# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:43 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1FKO |
| Title | : | CRYSTAL STRUCTURE OF NNRTI RESISTANT K103N MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH DMP-266(EFAVIRENZ) |
| Authors | : | Ren, J.; Milton, J.; Weaver, K.L.; Short, S.A.; Stuart, D.I.; Stammers, D.K. |
| Deposited on | : | 2000-08-10 |
| Resolution | : | 2.90 Å(reported) |

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

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

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

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

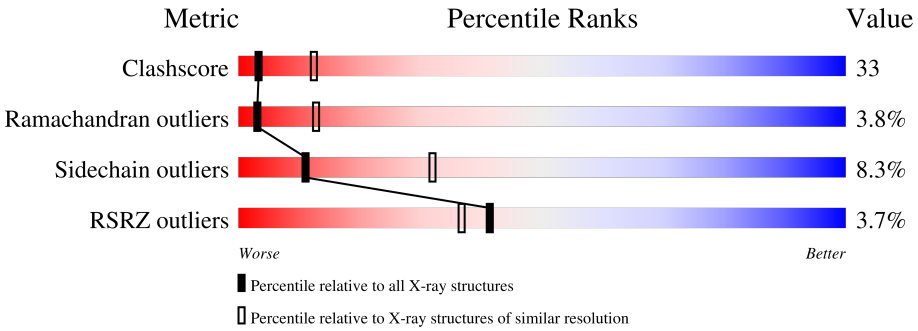
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.2 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 | 141614 | 2172 (2.90-2.90) |
| Ramachandran outliers | 138981 | 2115 (2.90-2.90) |
| Sidechain outliers | 138945 | 2117 (2.90-2.90) |
| RSRZ outliers | 127900 | 1906 (2.90-2.90) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 543 | 5% 39% 53% 7% |
| 2 | B | 440 | 2% 41% 44% 6% 8% |

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7777 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 HIV-1 RT, A-CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 543 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 4434 | 2867 | 739 | 820 | 8 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 103 | ASN | LEU | ENGINEERED MUTATION | UNP P04585 |

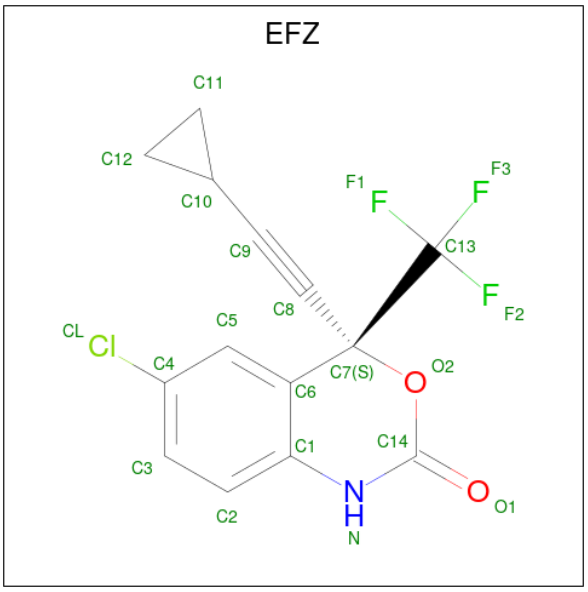
- Molecule 2 is a protein called HIV-1 RT, B-CHAIN.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 403 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3322 | 2157 | 554 | 604 | 7 | | | |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 103 | ASN | LEU | ENGINEERED MUTATION | UNP P04585 |

- Molecule 3 is (-)-6-CHLORO-4-CYCLOPROPYLETHYNYL-4-TRIFLUOROMETHYL-1,4-DIHYDRO-2H-3,1-BENZOXAZIN-2-ONE (three-letter code: EFZ) (formula: $C_{14}H_9ClF_3NO_2$).



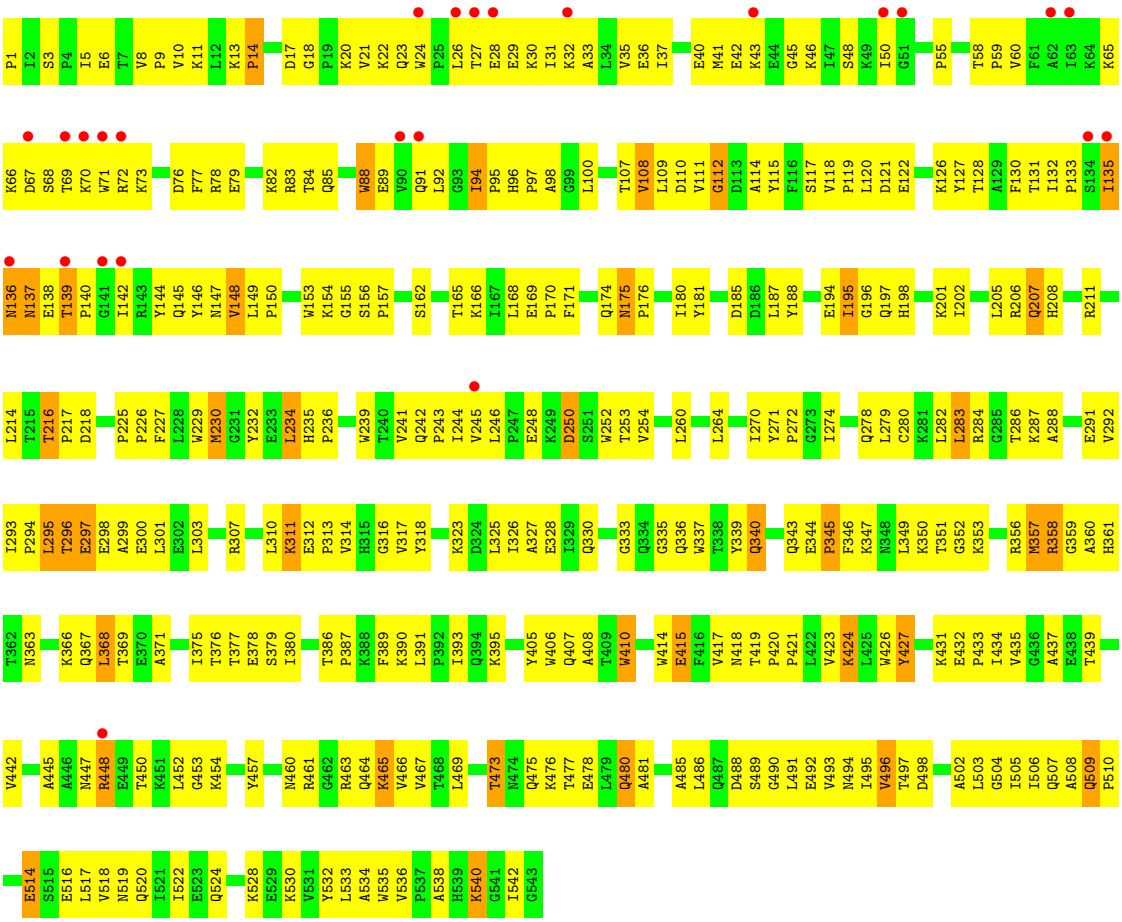

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1 | Total | C | Cl | F | N | O | 0 | 0 |
| | | | 21 | 14 | 1 | 3 | 1 | 2 | | |

# 3 Residue-property plots (i)

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

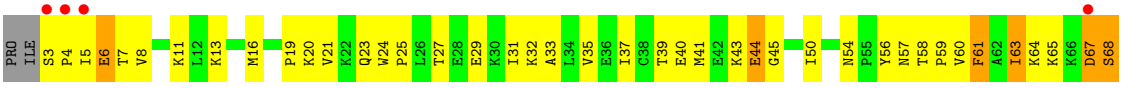
• Molecule 1: HIV-1 RT, A-CHAIN

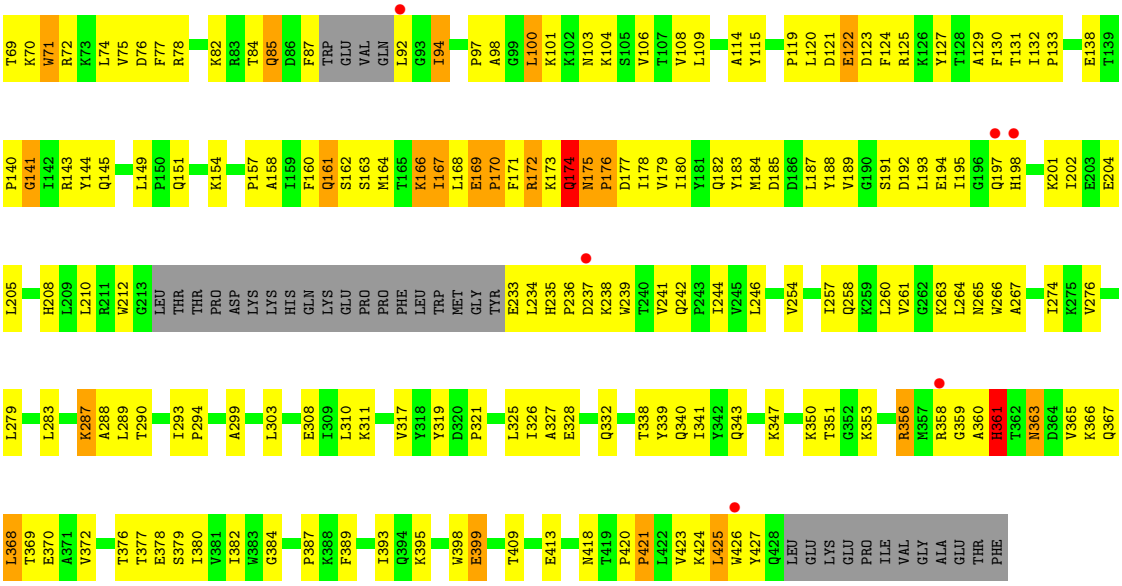
Chain A:


• Molecule 2: HIV-1 RT, B-CHAIN

Chain B:


