1:I:92:LYS:HB2 | 1:I:94:ASP:OD2 | 2.20 | 0.41 |
| 1:A:106:VAL:HG22 | 1:A:192:ILE:HG12 | 2.02 | 0.41 |
| 1:B:59:ILE:N | 1:B:60:PRO:CD | 2.84 | 0.41 |
| 1:D:134:GLY:HA2 | 1:D:170:LYS:O | 2.20 | 0.41 |
| 1:D:225:VAL:HG23 | 1:D:285:ALA:HB2 | 2.02 | 0.41 |
| 1:D:59:ILE:N | 1:D:60:PRO:CD | 2.84 | 0.41 |
| 1:E:152:LEU:HD21 | 1:E:288:VAL:HG12 | 2.03 | 0.41 |
| 1:E:109:THR:HG21 | 1:E:212:ARG:CG | 2.50 | 0.41 |
| 1:F:217:ARG:HG2 | 1:F:217:ARG:HH11 | 1.85 | 0.41 |
| 1:G:234:LYS:NZ | 1:G:234:LYS:CB | 2.79 | 0.41 |
| 1:B:131:ASN:CA | 1:B:170:LYS:HE3 | 2.51 | 0.41 |
| 1:C:149:ILE:O | 1:C:153:LYS:N | 2.47 | 0.41 |
| 1:C:55:TYR:CD1 | 1:C:249:LEU:HD13 | 2.56 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:79:ILE:HD12 | 1:C:93:LYS:CG | 2.46 | 0.41 |
| 1:C:90:ALA:HB2 | 1:C:95:TRP:CD2 | 2.55 | 0.41 |
| 1:F:178:ALA:CB | 1:F:192:ILE:HD11 | 2.50 | 0.41 |
| 1:F:255:GLN:NE2 | 1:F:268:ASN:H | 2.19 | 0.41 |
| 1:G:233:LEU:CD1 | 1:G:233:LEU:H | 2.33 | 0.41 |
| 1:G:69:ASN:C | 1:G:71:LEU:H | 2.24 | 0.41 |
| 1:I:298:HIS:HD2 | 3:I:456:HOH:O | 2.02 | 0.41 |
| 1:A:8:GLN:HG2 | 1:A:9:HIS:H | 1.86 | 0.41 |
| 1:B:103:ARG:NH2 | 3:B:403:HOH:O | 2.40 | 0.41 |
| 1:B:237:GLN:CD | 1:B:237:GLN:H | 2.22 | 0.41 |
| 1:C:236:SER:OG | 1:C:239:LYS:HE2 | 2.21 | 0.41 |
| 1:C:48:ARG:HD2 | 3:C:472:HOH:O | 2.21 | 0.41 |
| 1:D:107:TYR:CD1 | 1:D:117:LEU:HD21 | 2.55 | 0.41 |
| 1:D:18:ASP:O | 1:D:22:ARG:HG3 | 2.20 | 0.41 |
| 1:E:252:LYS:HE2 | 1:E:268:ASN:OD1 | 2.20 | 0.41 |
| 1:E:83:ARG:HG3 | 1:E:83:ARG:HH11 | 1.84 | 0.41 |
| 1:F:38:LEU:O | 1:F:42:ILE:HG13 | 2.20 | 0.41 |
| 1:H:2:ILE:O | 1:H:28:VAL:HA | 2.20 | 0.41 |
| 1:C:101:ARG:O | 1:C:225:VAL:HA | 2.21 | 0.41 |
| 1:C:268:ASN:HA | 1:C:269:PRO:HD2 | 1.94 | 0.41 |
| 1:C:225:VAL:HG23 | 1:C:285:ALA:HB2 | 2.02 | 0.41 |
| 1:D:65:LEU:CD2 | 1:D:65:LEU:N | 2.84 | 0.41 |
| 1:E:268:ASN:ND2 | 1:E:269:PRO:HD2 | 2.36 | 0.41 |
| 1:F:240:ASP:O | 1:F:244:LYS:HG3 | 2.20 | 0.41 |
| 1:A:51:ALA:HB3 | 1:A:233:LEU:HD22 | 2.02 | 0.41 |
| 1:A:71:LEU:HB2 | 1:A:94:ASP:HB2 | 2.02 | 0.41 |
| 1:C:236:SER:OG | 1:C:239:LYS:HG3 | 2.20 | 0.41 |
| 1:C:268:ASN:ND2 | 1:C:270:HIS:H | 2.18 | 0.41 |
| 1:C:5:TYR:HE2 | 1:C:41:GLN:HG2 | 1.86 | 0.41 |
| 1:G:164:GLY:O | 1:G:168:TYR:CE1 | 2.74 | 0.41 |