T69 K70 W71 R72 K73 L74 V75 D76 F77 R78 K82 R83 T84 Q85 D86 F87 TRP GLU VAL GLN L92 G93 I94 P97 A98 G99 L100 K101 K102 N103 K104 S105 V106 T107 V108 L109 A114 Y115 P119 L120 D121 E122 D123 F124 R125 K126 Y127 T128 A129 F130 T131 I132 P133 E138 T139
P140 G141 I142 R143 Y144 Q145 L149 P150 Q151 K154 P157 A158 I159 F160 Q161 S162 S163 M164 T165 K166 I167 L168 E169 P170 F171 R172 K173 Q174 N175 P176 D177 I178 V179 I180 Y181 Q182 Y183 M184 D185 D186 L187 Y188 V189 G190 S191 D192 L193 E194 I195 G196 Q197 H198 K201 I202 E203 E204
L205 H208 L209 L210 R211 W212 Q213 LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR E233 L234 H235 P236 D237 K238 W239 T240 V241 Q242 P243 I244 V245 L246 V254 I257 Q258 K259 L260 V261 G262 K263 L264 N265 W266 A267 I274 K275 V276
L279 L283 K287 A288 L289 T290 I293 P294 A299 L303 E308 I309 L310 K311 V317 Y318 Y319 D320 P321 L325 I326 A327 E328 Q332 T338 Y339 Q340 I341 Y342 Q343 K347 K350 T351 G352 K353 R356 M357 R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367
L368 T369 E370 A371 V372 T376 T377 E378 S379 I380 V381 I382 W383 G384 P387 K388 F389 I393 Q394 K395 W398 E399 T409 E413 N418 T419 P420 P421 L422 V423 K424 L425 W426 Y427 Q428 LEU GLU LYS GLU PRO ILE VAL GLY ALA GLU THR PHE

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 140.30Å 109.70Å 74.40Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.90<br>29.55 – 2.86 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 89.2 (30.00-2.90)<br>87.0 (29.55-2.86) | Depositor<br>EDS |
| $R_{merge}$ | 0.12 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 0.77 (at 2.85Å) | Xtriage |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.205 , 0.287<br>0.205 , (Not available) | Depositor<br>DCC |
| $R_{free}$ test set | No test flags present. | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 61.6 | Xtriage |
| Anisotropy | 0.650 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.29 , 84.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.30$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 7777 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 82.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.44 | 0/4543 | 0.68 | 0/6175 |
| 2 | B | 0.43 | 0/3414 | 0.69 | 0/4637 |
| All | All | 0.44 | 0/7957 | 0.68 | 0/10812 |

There are no bond length outliers.

There are no bond angle outliers.

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 | 4434 | 0 | 4477 | 305 | 0 |
| 2 | B | 3322 | 0 | 3352 | 227 | 0 |
| 3 | A | 21 | 0 | 9 | 0 | 0 |
| All | All | 7777 | 0 | 7838 | 513 | 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 33.

All (513) 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) |
|---|---|---|---|
| 2:B:72:ARG:HH21 | 2:B:409:THR:HG22 | 1.16 | 1.09 |
| 2:B:174:GLN:H | 2:B:176:PRO:HD3 | 1.22 | 1.02 |
| 2:B:173:LYS:HD2 | 2:B:176:PRO:HG2 | 1.44 | 0.99 |
| 1:A:380:ILE:HD11 | 1:A:386:THR:HG22 | 1.46 | 0.95 |
| 1:A:118:VAL:O | 1:A:148:VAL:HG22 | 1.72 | 0.89 |
| 1:A:410:TRP:CE3 | 2:B:363:ASN:HB2 | 2.07 | 0.89 |
| 1:A:226:PRO:HB3 | 1:A:235:HIS:CD2 | 2.08 | 0.89 |
| 1:A:323:LYS:HB2 | 1:A:343:GLN:NE2 | 1.90 | 0.85 |
| 1:A:461:ARG:HG3 | 1:A:461:ARG:HH11 | 1.42 | 0.85 |
| 1:A:239:TRP:CZ2 | 1:A:316:GLY:HA3 | 2.13 | 0.83 |
| 2:B:363:ASN:ND2 | 2:B:366:LYS:HB2 | 1.94 | 0.83 |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:NZ | 1.77 | 0.82 |
| 1:A:206:ARG:HH11 | 1:A:206:ARG:HG2 | 1.43 | 0.82 |
| 1:A:439:THR:HG21 | 2:B:289:LEU:HD13 | 1.63 | 0.81 |
| 2:B:274:ILE:HD11 | 2:B:310:LEU:HD21 | 1.63 | 0.81 |
| 1:A:283:LEU:O | 1:A:286:THR:HG23 | 1.81 | 0.80 |
| 2:B:175:ASN:N | 2:B:176:PRO:HD3 | 1.97 | 0.80 |
| 1:A:227:PHE:HB2 | 1:A:234:LEU:CD1 | 2.11 | 0.80 |
| 1:A:270:ILE:O | 1:A:272:PRO:HD3 | 1.81 | 0.80 |
| 2:B:233:GLU:O | 2:B:234:LEU:HD12 | 1.80 | 0.80 |
| 1:A:120:LEU:HD12 | 1:A:121:ASP:H | 1.46 | 0.79 |
| 2:B:163:SER:HA | 2:B:166:LYS:HE2 | 1.64 | 0.79 |
| 2:B:174:GLN:N | 2:B:176:PRO:HD3 | 1.97 | 0.79 |
| 1:A:390:LYS:HE2 | 1:A:415:GLU:OE2 | 1.84 | 0.78 |
| 1:A:150:PRO:HG2 | 1:A:153:TRP:CB | 2.15 | 0.77 |
| 1:A:490:GLY:H | 1:A:528:LYS:HZ1 | 1.29 | 0.77 |
| 1:A:9:PRO:HA | 1:A:121:ASP:OD2 | 1.85 | 0.77 |
| 2:B:106:VAL:O | 2:B:234:LEU:HB2 | 1.84 | 0.76 |
| 2:B:267:ALA:HB2 | 2:B:426:TRP:CH2 | 2.20 | 0.76 |
| 2:B:244:ILE:HG21 | 2:B:426:TRP:CZ2 | 2.19 | 0.76 |
| 2:B:173:LYS:HA | 2:B:176:PRO:HG3 | 1.68 | 0.76 |
| 2:B:163:SER:O | 2:B:167:ILE:HG13 | 1.87 | 0.75 |
| 1:A:457:TYR:CE2 | 1:A:465:LYS:HB3 | 2.23 | 0.74 |
| 1:A:50:ILE:HD13 | 1:A:145:GLN:HB3 | 1.70 | 0.74 |
| 1:A:317:VAL:HG22 | 1:A:318:TYR:H | 1.52 | 0.73 |
| 1:A:282:LEU:HD12 | 1:A:293:ILE:CG2 | 2.18 | 0.73 |
| 2:B:67:ASP:O | 2:B:68:SER:HB2 | 1.88 | 0.73 |
| 2:B:157:PRO:HG2 | 2:B:184:MET:HA | 1.70 | 0.73 |
| 1:A:21:VAL:HG12 | 1:A:22:LYS:H | 1.52 | 0.72 |
| 1:A:206:ARG:HE | 1:A:218:ASP:HA | 1.54 | 0.72 |
| 2:B:68:SER:OG | 2:B:70:LYS:HG2 | 1.89 | 0.72 |
| 1:A:356:ARG:HB2 | 1:A:367:GLN:NE2 | 2.05 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:157:PRO:CG | 2:B:184:MET:HA | 2.20 | 0.72 |
| 1:A:335:GLY:HA2 | 1:A:367:GLN:OE1 | 1.90 | 0.71 |
| 2:B:27:THR:O | 2:B:31:ILE:HG12 | 1.90 | 0.71 |
| 1:A:393:ILE:HB | 1:A:423:VAL:HG22 | 1.73 | 0.71 |
| 1:A:503:LEU:O | 1:A:507:GLN:HB2 | 1.89 | 0.71 |
| 2:B:7:THR:HG22 | 2:B:119:PRO:HG2 | 1.73 | 0.71 |
| 2:B:173:LYS:HA | 2:B:176:PRO:CG | 2.20 | 0.71 |
| 1:A:41:MET:HB2 | 1:A:46:LYS:HB2 | 1.73 | 0.71 |
| 1:A:126:LYS:HE3 | 1:A:127:TYR:CZ | 2.26 | 0.71 |
| 1:A:31:ILE:HG12 | 1:A:133:PRO:HG2 | 1.72 | 0.70 |
| 1:A:239:TRP:CE2 | 1:A:316:GLY:HA3 | 2.27 | 0.70 |
| 1:A:21:VAL:HG12 | 1:A:22:LYS:N | 2.06 | 0.69 |
| 2:B:387:PRO:HG2 | 2:B:389:PHE:CE1 | 2.27 | 0.69 |
| 1:A:150:PRO:HG2 | 1:A:153:TRP:HB2 | 1.75 | 0.69 |
| 1:A:244:ILE:HG23 | 1:A:310:LEU:HB3 | 1.74 | 0.69 |
| 1:A:282:LEU:HD12 | 1:A:293:ILE:HG21 | 1.74 | 0.69 |
| 1:A:297:GLU:O | 1:A:301:LEU:HD23 | 1.93 | 0.69 |
| 1:A:460:ASN:HD22 | 2:B:288:ALA:HB2 | 1.58 | 0.69 |
| 1:A:13:LYS:HE3 | 1:A:84:THR:O | 1.93 | 0.68 |
| 1:A:540:LYS:HB3 | 1:A:542:ILE:HD11 | 1.75 | 0.68 |
| 1:A:21:VAL:HG11 | 1:A:59:PRO:HD3 | 1.76 | 0.68 |
| 1:A:235:HIS:HB3 | 1:A:236:PRO:HD2 | 1.76 | 0.68 |
| 1:A:278:GLN:HG2 | 1:A:298:GLU:HB3 | 1.75 | 0.68 |
| 2:B:356:ARG:NH2 | 2:B:361:HIS:HB3 | 2.10 | 0.67 |
| 2:B:72:ARG:NH2 | 2:B:409:THR:HG22 | 2.01 | 0.67 |
| 2:B:235:HIS:O | 2:B:238:LYS:HB2 | 1.95 | 0.67 |
| 1:A:100:LEU:O | 1:A:318:TYR:HB3 | 1.95 | 0.66 |
| 1:A:33:ALA:O | 1:A:37:ILE:HD13 | 1.96 | 0.66 |
| 2:B:169:GLU:O | 2:B:172:ARG:HB2 | 1.95 | 0.66 |
| 1:A:366:LYS:O | 1:A:369:THR:HB | 1.95 | 0.66 |
| 2:B:13:LYS:HB2 | 2:B:16:MET:HG3 | 1.75 | 0.66 |
| 1:A:417:VAL:HG13 | 1:A:419:THR:HG22 | 1.78 | 0.65 |
| 1:A:225:PRO:HG3 | 1:A:227:PHE:CE2 | 2.31 | 0.65 |
| 2:B:266:TRP:HZ3 | 2:B:426:TRP:CD1 | 2.14 | 0.65 |
| 2:B:175:ASN:N | 2:B:176:PRO:CD | 2.58 | 0.65 |
| 1:A:360:ALA:HA | 1:A:514:GLU:HG2 | 1.78 | 0.65 |
| 1:A:445:ALA:H | 1:A:477:THR:HG21 | 1.60 | 0.65 |
| 1:A:130:PHE:CZ | 1:A:144:TYR:HB2 | 2.31 | 0.65 |
| 1:A:490:GLY:H | 1:A:528:LYS:NZ | 1.93 | 0.65 |
| 2:B:261:VAL:HG13 | 2:B:276:VAL:HG21 | 1.78 | 0.65 |
| 1:A:89:GLU:OE2 | 1:A:92:LEU:HA | 1.97 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:171:PHE:HB2 | 1:A:208:HIS:CE1 | 2.31 | 0.64 |
| 1:A:23:GLN:HE22 | 1:A:60:VAL:HB | 1.62 | 0.64 |
| 1:A:216:THR:OG1 | 1:A:217:PRO:HD2 | 1.98 | 0.64 |
| 1:A:485:ALA:O | 1:A:489:SER:HB3 | 1.96 | 0.64 |
| 2:B:21:VAL:HB | 2:B:59:PRO:HD3 | 1.80 | 0.64 |
| 1:A:122:GLU:H | 1:A:122:GLU:CD | 1.98 | 0.64 |
| 2:B:350:LYS:HE3 | 2:B:378:GLU:OE1 | 1.98 | 0.64 |
| 1:A:181:TYR:CD1 | 2:B:138:GLU:HA | 2.32 | 0.63 |
| 1:A:380:ILE:CD1 | 1:A:386:THR:HG22 | 2.25 | 0.63 |
| 2:B:201:LYS:HZ3 | 2:B:204:GLU:CD | 2.01 | 0.63 |
| 1:A:439:THR:CG2 | 2:B:289:LEU:HD13 | 2.27 | 0.63 |
| 1:A:156:SER:HB2 | 1:A:157:PRO:HD3 | 1.82 | 0.62 |
| 2:B:3:SER:N | 2:B:4:PRO:HD3 | 2.13 | 0.62 |
| 2:B:174:GLN:HG3 | 2:B:175:ASN:OD1 | 1.98 | 0.62 |
| 1:A:26:LEU:HD22 | 1:A:30:LYS:HE3 | 1.81 | 0.62 |
| 1:A:317:VAL:HG22 | 1:A:318:TYR:N | 2.15 | 0.62 |
| 1:A:330:GLN:NE2 | 1:A:340:GLN:OE1 | 2.31 | 0.62 |
| 1:A:248:GLU:HA | 1:A:307:ARG:NH2 | 2.14 | 0.62 |
| 2:B:328:GLU:O | 2:B:339:TYR:HA | 2.00 | 0.62 |
| 1:A:274:ILE:HD11 | 1:A:310:LEU:HD21 | 1.82 | 0.62 |
| 2:B:170:PRO:O | 2:B:174:GLN:HB3 | 2.00 | 0.61 |
| 1:A:206:ARG:HG2 | 1:A:206:ARG:NH1 | 2.10 | 0.61 |
| 2:B:120:LEU:HD22 | 2:B:125:ARG:HG3 | 1.82 | 0.61 |
| 2:B:175:ASN:H | 2:B:176:PRO:HD3 | 1.64 | 0.61 |
| 2:B:175:ASN:ND2 | 2:B:201:LYS:NZ | 2.47 | 0.61 |
| 1:A:174:GLN:C | 1:A:176:PRO:HD3 | 2.21 | 0.61 |
| 1:A:234:LEU:HD12 | 1:A:234:LEU:H | 1.65 | 0.61 |
| 1:A:260:LEU:HG | 1:A:264:LEU:HD23 | 1.82 | 0.61 |
| 2:B:242:GLN:HE22 | 2:B:353:LYS:HE3 | 1.64 | 0.61 |
| 2:B:360:ALA:HB2 | 2:B:366:LYS:HD2 | 1.82 | 0.61 |
| 1:A:340:GLN:HB3 | 1:A:351:THR:HG22 | 1.83 | 0.60 |
| 1:A:254:VAL:HG22 | 1:A:293:ILE:HD11 | 1.82 | 0.60 |
| 1:A:150:PRO:HG2 | 1:A:153:TRP:HB3 | 1.82 | 0.60 |
| 1:A:169:GLU:N | 1:A:170:PRO:HD2 | 2.16 | 0.60 |
| 1:A:325:LEU:O | 1:A:326:ILE:HD13 | 2.02 | 0.60 |
| 1:A:79:GLU:O | 1:A:83:ARG:HG3 | 1.99 | 0.60 |
| 2:B:124:PHE:CD1 | 2:B:127:TYR:HD2 | 2.20 | 0.60 |
| 2:B:266:TRP:CZ3 | 2:B:426:TRP:CD1 | 2.90 | 0.60 |
| 1:A:3:SER:HB3 | 1:A:119:PRO:HD3 | 1.83 | 0.60 |
| 2:B:158:ALA:O | 2:B:161:GLN:HB2 | 2.01 | 0.60 |
| 1:A:76:ASP:OD1 | 1:A:78:ARG:HG3 | 2.02 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:461:ARG:HH11 | 1:A:461:ARG:CG | 2.15 | 0.59 |
| 1:A:170:PRO:HG2 | 1:A:171:PHE:H | 1.67 | 0.59 |
| 1:A:407:GLN:HG2 | 2:B:393:ILE:HA | 1.85 | 0.59 |
| 2:B:308:GLU:O | 2:B:311:LYS:HB2 | 2.03 | 0.59 |
| 2:B:242:GLN:O | 2:B:242:GLN:HG3 | 2.03 | 0.59 |
| 2:B:267:ALA:CB | 2:B:426:TRP:CH2 | 2.85 | 0.59 |
| 2:B:356:ARG:CZ | 2:B:361:HIS:HB3 | 2.32 | 0.59 |
| 1:A:118:VAL:C | 1:A:148:VAL:HG22 | 2.22 | 0.59 |
| 2:B:114:ALA:HB1 | 2:B:160:PHE:CZ | 2.38 | 0.59 |
| 1:A:408:ALA:O | 2:B:393:ILE:HG13 | 2.04 | 0.58 |
| 1:A:50:ILE:HG23 | 1:A:145:GLN:HG2 | 1.85 | 0.58 |
| 1:A:498:ASP:HA | 1:A:536:VAL:O | 2.03 | 0.58 |
| 1:A:432:GLU:HB2 | 1:A:433:PRO:HD2 | 1.86 | 0.58 |
| 2:B:104:LYS:HB3 | 2:B:192:ASP:HA | 1.85 | 0.58 |
| 2:B:237:ASP:C | 2:B:239:TRP:N | 2.54 | 0.58 |
| 2:B:263:LYS:HE2 | 2:B:425:LEU:HB3 | 1.86 | 0.58 |
| 1:A:115:TYR:CE2 | 1:A:156:SER:HB3 | 2.38 | 0.58 |
| 2:B:161:GLN:OE1 | 2:B:161:GLN:HA | 2.02 | 0.58 |
| 1:A:139:THR:HB | 1:A:140:PRO:HD3 | 1.85 | 0.58 |
| 2:B:120:LEU:HD21 | 2:B:124:PHE:HD2 | 1.68 | 0.58 |
| 1:A:518:VAL:O | 1:A:522:ILE:HG13 | 2.04 | 0.58 |
| 2:B:20:LYS:HE2 | 2:B:56:TYR:CE1 | 2.39 | 0.57 |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:CE | 2.17 | 0.57 |
| 1:A:311:LYS:O | 1:A:313:PRO:HD3 | 2.03 | 0.57 |
| 1:A:426:TRP:O | 1:A:427:TYR:HB3 | 2.04 | 0.57 |
| 1:A:454:LYS:HA | 1:A:467:VAL:O | 2.04 | 0.57 |
| 2:B:120:LEU:HD23 | 2:B:121:ASP:N | 2.20 | 0.57 |
| 2:B:100:LEU:N | 2:B:100:LEU:HD23 | 2.20 | 0.57 |
| 2:B:365:VAL:O | 2:B:369:THR:HG23 | 2.05 | 0.57 |
| 1:A:24:TRP:HD1 | 1:A:24:TRP:H | 1.53 | 0.56 |
| 2:B:369:THR:HG22 | 2:B:398:TRP:CH2 | 2.40 | 0.56 |
| 1:A:208:HIS:HA | 1:A:211:ARG:HD3 | 1.88 | 0.56 |
| 2:B:237:ASP:C | 2:B:239:TRP:H | 2.08 | 0.56 |
| 1:A:270:ILE:HG23 | 1:A:271:TYR:N | 2.21 | 0.56 |
| 2:B:151:GLN:HB3 | 2:B:185:ASP:OD1 | 2.06 | 0.56 |
| 1:A:244:ILE:HG21 | 1:A:310:LEU:HD22 | 1.88 | 0.55 |
| 1:A:532:TYR:CE2 | 1:A:534:ALA:HB2 | 2.42 | 0.55 |
| 2:B:341:ILE:N | 2:B:341:ILE:HD12 | 2.21 | 0.55 |
| 1:A:486:LEU:HB3 | 1:A:524:GLN:CG | 2.35 | 0.55 |
| 1:A:229:TRP:O | 1:A:232:TYR:N | 2.40 | 0.55 |
| 1:A:287:LYS:HG2 | 1:A:291:GLU:OE2 | 2.06 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:214:LEU:N | 1:A:214:LEU:HD12 | 2.22 | 0.55 |
| 2:B:266:TRP:CZ3 | 2:B:426:TRP:CG | 2.95 | 0.55 |
| 2:B:108:VAL:HG22 | 2:B:188:TYR:CD2 | 2.42 | 0.55 |
| 1:A:97:PRO:HA | 1:A:100:LEU:HG | 1.87 | 0.54 |
| 1:A:23:GLN:HG2 | 1:A:131:THR:O | 2.07 | 0.54 |
| 1:A:31:ILE:HD12 | 1:A:135:ILE:HA | 1.87 | 0.54 |
| 2:B:29:GLU:HG3 | 2:B:71:TRP:CH2 | 2.42 | 0.54 |
| 1:A:171:PHE:HD1 | 1:A:208:HIS:HD1 | 1.55 | 0.54 |
| 1:A:295:LEU:HD23 | 1:A:299:ALA:HB3 | 1.89 | 0.54 |
| 2:B:115:TYR:HB3 | 2:B:149:LEU:HB2 | 1.87 | 0.54 |
| 2:B:173:LYS:HD2 | 2:B:176:PRO:CG | 2.29 | 0.54 |
| 2:B:246:LEU:HD22 | 2:B:260:LEU:HD11 | 1.89 | 0.54 |
| 1:A:226:PRO:HB3 | 1:A:235:HIS:NE2 | 2.22 | 0.54 |
| 1:A:434:ILE:HG22 | 1:A:437:ALA:HB2 | 1.88 | 0.54 |
| 1:A:17:ASP:O | 1:A:83:ARG:NE | 2.41 | 0.54 |
| 1:A:229:TRP:O | 1:A:230:MET:C | 2.46 | 0.54 |
| 1:A:434:ILE:CG2 | 1:A:437:ALA:HB2 | 2.38 | 0.54 |
| 2:B:244:ILE:HG21 | 2:B:426:TRP:CH2 | 2.43 | 0.54 |
| 2:B:366:LYS:HE2 | 2:B:370:GLU:OE2 | 2.07 | 0.54 |
| 1:A:516:GLU:HA | 1:A:519:ASN:HD22 | 1.73 | 0.53 |
| 1:A:246:LEU:HB2 | 1:A:307:ARG:NH1 | 2.23 | 0.53 |
| 1:A:21:VAL:CG1 | 1:A:59:PRO:HD3 | 2.39 | 0.53 |
| 1:A:241:VAL:HG23 | 1:A:314:VAL:O | 2.08 | 0.53 |
| 2:B:57:ASN:HA | 2:B:129:ALA:O | 2.08 | 0.53 |
| 2:B:43:LYS:O | 2:B:45:GLY:N | 2.42 | 0.53 |
| 1:A:356:ARG:HB2 | 1:A:367:GLN:HE22 | 1.72 | 0.53 |
| 1:A:395:LYS:HD3 | 1:A:414:TRP:CZ2 | 2.43 | 0.53 |
| 1:A:448:ARG:NH2 | 1:A:473:THR:OG1 | 2.41 | 0.53 |
| 2:B:176:PRO:C | 2:B:178:ILE:H | 2.12 | 0.53 |
| 1:A:120:LEU:HD12 | 1:A:121:ASP:N | 2.21 | 0.53 |
| 1:A:465:LYS:HG2 | 1:A:466:VAL:N | 2.22 | 0.53 |
| 1:A:502:ALA:O | 1:A:503:LEU:C | 2.45 | 0.53 |
| 1:A:78:ARG:O | 1:A:82:LYS:HG3 | 2.09 | 0.53 |
| 1:A:442:VAL:CG1 | 1:A:485:ALA:HB2 | 2.38 | 0.53 |
| 2:B:395:LYS:HG2 | 2:B:399:GLU:HG3 | 1.90 | 0.53 |
| 1:A:112:GLY:H | 1:A:185:ASP:HB3 | 1.74 | 0.52 |
| 2:B:94:ILE:HG23 | 2:B:94:ILE:O | 2.09 | 0.52 |
| 2:B:191:SER:HB2 | 2:B:193:LEU:HD13 | 1.90 | 0.52 |
| 1:A:128:THR:HB | 1:A:146:TYR:HB2 | 1.91 | 0.52 |
| 1:A:410:TRP:CZ3 | 2:B:363:ASN:HB2 | 2.42 | 0.52 |
| 2:B:72:ARG:HG3 | 2:B:72:ARG:HH11 | 1.74 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:106:VAL:HA | 2:B:189:VAL:O | 2.08 | 0.52 |
| 1:A:50:ILE:CG2 | 1:A:145:GLN:HG2 | 2.40 | 0.52 |
| 2:B:242:GLN:NE2 | 2:B:353:LYS:HE3 | 2.24 | 0.52 |
| 2:B:160:PHE:O | 2:B:160:PHE:CD1 | 2.62 | 0.52 |
| 1:A:108:VAL:C | 1:A:109:LEU:HD12 | 2.30 | 0.52 |
| 1:A:122:GLU:N | 1:A:122:GLU:OE1 | 2.43 | 0.52 |
| 1:A:171:PHE:CZ | 1:A:205:LEU:HB2 | 2.45 | 0.52 |
| 1:A:195:ILE:CG1 | 1:A:196:GLY:N | 2.72 | 0.52 |
| 1:A:417:VAL:HG13 | 1:A:417:VAL:O | 2.08 | 0.52 |
| 1:A:460:ASN:ND2 | 2:B:288:ALA:HB2 | 2.23 | 0.52 |
| 1:A:503:LEU:HD22 | 1:A:535:TRP:CB | 2.39 | 0.52 |
| 2:B:130:PHE:CZ | 2:B:144:TYR:HB2 | 2.45 | 0.52 |
| 1:A:296:THR:HG23 | 1:A:299:ALA:CB | 2.39 | 0.52 |
| 2:B:54:ASN:O | 2:B:143:ARG:NH2 | 2.42 | 0.52 |
| 1:A:497:THR:O | 1:A:535:TRP:HA | 2.10 | 0.52 |
| 2:B:205:LEU:HD13 | 2:B:205:LEU:C | 2.30 | 0.52 |
| 2:B:420:PRO:O | 2:B:423:VAL:HG22 | 2.10 | 0.52 |
| 1:A:88:TRP:HA | 1:A:88:TRP:CE3 | 2.45 | 0.51 |
| 1:A:486:LEU:HB3 | 1:A:524:GLN:HG2 | 1.93 | 0.51 |
| 2:B:5:ILE:HG22 | 2:B:6:GLU:N | 2.25 | 0.51 |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:HZ1 | 1.54 | 0.51 |
| 2:B:179:VAL:C | 2:B:180:ILE:HD12 | 2.31 | 0.51 |
| 2:B:274:ILE:HD11 | 2:B:310:LEU:CD2 | 2.38 | 0.51 |
| 1:A:96:HIS:HD1 | 1:A:97:PRO:HD2 | 1.75 | 0.51 |
| 1:A:293:ILE:HG23 | 1:A:294:PRO:HD2 | 1.91 | 0.51 |
| 1:A:466:VAL:HG22 | 1:A:467:VAL:N | 2.25 | 0.51 |
| 2:B:387:PRO:HG2 | 2:B:389:PHE:CZ | 2.45 | 0.51 |
| 1:A:37:ILE:O | 1:A:40:GLU:HB3 | 2.10 | 0.51 |
| 1:A:96:HIS:ND1 | 1:A:97:PRO:HD2 | 2.25 | 0.51 |
| 1:A:296:THR:HG23 | 1:A:299:ALA:HB2 | 1.92 | 0.51 |
| 2:B:100:LEU:H | 2:B:100:LEU:CD2 | 2.23 | 0.51 |
| 1:A:1:PRO:H2 | 1:A:46:LYS:NZ | 2.09 | 0.50 |
| 1:A:476:LYS:O | 1:A:480:GLN:HB2 | 2.11 | 0.50 |
| 1:A:350:LYS:HG2 | 1:A:351:THR:N | 2.27 | 0.50 |
| 2:B:40:GLU:O | 2:B:44:GLU:HG3 | 2.12 | 0.50 |
| 2:B:241:VAL:HG13 | 2:B:351:THR:OG1 | 2.11 | 0.50 |
| 2:B:122:GLU:HA | 2:B:125:ARG:HD2 | 1.93 | 0.50 |
| 1:A:303:LEU:O | 1:A:303:LEU:HD23 | 2.12 | 0.50 |
| 2:B:326:ILE:O | 2:B:341:ILE:HA | 2.12 | 0.50 |
| 2:B:43:LYS:C | 2:B:45:GLY:H | 2.15 | 0.50 |
| 2:B:359:GLY:C | 2:B:361:HIS:H | 2.16 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:363:ASN:HD21 | 2:B:366:LYS:HB2 | 1.74 | 0.50 |
| 2:B:40:GLU:HG2 | 2:B:44:GLU:OE2 | 2.12 | 0.49 |
| 2:B:236:PRO:C | 2:B:238:LYS:H | 2.15 | 0.49 |
| 1:A:21:VAL:CG1 | 1:A:22:LYS:N | 2.75 | 0.49 |
| 1:A:344:GLU:O | 1:A:347:LYS:HB2 | 2.11 | 0.49 |
| 2:B:84:THR:HG22 | 2:B:154:LYS:HE2 | 1.94 | 0.49 |
| 2:B:368:LEU:O | 2:B:372:VAL:HG23 | 2.12 | 0.49 |
| 1:A:48:SER:O | 1:A:144:TYR:HA | 2.13 | 0.49 |
| 1:A:410:TRP:CD2 | 2:B:363:ASN:HB2 | 2.46 | 0.49 |