| 1:G:70:LEU:C | 1:G:234:LYS:HG2 | 2.41 | 0.41 |
| 1:G:265:TYR:CE2 | 1:G:277:LEU:HB3 | 2.55 | 0.41 |
| 1:G:2:ILE:CD1 | 1:G:28:VAL:HG22 | 2.47 | 0.41 |
| 1:H:137:PRO:HA | 1:H:142:PHE:CD2 | 2.56 | 0.41 |
| 1:H:6:ASN:O | 1:H:32:SER:HA | 2.19 | 0.41 |
| 1:B:202:ARG:HH22 | 1:B:274:THR:C | 2.25 | 0.41 |
| 1:C:303:LEU:HG | 1:C:309:LYS:H | 1.86 | 0.41 |
| 1:D:124:TYR:HB2 | 3:D:501:HOH:O | 2.21 | 0.41 |
| 1:D:184:ASN:HB2 | 1:D:186:GLU:CG | 2.51 | 0.41 |
| 1:D:51:ALA:HB3 | 1:D:233:LEU:CD2 | 2.51 | 0.41 |
| 1:E:151:LYS:CE | 1:E:295:GLU:OE1 | 2.68 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:46:GLY:O | 1:F:48:ARG:N | 2.54 | 0.41 |
| 1:H:144:GLU:OE2 | 1:H:291:THR:HG21 | 2.20 | 0.41 |
| 1:B:147:VAL:HG11 | 1:B:291:THR:HG23 | 2.03 | 0.41 |
| 1:C:92:LYS:O | 1:C:93:LYS:CB | 2.69 | 0.41 |
| 1:D:103:ARG:HD3 | 3:D:431:HOH:O | 2.21 | 0.41 |
| 1:D:175:ASN:HD22 | 1:D:192:ILE:HG22 | 1.86 | 0.41 |
| 1:F:85:LYS:HB3 | 1:F:86:GLY:H | 1.55 | 0.41 |
| 1:G:104:VAL:CG1 | 1:G:105:VAL:N | 2.83 | 0.41 |
| 1:H:111:LYS:HD2 | 1:H:188:ASP:OD1 | 2.21 | 0.41 |
| 1:H:60:PRO:HA | 1:H:63:ALA:HB3 | 2.01 | 0.41 |
| 1:H:74:LEU:HA | 1:H:75:PRO:HD3 | 1.91 | 0.41 |
| 1:I:136:VAL:O | 1:I:139:SER:HB3 | 2.20 | 0.41 |
| 1:I:255:GLN:HG3 | 1:I:268:ASN:CB | 2.51 | 0.41 |
| 1:B:2:ILE:HG22 | 1:B:52:ASP:OD1 | 2.20 | 0.41 |
| 1:B:71:LEU:HD12 | 1:B:94:ASP:OD2 | 2.21 | 0.41 |
| 1:C:166:LYS:HD3 | 1:C:166:LYS:C | 2.40 | 0.41 |
| 1:D:106:VAL:HG21 | 1:D:179:LEU:CD1 | 2.51 | 0.41 |
| 1:D:181:ALA:HA | 1:D:186:GLU:OE1 | 2.20 | 0.41 |
| 1:E:262:ARG:HE | 1:E:264:GLU:CD | 2.24 | 0.41 |
| 1:G:3:THR:HB | 1:G:50:PRO:O | 2.20 | 0.41 |
| 1:H:143:LEU:HD11 | 1:H:299:ALA:HB3 | 2.03 | 0.41 |
| 1:H:218:HIS:O | 1:H:219:ARG:HB2 | 2.21 | 0.41 |
| 1:A:57:GLU:HG2 | 1:A:101:ARG:HH12 | 1.86 | 0.40 |
| 1:C:304:GLU:CG | 1:C:309:LYS:HG3 | 2.51 | 0.40 |
| 1:G:111:LYS:HD2 | 3:G:455:HOH:O | 2.20 | 0.40 |
| 1:G:9:HIS:HB2 | 1:G:262:ARG:HD2 | 2.03 | 0.40 |
| 1:H:178:ALA:O | 1:H:182:VAL:HG23 | 2.21 | 0.40 |
| 1:H:106:VAL:HG12 | 1:H:192:ILE:CD1 | 2.51 | 0.40 |
| 1:H:117:LEU:HD23 | 1:H:214:ASN:CG | 2.42 | 0.40 |
| 1:I:90:ALA:HB2 | 1:I:95:TRP:CD2 | 2.55 | 0.40 |
| 1:A:217:ARG:HB3 | 1:A:284:GLU:OE2 | 2.20 | 0.40 |
| 1:C:52:ASP:HB3 | 1:C:242:ALA:HB2 | 2.03 | 0.40 |
| 1:G:182:VAL:HG12 | 1:G:211:THR:HG22 | 2.04 | 0.40 |
| 1:G:256:ARG:NH1 | 1:G:256:ARG:CB | 2.85 | 0.40 |
| 1:I:20:PHE:HZ | 1:I:26:ILE:HD12 | 1.86 | 0.40 |
| 1:A:206:VAL:O | 1:A:209:VAL:HG22 | 2.21 | 0.40 |
| 1:C:10:LYS:O | 1:C:14:GLN:HG2 | 2.21 | 0.40 |
| 2:C:400:ZRC:O2A | 2:C:400:ZRC:O23 | 2.39 | 0.40 |
| 1:G:39:ALA:HA | 1:G:65:LEU:HD11 | 2.03 | 0.40 |
| 1:H:149:ILE:HG12 | 1:H:221:PRO:HB3 | 2.03 | 0.40 |
| 1:H:59:ILE:H | 1:H:60:PRO:HD2 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:I:112:LEU:C | 1:I:112:LEU:HD12 | 2.41 | 0.40 |
| 1:I:74:LEU:HA | 1:I:75:PRO:HD3 | 1.87 | 0.40 |
| 1:B:21:THR:O | 1:B:25:GLY:N | 2.46 | 0.40 |
| 1:B:297:GLU:O | 1:B:301:ARG:HG2 | 2.21 | 0.40 |
| 1:C:52:ASP:CA | 1:C:236:SER:HB2 | 2.45 | 0.40 |
| 1:D:127:PRO:HG3 | 1:D:168:TYR:CZ | 2.55 | 0.40 |
| 1:G:202:ARG:NH2 | 1:G:274:THR:CG2 | 2.74 | 0.40 |
| 1:H:2:ILE:CG2 | 1:H:28:VAL:HG12 | 2.51 | 0.40 |
| 1:H:33:ALA:HB3 | 1:H:38:LEU:CG | 2.49 | 0.40 |
| 1:I:35:GLY:HA3 | 1:I:57:GLU:OE2 | 2.21 | 0.40 |
| 1:C:251:GLY:O | 1:C:255:GLN:HG2 | 2.22 | 0.40 |
| 1:D:180:GLN:HE21 | 1:D:184:ASN:CG | 2.23 | 0.40 |
| 1:I:255:GLN:HB3 | 1:I:271:VAL:HG21 | 2.03 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1 | A | 307/309 (99%) | 288 (94%) | 19 (6%) | 0 | 100 | 100 |
| 1 | B | 307/309 (99%) | 288 (94%) | 17 (6%) | 2 (1%) | 25 | 6 |
| 1 | C | 307/309 (99%) | 283 (92%) | 20 (6%) | 4 (1%) | 14 | 2 |
| 1 | D | 307/309 (99%) | 291 (95%) | 14 (5%) | 2 (1%) | 25 | 6 |
| 1 | E | 307/309 (99%) | 291 (95%) | 12 (4%) | 4 (1%) | 14 | 2 |
| 1 | F | 307/309 (99%) | 292 (95%) | 13 (4%) | 2 (1%) | 25 | 6 |
| 1 | G | 307/309 (99%) | 281 (92%) | 23 (8%) | 3 (1%) | 18 | 3 |
| 1 | H | 307/309 (99%) | 287 (94%) | 18 (6%) | 2 (1%) | 25 | 6 |
| 1 | I | 307/309 (99%) | 291 (95%) | 15 (5%) | 1 (0%) | 44 | 19 |
| All | All | 2763/2781 (99%) | 2592 (94%) | 151 (6%) | 20 (1%) | 25 | 6 |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 195 | TYR |
| 1 | F | 85 | LYS |
| 1 | C | 46 | GLY |
| 1 | D | 252 | LYS |
| 1 | F | 47 | SER |
| 1 | G | 8 | GLN |
| 1 | G | 206 | VAL |
| 1 | H | 308 | MET |
| 1 | I | 23 | ALA |
| 1 | E | 114 | GLU |
| 1 | B | 93 | LYS |
| 1 | C | 47 | SER |
| 1 | C | 114 | GLU |
| 1 | E | 217 | ARG |
| 1 | B | 217 | ARG |
| 1 | E | 35 | GLY |