| 2:B:97:PRO:HG2 | 2:B:100:LEU:CD2 | 2.42 | 0.49 |
| 2:B:175:ASN:ND2 | 2:B:201:LYS:HZ2 | 2.10 | 0.49 |
| 1:A:120:LEU:HD21 | 1:A:128:THR:HG21 | 1.93 | 0.49 |
| 1:A:148:VAL:HG13 | 1:A:149:LEU:N | 2.27 | 0.49 |
| 1:A:406:TRP:CH2 | 2:B:418:ASN:HA | 2.46 | 0.49 |
| 2:B:11:LYS:O | 2:B:85:GLN:HG2 | 2.12 | 0.49 |
| 2:B:201:LYS:O | 2:B:204:GLU:HB3 | 2.12 | 0.49 |
| 2:B:423:VAL:O | 2:B:427:TYR:HD2 | 1.95 | 0.49 |
| 1:A:244:ILE:CG2 | 1:A:310:LEU:HB3 | 2.42 | 0.49 |
| 2:B:98:ALA:O | 2:B:101:LYS:HB3 | 2.12 | 0.49 |
| 2:B:175:ASN:O | 2:B:177:ASP:N | 2.45 | 0.49 |
| 2:B:308:GLU:HA | 2:B:311:LYS:HD2 | 1.95 | 0.49 |
| 2:B:356:ARG:HH12 | 2:B:359:GLY:H | 1.60 | 0.49 |
| 1:A:424:LYS:HE3 | 1:A:426:TRP:CD2 | 2.48 | 0.49 |
| 2:B:167:ILE:HG23 | 2:B:212:TRP:CD1 | 2.48 | 0.49 |
| 2:B:168:LEU:C | 2:B:170:PRO:HD2 | 2.34 | 0.48 |
| 1:A:154:LYS:O | 1:A:157:PRO:HD2 | 2.12 | 0.48 |
| 2:B:72:ARG:HH22 | 2:B:151:GLN:NE2 | 2.11 | 0.48 |
| 2:B:350:LYS:HG2 | 2:B:351:THR:N | 2.29 | 0.48 |
| 1:A:516:GLU:O | 1:A:520:GLN:HG2 | 2.12 | 0.48 |
| 1:A:59:PRO:HG2 | 1:A:76:ASP:HB3 | 1.94 | 0.48 |
| 1:A:457:TYR:CZ | 1:A:465:LYS:HB3 | 2.49 | 0.48 |
| 2:B:254:VAL:HB | 2:B:289:LEU:HA | 1.95 | 0.48 |
| 1:A:110:ASP:O | 1:A:217:PRO:HD3 | 2.13 | 0.48 |
| 2:B:197:GLN:O | 2:B:201:LYS:HB2 | 2.13 | 0.48 |
| 2:B:140:PRO:O | 2:B:141:GLY:O | 2.30 | 0.48 |
| 1:A:8:VAL:O | 1:A:10:VAL:HG23 | 2.13 | 0.48 |
| 1:A:111:VAL:HG23 | 1:A:112:GLY:N | 2.29 | 0.48 |
| 1:A:31:ILE:O | 1:A:35:VAL:HG23 | 2.14 | 0.48 |
| 1:A:111:VAL:CG2 | 1:A:112:GLY:N | 2.76 | 0.48 |
| 1:A:171:PHE:CE1 | 1:A:205:LEU:HA | 2.48 | 0.48 |
| 2:B:205:LEU:HD13 | 2:B:205:LEU:O | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:208:HIS:O | 1:A:211:ARG:HB2 | 2.14 | 0.48 |
| 1:A:180:ILE:HA | 1:A:188:TYR:O | 2.14 | 0.47 |
| 2:B:363:ASN:CG | 2:B:366:LYS:HB2 | 2.34 | 0.47 |
| 1:A:205:LEU:O | 1:A:208:HIS:HB3 | 2.14 | 0.47 |
| 1:A:503:LEU:HD13 | 1:A:535:TRP:HB2 | 1.95 | 0.47 |
| 1:A:11:LYS:O | 1:A:85:GLN:HB3 | 2.14 | 0.47 |
| 1:A:21:VAL:CG1 | 1:A:22:LYS:H | 2.22 | 0.47 |
| 2:B:171:PHE:HA | 2:B:174:GLN:HG2 | 1.96 | 0.47 |
| 2:B:201:LYS:NZ | 2:B:204:GLU:OE2 | 2.46 | 0.47 |
| 2:B:317:VAL:HG12 | 2:B:347:LYS:HB3 | 1.96 | 0.47 |
| 2:B:339:TYR:C | 2:B:340:GLN:NE2 | 2.67 | 0.47 |
| 1:A:478:GLU:O | 1:A:481:ALA:HB3 | 2.14 | 0.47 |
| 1:A:494:ASN:HB3 | 2:B:289:LEU:HD22 | 1.95 | 0.47 |
| 1:A:171:PHE:HB2 | 1:A:208:HIS:ND1 | 2.29 | 0.47 |
| 2:B:157:PRO:HG3 | 2:B:184:MET:HA | 1.95 | 0.47 |
| 2:B:166:LYS:O | 2:B:168:LEU:N | 2.47 | 0.47 |
| 2:B:172:ARG:HG3 | 2:B:172:ARG:HH11 | 1.80 | 0.47 |
| 2:B:198:HIS:O | 2:B:202:ILE:HG12 | 2.14 | 0.47 |
| 1:A:254:VAL:HG21 | 1:A:288:ALA:O | 2.14 | 0.47 |
| 1:A:333:GLY:H | 1:A:336:GLN:HB3 | 1.80 | 0.47 |
| 1:A:109:LEU:HD12 | 1:A:109:LEU:N | 2.29 | 0.47 |
| 1:A:162:SER:O | 1:A:165:THR:N | 2.48 | 0.47 |
| 1:A:174:GLN:O | 1:A:176:PRO:HD3 | 2.14 | 0.47 |
| 1:A:297:GLU:HA | 1:A:300:GLU:HB2 | 1.95 | 0.47 |
| 1:A:461:ARG:HG3 | 1:A:461:ARG:NH1 | 2.21 | 0.47 |
| 1:A:498:ASP:HB2 | 1:A:538:ALA:HB2 | 1.97 | 0.47 |
| 1:A:516:GLU:HA | 1:A:516:GLU:OE2 | 2.14 | 0.47 |
| 1:A:516:GLU:O | 1:A:519:ASN:HB2 | 2.14 | 0.47 |
| 1:A:60:VAL:CG2 | 1:A:130:PHE:HB2 | 2.45 | 0.47 |
| 1:A:114:ALA:O | 1:A:117:SER:HB2 | 2.15 | 0.47 |
| 1:A:345:PRO:HB2 | 1:A:346:PHE:CD1 | 2.49 | 0.47 |
| 2:B:72:ARG:NH2 | 2:B:151:GLN:NE2 | 2.63 | 0.47 |
| 1:A:20:LYS:HG2 | 1:A:55:PRO:O | 2.14 | 0.47 |
| 1:A:30:LYS:HG2 | 1:A:71:TRP:CH2 | 2.50 | 0.47 |
| 1:A:139:THR:HB | 1:A:140:PRO:CD | 2.44 | 0.47 |
| 1:A:181:TYR:CE1 | 2:B:138:GLU:HA | 2.49 | 0.47 |
| 1:A:300:GLU:OE2 | 1:A:300:GLU:HA | 2.15 | 0.47 |
| 2:B:100:LEU:O | 2:B:236:PRO:HG2 | 2.15 | 0.47 |
| 1:A:445:ALA:N | 1:A:477:THR:HG21 | 2.29 | 0.46 |
| 1:A:207:GLN:O | 1:A:211:ARG:HG3 | 2.15 | 0.46 |
| 1:A:405:TYR:CE2 | 1:A:407:GLN:HB3 | 2.50 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:131:THR:OG1 | 2:B:143:ARG:HD2 | 2.15 | 0.46 |
| 2:B:178:ILE:HG22 | 2:B:180:ILE:CD1 | 2.46 | 0.46 |
| 1:A:340:GLN:CB | 1:A:351:THR:HG22 | 2.45 | 0.46 |
| 2:B:325:LEU:HD12 | 2:B:343:GLN:CG | 2.45 | 0.46 |
| 2:B:35:VAL:O | 2:B:39:THR:HG23 | 2.16 | 0.46 |
| 2:B:78:ARG:O | 2:B:82:LYS:HD3 | 2.16 | 0.46 |
| 1:A:88:TRP:HA | 1:A:88:TRP:HE3 | 1.81 | 0.46 |
| 1:A:187:LEU:HD12 | 1:A:187:LEU:HA | 1.80 | 0.46 |
| 2:B:100:LEU:N | 2:B:100:LEU:CD2 | 2.78 | 0.46 |
| 2:B:377:THR:O | 2:B:378:GLU:C | 2.53 | 0.46 |
| 1:A:89:GLU:HG3 | 1:A:89:GLU:O | 2.16 | 0.46 |
| 2:B:171:PHE:O | 2:B:172:ARG:O | 2.34 | 0.46 |
| 1:A:380:ILE:HG22 | 2:B:25:PRO:HB2 | 1.96 | 0.46 |
| 2:B:101:LYS:HD2 | 2:B:382:ILE:HG23 | 1.97 | 0.46 |
| 1:A:37:ILE:HG21 | 1:A:73:LYS:HD3 | 1.98 | 0.45 |
| 1:A:65:LYS:HG3 | 1:A:68:SER:HB3 | 1.98 | 0.45 |
| 2:B:7:THR:CG2 | 2:B:119:PRO:HG2 | 2.45 | 0.45 |
| 2:B:366:LYS:O | 2:B:370:GLU:HG3 | 2.16 | 0.45 |
| 1:A:447:ASN:HB3 | 1:A:450:THR:OG1 | 2.16 | 0.45 |
| 2:B:67:ASP:O | 2:B:68:SER:CB | 2.58 | 0.45 |
| 2:B:379:SER:CB | 2:B:387:PRO:HD3 | 2.46 | 0.45 |
| 2:B:380:ILE:O | 2:B:384:GLY:N | 2.48 | 0.45 |
| 1:A:376:THR:O | 1:A:379:SER:HB2 | 2.17 | 0.45 |
| 2:B:5:ILE:HG22 | 2:B:6:GLU:H | 1.81 | 0.45 |
| 1:A:420:PRO:HA | 1:A:421:PRO:C | 2.36 | 0.45 |
| 1:A:508:ALA:O | 1:A:510:PRO:N | 2.50 | 0.45 |
| 2:B:64:LYS:HE3 | 2:B:71:TRP:CZ2 | 2.52 | 0.45 |
| 2:B:85:GLN:O | 2:B:85:GLN:HG3 | 2.15 | 0.45 |
| 1:A:234:LEU:HD12 | 1:A:234:LEU:N | 2.31 | 0.45 |
| 2:B:100:LEU:HD23 | 2:B:100:LEU:H | 1.81 | 0.45 |
| 1:A:375:ILE:O | 1:A:376:THR:C | 2.53 | 0.45 |
| 2:B:376:THR:O | 2:B:380:ILE:HG13 | 2.16 | 0.45 |
| 1:A:65:LYS:HB3 | 1:A:72:ARG:HD3 | 1.98 | 0.45 |
| 2:B:257:ILE:HB | 2:B:283:LEU:HD11 | 1.97 | 0.45 |
| 2:B:175:ASN:HD21 | 2:B:201:LYS:HE3 | 1.81 | 0.45 |
| 1:A:23:GLN:HE22 | 1:A:60:VAL:CB | 2.29 | 0.45 |
| 1:A:253:THR:HA | 1:A:292:VAL:HA | 1.98 | 0.45 |
| 2:B:359:GLY:HA2 | 2:B:361:HIS:CE1 | 2.51 | 0.45 |
| 1:A:496:VAL:HA | 1:A:534:ALA:O | 2.16 | 0.44 |
| 1:A:508:ALA:O | 1:A:509:GLN:C | 2.55 | 0.44 |
| 2:B:267:ALA:HB2 | 2:B:426:TRP:CZ3 | 2.53 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:142:ILE:N | 1:A:142:ILE:HD12 | 2.31 | 0.44 |
| 1:A:350:LYS:HE3 | 1:A:378:GLU:OE2 | 2.16 | 0.44 |
| 2:B:61:PHE:N | 2:B:61:PHE:CD2 | 2.85 | 0.44 |
| 1:A:175:ASN:OD1 | 1:A:201:LYS:HE2 | 2.18 | 0.44 |
| 1:A:311:LYS:O | 1:A:313:PRO:CD | 2.64 | 0.44 |
| 1:A:358:ARG:HB2 | 1:A:358:ARG:NH1 | 2.32 | 0.44 |
| 1:A:488:ASP:OD2 | 1:A:488:ASP:N | 2.47 | 0.44 |
| 1:A:92:LEU:HD22 | 2:B:141:GLY:H | 1.82 | 0.44 |
| 1:A:328:GLU:O | 1:A:339:TYR:HA | 2.17 | 0.44 |
| 1:A:505:ILE:HG22 | 1:A:506:ILE:N | 2.31 | 0.44 |
| 2:B:169:GLU:HA | 2:B:172:ARG:HB2 | 1.98 | 0.44 |
| 1:A:23:GLN:NE2 | 1:A:131:THR:O | 2.44 | 0.44 |
| 1:A:69:THR:O | 1:A:69:THR:HG22 | 2.18 | 0.44 |
| 1:A:424:LYS:HE3 | 1:A:426:TRP:CE3 | 2.53 | 0.43 |
| 1:A:495:ILE:O | 1:A:533:LEU:HD12 | 2.17 | 0.43 |
| 1:A:66:LYS:HD3 | 1:A:66:LYS:HA | 1.84 | 0.43 |
| 2:B:32:LYS:O | 2:B:35:VAL:HG22 | 2.18 | 0.43 |
| 1:A:31:ILE:HD13 | 1:A:133:PRO:O | 2.17 | 0.43 |
| 1:A:32:LYS:O | 1:A:36:GLU:HG3 | 2.18 | 0.43 |
| 1:A:66:LYS:O | 1:A:67:ASP:CB | 2.66 | 0.43 |
| 1:A:252:TRP:CD1 | 1:A:295:LEU:HD12 | 2.53 | 0.43 |
| 1:A:463:ARG:HG2 | 1:A:464:GLN:N | 2.34 | 0.43 |
| 2:B:319:TYR:CE1 | 2:B:321:PRO:HG3 | 2.53 | 0.43 |
| 2:B:356:ARG:HB2 | 2:B:367:GLN:HG2 | 2.00 | 0.43 |
| 1:A:248:GLU:HA | 1:A:307:ARG:HH22 | 1.83 | 0.43 |
| 2:B:353:LYS:HE3 | 2:B:353:LYS:HB2 | 1.77 | 0.43 |
| 2:B:413:GLU:HA | 2:B:413:GLU:OE2 | 2.17 | 0.43 |
| 1:A:386:THR:HA | 1:A:387:PRO:HD3 | 1.81 | 0.43 |
| 1:A:407:GLN:CG | 2:B:393:ILE:HA | 2.47 | 0.43 |
| 1:A:536:VAL:HG11 | 2:B:258:GLN:HG2 | 2.00 | 0.43 |
| 2:B:19:PRO:O | 2:B:56:TYR:HB3 | 2.19 | 0.43 |
| 2:B:279:LEU:HD23 | 2:B:299:ALA:HB1 | 2.00 | 0.43 |
| 1:A:419:THR:HG23 | 1:A:419:THR:O | 2.18 | 0.43 |
| 1:A:175:ASN:N | 1:A:175:ASN:ND2 | 2.66 | 0.43 |
| 1:A:453:GLY:O | 1:A:469:LEU:N | 2.39 | 0.43 |
| 2:B:129:ALA:HA | 2:B:144:TYR:O | 2.18 | 0.43 |
| 2:B:182:GLN:HB2 | 2:B:187:LEU:CD1 | 2.49 | 0.43 |
| 1:A:77:PHE:O | 1:A:78:ARG:C | 2.54 | 0.43 |
| 2:B:340:GLN:C | 2:B:341:ILE:HD12 | 2.39 | 0.43 |
| 2:B:395:LYS:HG2 | 2:B:399:GLU:CG | 2.49 | 0.43 |
| 1:A:254:VAL:HG13 | 1:A:286:THR:HG21 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:282:LEU:N | 1:A:282:LEU:HD22 | 2.34 | 0.43 |
| 2:B:120:LEU:HD22 | 2:B:125:ARG:CG | 2.46 | 0.43 |
| 1:A:339:TYR:CE2 | 1:A:352:GLY:HA3 | 2.54 | 0.43 |
| 2:B:37:ILE:O | 2:B:41:MET:HG3 | 2.18 | 0.43 |
| 2:B:183:TYR:HB3 | 2:B:188:TYR:HE1 | 1.83 | 0.43 |
| 1:A:23:GLN:NE2 | 1:A:60:VAL:HB | 2.32 | 0.42 |
| 1:A:356:ARG:HG2 | 1:A:356:ARG:HH11 | 1.84 | 0.42 |
| 2:B:58:THR:HG23 | 2:B:76:ASP:O | 2.19 | 0.42 |
| 2:B:60:VAL:HG11 | 2:B:130:PHE:CD1 | 2.54 | 0.42 |
| 2:B:332:GLN:HG3 | 2:B:338:THR:HG23 | 2.01 | 0.42 |
| 1:A:136:ASN:O | 1:A:137:ASN:HB3 | 2.19 | 0.42 |
| 1:A:393:ILE:HB | 1:A:423:VAL:CG2 | 2.44 | 0.42 |
| 1:A:486:LEU:HB3 | 1:A:524:GLN:HG3 | 2.01 | 0.42 |
| 1:A:536:VAL:CG1 | 2:B:258:GLN:HG2 | 2.50 | 0.42 |
| 2:B:421:PRO:O | 2:B:425:LEU:HD22 | 2.19 | 0.42 |
| 1:A:131:THR:HG22 | 1:A:132:ILE:N | 2.33 | 0.42 |
| 1:A:314:VAL:O | 1:A:314:VAL:HG13 | 2.18 | 0.42 |
| 2:B:178:ILE:HG22 | 2:B:180:ILE:HD12 | 2.00 | 0.42 |
| 1:A:337:TRP:O | 1:A:353:LYS:HA | 2.19 | 0.42 |
| 1:A:356:ARG:NH2 | 1:A:371:ALA:HA | 2.34 | 0.42 |
| 1:A:442:VAL:HG11 | 1:A:485:ALA:HB2 | 2.01 | 0.42 |
| 1:A:198:HIS:NE2 | 1:A:202:ILE:HD11 | 2.35 | 0.42 |
| 1:A:270:ILE:HG23 | 1:A:271:TYR:CD2 | 2.55 | 0.42 |
| 1:A:307:ARG:HH11 | 1:A:307:ARG:HG2 | 1.84 | 0.42 |
| 1:A:31:ILE:CD1 | 1:A:135:ILE:HA | 2.49 | 0.42 |
| 1:A:115:TYR:OH | 1:A:157:PRO:HA | 2.19 | 0.42 |
| 2:B:132:ILE:HA | 2:B:133:PRO:HD2 | 1.80 | 0.42 |
| 2:B:158:ALA:O | 2:B:161:GLN:N | 2.52 | 0.42 |
| 1:A:41:MET:SD | 1:A:73:LYS:HE2 | 2.59 | 0.42 |
| 1:A:142:ILE:HG22 | 1:A:144:TYR:CE1 | 2.55 | 0.42 |
| 2:B:274:ILE:CD1 | 2:B:310:LEU:HD21 | 2.42 | 0.42 |
| 1:A:13:LYS:HB3 | 1:A:14:PRO:HD2 | 2.02 | 0.42 |
| 1:A:119:PRO:HA | 1:A:148:VAL:HG23 | 2.01 | 0.42 |
| 1:A:517:LEU:O | 1:A:520:GLN:HB2 | 2.20 | 0.42 |
| 2:B:75:VAL:HG11 | 2:B:77:PHE:CZ | 2.55 | 0.42 |
| 2:B:168:LEU:O | 2:B:169:GLU:C | 2.58 | 0.42 |
| 2:B:63:ILE:HD12 | 2:B:74:LEU:HD22 | 2.01 | 0.42 |
| 2:B:201:LYS:HA | 2:B:201:LYS:HD2 | 1.84 | 0.42 |
| 2:B:293:ILE:HG23 | 2:B:294:PRO:HD2 | 2.00 | 0.42 |
| 2:B:327:ALA:HA | 2:B:340:GLN:O | 2.20 | 0.42 |
| 2:B:395:LYS:O | 2:B:399:GLU:CG | 2.68 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:461:ARG:CG | 1:A:461:ARG:NH1 | 2.78 | 0.42 |
| 2:B:303:LEU:HD23 | 2:B:303:LEU:C | 2.40 | 0.42 |
| 1:A:37:ILE:HD12 | 1:A:37:ILE:N | 2.35 | 0.41 |
| 1:A:297:GLU:O | 1:A:300:GLU:HB2 | 2.19 | 0.41 |
| 2:B:20:LYS:HE2 | 2:B:56:TYR:HE1 | 1.84 | 0.41 |
| 2:B:264:LEU:O | 2:B:265:ASN:C | 2.58 | 0.41 |
| 2:B:287:LYS:HE2 | 2:B:293:ILE:HD11 | 2.00 | 0.41 |
| 1:A:5:ILE:HG12 | 1:A:6:GLU:N | 2.35 | 0.41 |
| 1:A:26:LEU:HB2 | 1:A:31:ILE:CG1 | 2.50 | 0.41 |
| 2:B:50:ILE:CG2 | 2:B:145:GLN:HB3 | 2.51 | 0.41 |
| 1:A:166:LYS:C | 1:A:168:LEU:N | 2.74 | 0.41 |
| 1:A:227:PHE:O | 1:A:234:LEU:HD12 | 2.21 | 0.41 |
| 1:A:244:ILE:CG2 | 1:A:310:LEU:HD22 | 2.50 | 0.41 |
| 1:A:377:THR:O | 1:A:378:GLU:C | 2.56 | 0.41 |
| 2:B:23:GLN:OE1 | 2:B:59:PRO:HA | 2.19 | 0.41 |
| 1:A:68:SER:C | 1:A:70:LYS:H | 2.24 | 0.41 |
| 1:A:244:ILE:HD12 | 1:A:245:VAL:H | 1.85 | 0.41 |
| 1:A:3:SER:OG | 1:A:5:ILE:HG22 | 2.19 | 0.41 |
| 1:A:58:THR:CG2 | 1:A:59:PRO:HD2 | 2.51 | 0.41 |
| 1:A:253:THR:HA | 1:A:291:GLU:O | 2.20 | 0.41 |
| 1:A:283:LEU:O | 1:A:284:ARG:C | 2.58 | 0.41 |
| 1:A:94:ILE:HD13 | 1:A:95:PRO:CD | 2.50 | 0.41 |
| 1:A:122:GLU:CD | 1:A:122:GLU:N | 2.72 | 0.41 |
| 1:A:227:PHE:HB2 | 1:A:234:LEU:HD12 | 1.95 | 0.41 |
| 2:B:325:LEU:HD12 | 2:B:325:LEU:HA | 1.85 | 0.41 |
| 2:B:325:LEU:HD12 | 2:B:343:GLN:HG3 | 2.03 | 0.41 |
| 1:A:46:LYS:O | 1:A:147:ASN:HB3 | 2.21 | 0.41 |
| 1:A:98:ALA:HB2 | 1:A:349:LEU:O | 2.21 | 0.41 |
| 2:B:37:ILE:O | 2:B:37:ILE:CG2 | 2.68 | 0.41 |
| 1:A:40:GLU:O | 1:A:43:LYS:HG2 | 2.21 | 0.41 |
| 1:A:65:LYS:HB3 | 1:A:72:ARG:NE | 2.36 | 0.41 |
| 1:A:435:VAL:HA | 2:B:290:THR:HG21 | 2.02 | 0.41 |
| 2:B:32:LYS:O | 2:B:33:ALA:C | 2.59 | 0.41 |
| 2:B:237:ASP:O | 2:B:239:TRP:N | 2.54 | 0.41 |
| 2:B:241:VAL:HG22 | 2:B:350:LYS:HA | 2.02 | 0.41 |
| 2:B:319:TYR:O | 2:B:321:PRO:HD3 | 2.21 | 0.41 |
| 2:B:368:LEU:HD23 | 2:B:368:LEU:HA | 1.92 | 0.41 |
| 1:A:368:LEU:HD21 | 1:A:391:LEU:HD22 | 2.03 | 0.41 |
| 1:A:169:GLU:N | 1:A:170:PRO:CD | 2.84 | 0.40 |
| 1:A:492:GLU:HA | 1:A:530:LYS:O | 2.20 | 0.40 |
| 1:A:532:TYR:HE2 | 1:A:534:ALA:HB2 | 1.85 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:244:ILE:HG21 | 2:B:426:TRP:CE2 | 2.56 | 0.40 |
| 1:A:94:ILE:HD13 | 1:A:95:PRO:HD2 | 2.03 | 0.40 |
| 1:A:153:TRP:CZ3 | 1:A:155:GLY:HA3 | 2.56 | 0.40 |
| 1:A:207:GLN:HA | 1:A:207:GLN:HE21 | 1.86 | 0.40 |
| 1:A:502:ALA:O | 1:A:504:GLY:N | 2.54 | 0.40 |
| 2:B:376:THR:HG23 | 2:B:387:PRO:HD2 | 2.03 | 0.40 |
| 1:A:27:THR:HG22 | 1:A:28:GLU:N | 2.36 | 0.40 |
| 1:A:357:MET:O | 1:A:359:GLY:N | 2.55 | 0.40 |
| 2:B:50:ILE:HG21 | 2:B:145:GLN:HB3 | 2.03 | 0.40 |
| 2:B:72:ARG:HH21 | 2:B:409:THR:CG2 | 2.07 | 0.40 |
| 2:B:166:LYS:O | 2:B:167:ILE:C | 2.59 | 0.40 |
| 2:B:205:LEU:O | 2:B:208:HIS:HB3 | 2.21 | 0.40 |
| 2:B:369:THR:HG22 | 2:B:398:TRP:CZ3 | 2.55 | 0.40 |
| 1:A:45:GLY:O | 1:A:147:ASN:ND2 | 2.46 | 0.40 |
| 1:A:195:ILE:HG12 | 1:A:196:GLY:N | 2.36 | 0.40 |
| 1:A:317:VAL:CG2 | 1:A:318:TYR:N | 2.84 | 0.40 |
| 1:A:540:LYS:HB3 | 1:A:542:ILE:CD1 | 2.47 | 0.40 |
| 2:B:187:LEU:HD12 | 2:B:187:LEU:HA | 1.97 | 0.40 |
| 1:A:232:TYR:N | 1:A:232:TYR:CD1 | 2.89 | 0.40 |
| 1:A:327:ALA:HB3 | 1:A:389:PHE:CD2 | 2.57 | 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 | 540/543 (99%) | 453 (84%) | 69 (13%) | 18 (3%) | 4 15 |
| 2 | B | 397/440 (90%) | 338 (85%) | 41 (10%) | 18 (4%) | 2 9 |
| All | All | 937/983 (95%) | 791 (84%) | 110 (12%) | 36 (4%) | 3 13 |