| 1 | H | 2 | ILE |
| 1 | E | 42 | ILE |
| 1 | G | 2 | ILE |
| 1 | D | 192 | ILE |

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 | 245/245 (100%) | 233 (95%) | 12 (5%) | 29 | 4 |
| 1 | B | 245/245 (100%) | 233 (95%) | 12 (5%) | 29 | 4 |
| 1 | C | 245/245 (100%) | 234 (96%) | 11 (4%) | 32 | 6 |
| 1 | D | 245/245 (100%) | 233 (95%) | 12 (5%) | 29 | 4 |
| 1 | E | 245/245 (100%) | 236 (96%) | 9 (4%) | 39 | 9 |
| 1 | F | 245/245 (100%) | 235 (96%) | 10 (4%) | 35 | 7 |
| 1 | G | 245/245 (100%) | 238 (97%) | 7 (3%) | 48 | 15 |
| 1 | H | 245/245 (100%) | 235 (96%) | 10 (4%) | 35 | 7 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|-----|-------|------------------|------------|----------|-------------|
| 1 | I | 245/245 (100%) | 232 (95%) | 13 (5%) | 26 4 |
| All | All | 2205/2205 (100%) | 2109 (96%) | 96 (4%) | 33 6 |

All (96) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 45 | GLU |
| 1 | A | 60 | PRO |
| 1 | A | 80 | ASN |
| 1 | A | 101 | ARG |
| 1 | A | 103 | ARG |
| 1 | A | 106 | VAL |
| 1 | A | 115 | LYS |
| 1 | A | 146 | ILE |
| 1 | A | 187 | ILE |
| 1 | A | 191 | LEU |
| 1 | A | 216 | VAL |
| 1 | A | 301 | ARG |
| 1 | B | 1 | ASP |
| 1 | B | 14 | GLN |
| 1 | B | 93 | LYS |
| 1 | B | 103 | ARG |
| 1 | B | 175 | ASN |
| 1 | B | 183 | GLU |
| 1 | B | 188 | ASP |
| 1 | B | 211 | THR |
| 1 | B | 237 | GLN |
| 1 | B | 239 | LYS |
| 1 | B | 253 | GLU |
| 1 | B | 278 | GLU |
| 1 | C | 8 | GLN |
| 1 | C | 18 | ASP |
| 1 | C | 103 | ARG |
| 1 | C | 174 | LYS |
| 1 | C | 188 | ASP |
| 1 | C | 207 | GLN |
| 1 | C | 211 | THR |
| 1 | C | 239 | LYS |
| 1 | C | 253 | GLU |
| 1 | C | 259 | THR |
| 1 | C | 268 | ASN |
| 1 | D | 53 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | D | 103 | ARG |
| 1 | D | 115 | LYS |
| 1 | D | 132 | ARG |
| 1 | D | 167 | GLU |
| 1 | D | 214 | ASN |
| 1 | D | 216 | VAL |
| 1 | D | 240 | ASP |
| 1 | D | 256 | ARG |
| 1 | D | 264 | GLU |
| 1 | D | 268 | ASN |
| 1 | D | 287 | GLN |
| 1 | E | 103 | ARG |
| 1 | E | 139 | SER |
| 1 | E | 188 | ASP |
| 1 | E | 200 | PHE |
| 1 | E | 219 | ARG |
| 1 | E | 252 | LYS |
| 1 | E | 259 | THR |
| 1 | E | 268 | ASN |
| 1 | E | 280 | ILE |
| 1 | F | 8 | GLN |
| 1 | F | 11 | GLU |
| 1 | F | 111 | LYS |
| 1 | F | 114 | GLU |
| 1 | F | 115 | LYS |
| 1 | F | 174 | LYS |
| 1 | F | 191 | LEU |
| 1 | F | 240 | ASP |
| 1 | F | 280 | ILE |
| 1 | F | 287 | GLN |
| 1 | G | 55 | TYR |
| 1 | G | 94 | ASP |
| 1 | G | 103 | ARG |
| 1 | G | 168 | TYR |
| 1 | G | 278 | GLU |
| 1 | G | 288 | VAL |
| 1 | G | 294 | SER |
| 1 | H | 2 | ILE |
| 1 | H | 3 | THR |
| 1 | H | 103 | ARG |
| 1 | H | 117 | LEU |
| 1 | H | 180 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 192 | ILE |
| 1 | H | 233 | LEU |
| 1 | H | 256 | ARG |
| 1 | H | 287 | GLN |
| 1 | H | 301 | ARG |
| 1 | I | 30 | LEU |
| 1 | I | 36 | ASP |
| 1 | I | 57 | GLU |
| 1 | I | 71 | LEU |
| 1 | I | 72 | GLU |
| 1 | I | 80 | ASN |
| 1 | I | 188 | ASP |
| 1 | I | 212 | ARG |
| 1 | I | 213 | LEU |
| 1 | I | 253 | GLU |
| 1 | I | 264 | GLU |
| 1 | I | 287 | GLN |
| 1 | I | 301 | ARG |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 8 | GLN |
| 1 | A | 14 | GLN |
| 1 | A | 58 | GLN |
| 1 | A | 131 | ASN |
| 1 | A | 208 | ASN |
| 1 | A | 210 | HIS |
| 1 | A | 238 | ASN |
| 1 | A | 298 | HIS |
| 1 | B | 123 | ASN |
| 1 | B | 175 | ASN |
| 1 | B | 193 | ASN |
| 1 | B | 214 | ASN |
| 1 | B | 237 | GLN |
| 1 | B | 270 | HIS |
| 1 | B | 298 | HIS |
| 1 | C | 8 | GLN |
| 1 | C | 9 | HIS |
| 1 | C | 123 | ASN |
| 1 | C | 131 | ASN |
| 1 | C | 175 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | C | 180 | GLN |
| 1 | C | 237 | GLN |
| 1 | C | 255 | GLN |
| 1 | C | 268 | ASN |
| 1 | C | 270 | HIS |
| 1 | C | 298 | HIS |
| 1 | D | 14 | GLN |
| 1 | D | 80 | ASN |
| 1 | D | 123 | ASN |
| 1 | D | 175 | ASN |
| 1 | D | 180 | GLN |
| 1 | D | 193 | ASN |
| 1 | D | 218 | HIS |
| 1 | D | 268 | ASN |
| 1 | D | 298 | HIS |
| 1 | E | 6 | ASN |
| 1 | E | 180 | GLN |
| 1 | E | 238 | ASN |
| 1 | E | 255 | GLN |
| 1 | E | 270 | HIS |
| 1 | E | 298 | HIS |
| 1 | F | 37 | GLN |
| 1 | F | 123 | ASN |
| 1 | F | 184 | ASN |
| 1 | F | 218 | HIS |
| 1 | F | 238 | ASN |
| 1 | F | 255 | GLN |
| 1 | F | 270 | HIS |
| 1 | F | 298 | HIS |
| 1 | G | 31 | ASN |
| 1 | G | 58 | GLN |
| 1 | G | 69 | ASN |
| 1 | G | 123 | ASN |
| 1 | G | 175 | ASN |
| 1 | G | 184 | ASN |
| 1 | G | 208 | ASN |
| 1 | G | 237 | GLN |
| 1 | G | 255 | GLN |
| 1 | G | 298 | HIS |