All (36) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 68 | SER |
| 2 | B | 172 | ARG |
| 1 | A | 112 | GLY |
| 1 | A | 230 | MET |
| 1 | A | 491 | LEU |
| 2 | B | 44 | GLU |
| 2 | B | 103 | ASN |
| 2 | B | 141 | GLY |
| 2 | B | 167 | ILE |
| 2 | B | 174 | GLN |
| 1 | A | 18 | GLY |
| 1 | A | 139 | THR |
| 1 | A | 312 | GLU |
| 1 | A | 358 | ARG |
| 2 | B | 122 | GLU |
| 2 | B | 166 | LYS |
| 2 | B | 176 | PRO |
| 1 | A | 250 | ASP |
| 1 | A | 427 | TYR |
| 2 | B | 361 | HIS |
| 1 | A | 138 | GLU |
| 1 | A | 357 | MET |
| 1 | A | 418 | ASN |
| 2 | B | 162 | SER |
| 1 | A | 242 | GLN |
| 2 | B | 175 | ASN |
| 2 | B | 356 | ARG |
| 1 | A | 509 | GLN |
| 2 | B | 195 | ILE |
| 2 | B | 421 | PRO |
| 1 | A | 135 | ILE |
| 1 | A | 243 | PRO |
| 1 | A | 345 | PRO |
| 1 | A | 14 | PRO |
| 2 | B | 169 | GLU |
| 2 | B | 170 | PRO |