| 1 | G | 305 | GLN |
| 1 | H | 9 | HIS |
| 1 | H | 14 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | H | 37 | GLN |
| 1 | H | 41 | GLN |
| 1 | H | 80 | ASN |
| 1 | H | 175 | ASN |
| 1 | H | 180 | GLN |
| 1 | H | 208 | ASN |
| 1 | H | 214 | ASN |
| 1 | H | 255 | GLN |
| 1 | H | 268 | ASN |
| 1 | H | 270 | HIS |
| 1 | H | 287 | GLN |
| 1 | H | 298 | HIS |
| 1 | I | 6 | ASN |
| 1 | I | 8 | GLN |
| 1 | I | 31 | ASN |
| 1 | I | 69 | ASN |
| 1 | I | 80 | ASN |
| 1 | I | 175 | ASN |
| 1 | I | 184 | ASN |
| 1 | I | 193 | ASN |
| 1 | I | 207 | GLN |
| 1 | I | 238 | ASN |
| 1 | I | 298 | HIS |
| 1 | I | 305 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 2 | ZRC | A | 400 | 1 | 1,23,25 | 0.11 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | B | 400 | 1 | 1,23,25 | 0.25 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | C | 400 | 1 | 1,23,25 | 0.02 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | D | 400 | 1 | 1,23,25 | 0.04 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | E | 400 | 1 | 1,23,25 | 0.01 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | F | 400 | 1 | 1,23,25 | 0.02 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | G | 400 | 1 | 1,23,25 | 0.12 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | H | 400 | 1 | 1,23,25 | 0.23 | 0 | 0,66,78 | 0.00 | - |
| 2 | ZRC | I | 400 | 1 | 1,23,25 | 0.20 | 0 | 0,66,78 | 0.00 | - |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2 | ZRC | A | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | B | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | C | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | D | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | E | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | F | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | G | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | H | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |
| 2 | ZRC | I | 400 | 1 | - | 0/0/89/99 | 0/0/5/5 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | B | 400 | ZRC | 1 | 0 |
| 2 | C | 400 | ZRC | 1 | 0 |
| 2 | D | 400 | ZRC | 2 | 0 |
| 2 | H | 400 | ZRC | 1 | 0 |
| 2 | I | 400 | ZRC | 1 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.