### 5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 485/485 (100%) | 443 (91%) | 42 (9%) | 10 30 |
| 2 | B | 366/400 (92%) | 337 (92%) | 29 (8%) | 12 34 |
| All | All | 851/885 (96%) | 780 (92%) | 71 (8%) | 11 32 |

All (71) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 29 | GLU |
| 1 | A | 42 | GLU |
| 1 | A | 88 | TRP |
| 1 | A | 91 | GLN |
| 1 | A | 94 | ILE |
| 1 | A | 107 | THR |
| 1 | A | 108 | VAL |
| 1 | A | 136 | ASN |
| 1 | A | 137 | ASN |
| 1 | A | 148 | VAL |
| 1 | A | 175 | ASN |
| 1 | A | 194 | GLU |
| 1 | A | 195 | ILE |
| 1 | A | 197 | GLN |
| 1 | A | 207 | GLN |
| 1 | A | 216 | THR |
| 1 | A | 234 | LEU |
| 1 | A | 250 | ASP |
| 1 | A | 279 | LEU |
| 1 | A | 283 | LEU |
| 1 | A | 295 | LEU |
| 1 | A | 296 | THR |
| 1 | A | 297 | GLU |
| 1 | A | 311 | LYS |
| 1 | A | 340 | GLN |
| 1 | A | 361 | HIS |
| 1 | A | 363 | ASN |
| 1 | A | 368 | LEU |
| 1 | A | 410 | TRP |
| 1 | A | 415 | GLU |
| 1 | A | 424 | LYS |
| 1 | A | 431 | LYS |
| 1 | A | 448 | ARG |
| 1 | A | 452 | LEU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 465 | LYS |
| 1 | A | 473 | THR |
| 1 | A | 475 | GLN |
| 1 | A | 480 | GLN |
| 1 | A | 493 | VAL |
| 1 | A | 496 | VAL |
| 1 | A | 514 | GLU |
| 1 | A | 540 | LYS |
| 2 | B | 6 | GLU |
| 2 | B | 8 | VAL |
| 2 | B | 24 | TRP |
| 2 | B | 61 | PHE |
| 2 | B | 63 | ILE |
| 2 | B | 65 | LYS |
| 2 | B | 67 | ASP |
| 2 | B | 69 | THR |
| 2 | B | 71 | TRP |
| 2 | B | 85 | GLN |
| 2 | B | 87 | PHE |
| 2 | B | 92 | LEU |
| 2 | B | 94 | ILE |
| 2 | B | 100 | LEU |
| 2 | B | 109 | LEU |
| 2 | B | 123 | ASP |
| 2 | B | 161 | GLN |
| 2 | B | 164 | MET |
| 2 | B | 174 | GLN |
| 2 | B | 194 | GLU |
| 2 | B | 210 | LEU |
| 2 | B | 287 | LYS |
| 2 | B | 358 | ARG |
| 2 | B | 361 | HIS |
| 2 | B | 363 | ASN |
| 2 | B | 368 | LEU |
| 2 | B | 399 | GLU |
| 2 | B | 424 | LYS |
| 2 | B | 425 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 137 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 161 | GLN |
| 1 | A | 332 | GLN |
| 1 | A | 475 | GLN |
| 1 | A | 480 | GLN |
| 1 | A | 519 | ASN |
| 2 | B | 57 | ASN |
| 2 | B | 85 | GLN |
| 2 | B | 151 | GLN |
| 2 | B | 174 | GLN |
| 2 | B | 175 | ASN |
| 2 | B | 207 | GLN |
| 2 | B | 242 | GLN |
| 2 | B | 361 | 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)

1 non-standard protein/DNA/RNA residue is 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 | $\#\|Z\| > 2$ |
| 1 | CSD | A | 280 | 1 | 3,7,8 | 1.08 | 0 | 1,8,10 | 7.80 | 1 (100%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | CSD | A | 280 | 1 | - | 2/2/6/8 | - |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 280 | CSD | OD1-SG-CB | 7.80 | 120.38 | 105.54 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 1 | A | 280 | CSD | N-CA-CB-SG |
| 1 | A | 280 | CSD | CA-CB-SG-OD1 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

1 ligand is 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 | $\#\|Z\| > 2$ |
| 3 | EFZ | A | 999 | - | 23,23,23 | 2.60 | 6 (26%) | 36,36,36 | 1.38 | 2 (5%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 3 | EFZ | A | 999 | - | - | 0/10/32/32 | 0/3/3/3 |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 3 | A | 999 | EFZ | C10-C9 | 7.43 | 1.71 | 1.46 |
| 3 | A | 999 | EFZ | C12-C11 | -5.30 | 1.28 | 1.48 |
| 3 | A | 999 | EFZ | C7-C6 | 4.64 | 1.57 | 1.51 |
| 3 | A | 999 | EFZ | C12-C10 | -3.68 | 1.24 | 1.48 |
| 3 | A | 999 | EFZ | C11-C10 | -3.68 | 1.24 | 1.48 |
| 3 | A | 999 | EFZ | C1-N | 2.09 | 1.43 | 1.39 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 3 | A | 999 | EFZ | C12-C10-C9 | -4.89 | 105.79 | 119.06 |
| 3 | A | 999 | EFZ | C11-C10-C9 | -4.87 | 105.83 | 119.06 |

There are no chirality outliers.

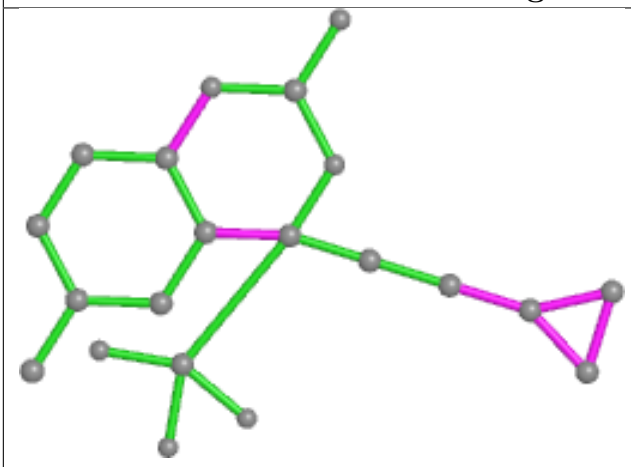
There are no torsion outliers.

There are no ring outliers.

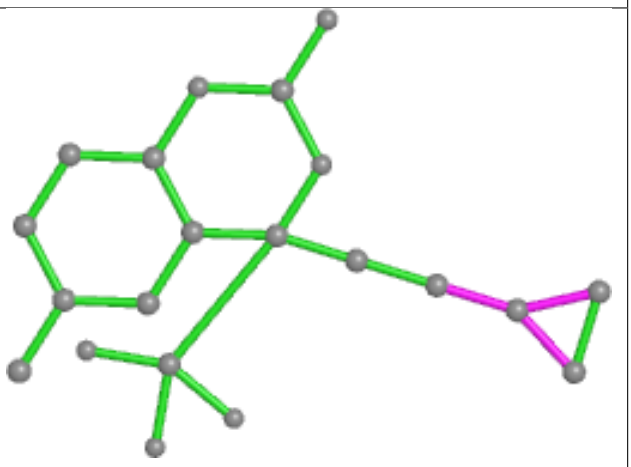
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

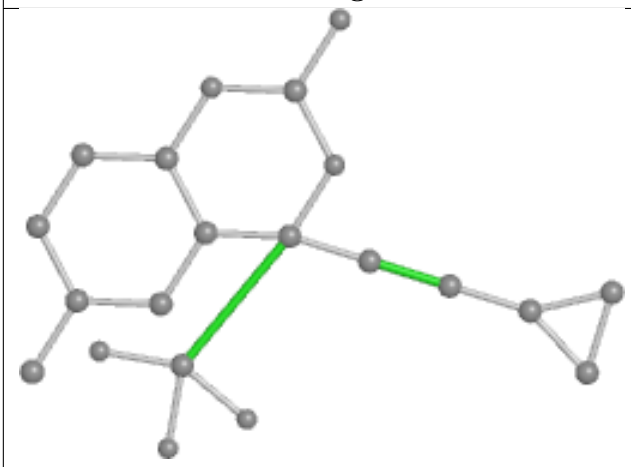
**Ligand EFZ A 999**



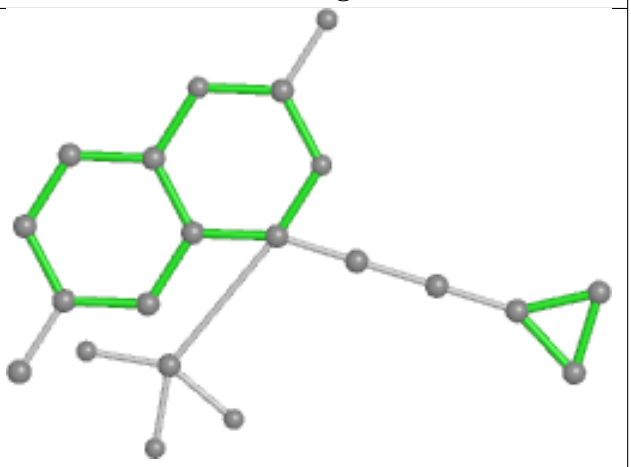
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | A | 542/543 (99%) | -0.11 | 25 (4%) | 32 | 29 | 26, 79, 148, 150 | 0 |
| 2 | B | 403/440 (91%) | -0.21 | 10 (2%) | 57 | 55 | 31, 72, 132, 150 | 0 |
| All | All | 945/983 (96%) | -0.15 | 35 (3%) | 41 | 37 | 26, 76, 145, 150 | 0 |

All (35) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 2 | B | 92 | LEU | 5.8 |
| 2 | B | 3 | SER | 5.6 |
| 1 | A | 43 | LYS | 5.1 |
| 1 | A | 135 | ILE | 4.3 |
| 1 | A | 69 | THR | 4.0 |
| 1 | A | 134 | SER | 3.9 |
| 1 | A | 71 | TRP | 3.9 |
| 1 | A | 50 | ILE | 3.9 |
| 2 | B | 5 | ILE | 3.9 |
| 1 | A | 90 | VAL | 3.7 |
| 1 | A | 62 | ALA | 3.6 |
| 1 | A | 63 | ILE | 3.5 |
| 2 | B | 426 | TRP | 3.4 |
| 1 | A | 136 | ASN | 3.4 |
| 1 | A | 67 | ASP | 3.3 |
| 1 | A | 28 | GLU | 3.2 |
| 2 | B | 4 | PRO | 3.2 |
| 1 | A | 141 | GLY | 3.0 |
| 1 | A | 91 | GLN | 2.8 |
| 1 | A | 51 | GLY | 2.8 |
| 2 | B | 198 | HIS | 2.7 |
| 1 | A | 32 | LYS | 2.6 |
| 1 | A | 245 | VAL | 2.4 |
| 2 | B | 197 | GLN | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 448 | ARG | 2.4 |
| 1 | A | 142 | ILE | 2.4 |
| 1 | A | 139 | THR | 2.4 |
| 1 | A | 24 | TRP | 2.3 |
| 1 | A | 26 | LEU | 2.3 |
| 1 | A | 70 | LYS | 2.3 |
| 1 | A | 27 | THR | 2.1 |
| 1 | A | 72 | ARG | 2.1 |
| 2 | B | 237 | ASP | 2.0 |
| 2 | B | 358 | ARG | 2.0 |
| 2 | B | 67 | ASP | 2.0 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 1 | CSD | A | 280 | 8/9 | 0.93 | 0.15 | 73,76,84,90 | 0 |

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

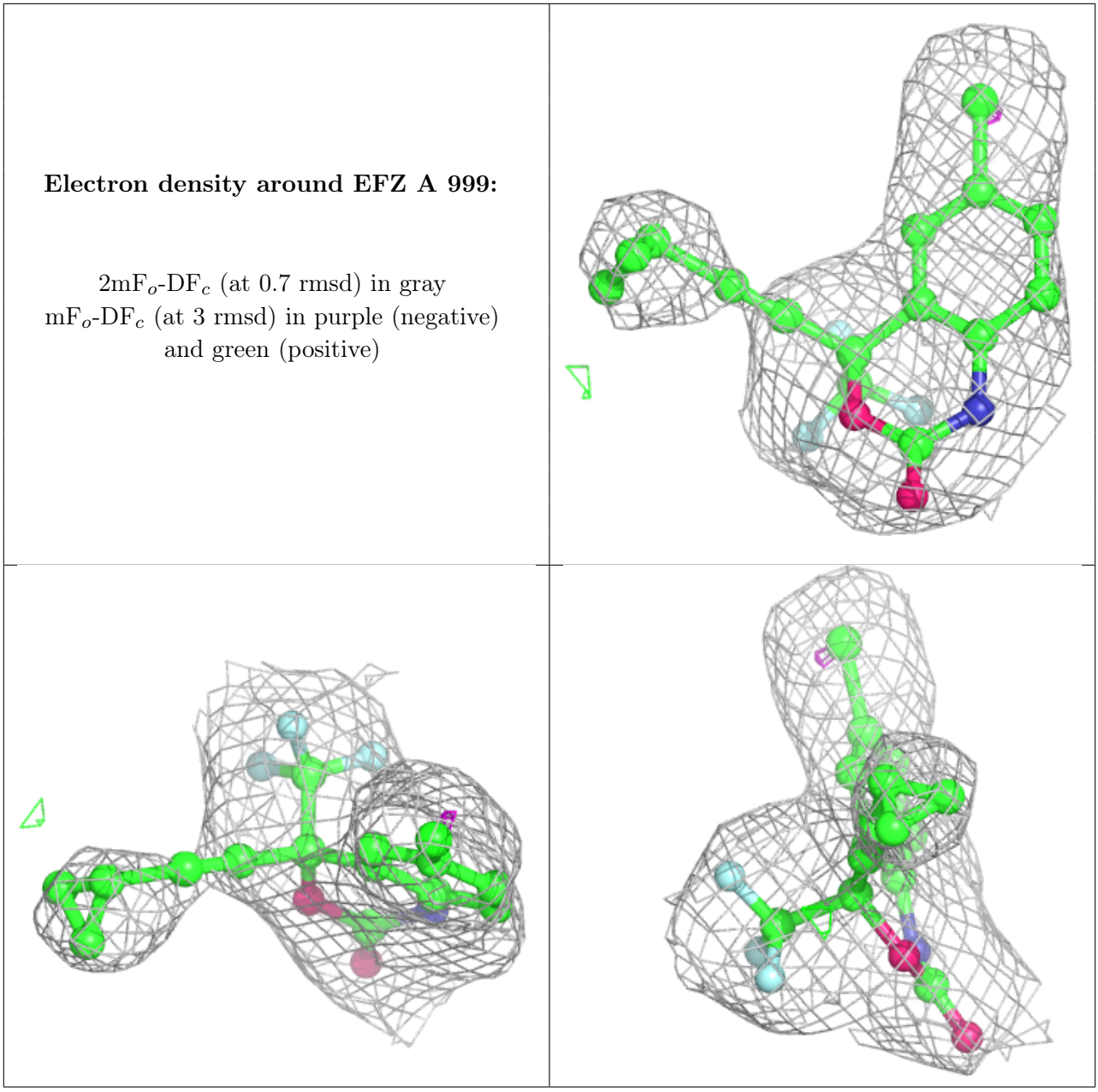
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, $95^{th}$ percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | EFZ | A | 999 | 21/21 | 0.95 | 0.18 | 50,71,80,83 | 0 |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around EFZ A 999:**

$2mF_o$-$DF_c$ (at 0.7 rmsd) in gray
$mF_o$-$DF_c$ (at 3 rmsd) in purple (negative) and green (positive)



## 6.5 Other polymers

There are no such residues in this entry.