



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:42 am BST

PDB ID : 2PNR
Title : Crystal Structure of the asymmetric Pdk3-l2 Complex
Authors : Vassilyev, D.G.; Steussy, C.N.; Devedjiev, Y.
Deposited on : 2007-04-25
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

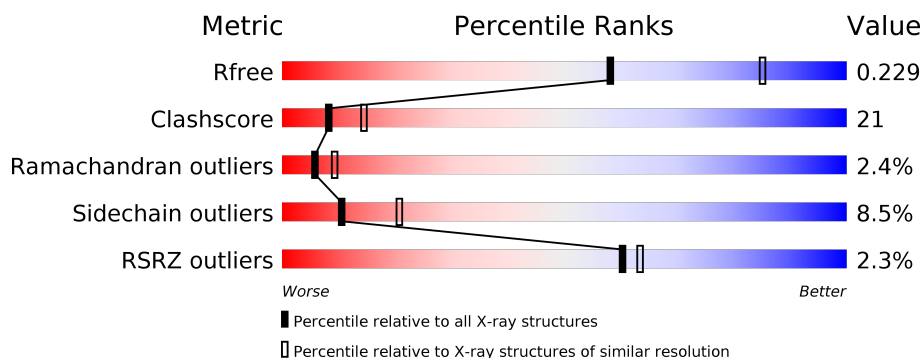
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 4661 (2.50-2.50) |
| Clashscore | 141614 | 5346 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 419 | <div> <div>3%</div> <div> <div></div> <div>52%</div> <div>32%</div> <div>5%</div> <div>11%</div> </div> </div> |
| 1 | B | 419 | <div> <div>2%</div> <div> <div></div> <div>46%</div> <div>30%</div> <div>5%</div> <div>19%</div> </div> </div> |
| 1 | E | 419 | <div> <div>2%</div> <div> <div></div> <div>53%</div> <div>33%</div> <div>•</div> <div>11%</div> </div> </div> |
| 1 | F | 419 | <div> <div>•</div> <div> <div></div> <div>47%</div> <div>30%</div> <div>•</div> <div>19%</div> </div> </div> |
| 2 | C | 128 | <div> <div>2%</div> <div> <div></div> <div>30%</div> <div>26%</div> <div>5%</div> <div>38%</div> </div> </div> |
| 2 | G | 128 | <div> <div> <div></div> <div>35%</div> <div>22%</div> <div>5%</div> <div>38%</div> </div> </div> |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13603 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 [Pyruvate dehydrogenase [lipoamide]] kinase isozyme 3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 374 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3038 | 1956 | 508 | 562 | 12 | | | |
| 1 | B | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2789 | 1796 | 467 | 513 | 13 | | | |
| 1 | E | 374 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3038 | 1956 | 508 | 562 | 12 | | | |
| 1 | F | 341 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2789 | 1796 | 467 | 513 | 13 | | | |

There are 84 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| A | -12 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| A | -11 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| A | -10 | SER | - | CLONING ARTIFACT | UNP Q15120 |
| A | -9 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -8 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -7 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -6 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -5 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -4 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| A | -3 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| A | -2 | MET | - | CLONING ARTIFACT | UNP Q15120 |
| A | -1 | ALA | - | CLONING ARTIFACT | UNP Q15120 |
| A | 0 | ARG | - | CLONING ARTIFACT | UNP Q15120 |
| A | 1 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| A | 2 | GLU | - | CLONING ARTIFACT | UNP Q15120 |
| A | 3 | ASN | - | CLONING ARTIFACT | UNP Q15120 |
| A | 4 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| A | 5 | TYR | - | CLONING ARTIFACT | UNP Q15120 |
| A | 6 | PHE | - | CLONING ARTIFACT | UNP Q15120 |
| A | 7 | GLN | - | CLONING ARTIFACT | UNP Q15120 |
| A | 8 | GLY | - | CLONING ARTIFACT | UNP Q15120 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| B | -12 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| B | -11 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| B | -10 | SER | - | CLONING ARTIFACT | UNP Q15120 |
| B | -9 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -8 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -7 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -6 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -5 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -4 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| B | -3 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| B | -2 | MET | - | CLONING ARTIFACT | UNP Q15120 |
| B | -1 | ALA | - | CLONING ARTIFACT | UNP Q15120 |
| B | 0 | ARG | - | CLONING ARTIFACT | UNP Q15120 |
| B | 1 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| B | 2 | GLU | - | CLONING ARTIFACT | UNP Q15120 |
| B | 3 | ASN | - | CLONING ARTIFACT | UNP Q15120 |
| B | 4 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| B | 5 | TYR | - | CLONING ARTIFACT | UNP Q15120 |
| B | 6 | PHE | - | CLONING ARTIFACT | UNP Q15120 |
| B | 7 | GLN | - | CLONING ARTIFACT | UNP Q15120 |
| B | 8 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| E | -12 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| E | -11 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| E | -10 | SER | - | CLONING ARTIFACT | UNP Q15120 |
| E | -9 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -8 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -7 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -6 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -5 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -4 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| E | -3 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| E | -2 | MET | - | CLONING ARTIFACT | UNP Q15120 |
| E | -1 | ALA | - | CLONING ARTIFACT | UNP Q15120 |
| E | 0 | ARG | - | CLONING ARTIFACT | UNP Q15120 |
| E | 1 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| E | 2 | GLU | - | CLONING ARTIFACT | UNP Q15120 |
| E | 3 | ASN | - | CLONING ARTIFACT | UNP Q15120 |
| E | 4 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| E | 5 | TYR | - | CLONING ARTIFACT | UNP Q15120 |
| E | 6 | PHE | - | CLONING ARTIFACT | UNP Q15120 |
| E | 7 | GLN | - | CLONING ARTIFACT | UNP Q15120 |
| E | 8 | GLY | - | CLONING ARTIFACT | UNP Q15120 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| F | -12 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| F | -11 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| F | -10 | SER | - | CLONING ARTIFACT | UNP Q15120 |
| F | -9 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -8 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -7 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -6 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -5 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -4 | HIS | - | CLONING ARTIFACT | UNP Q15120 |
| F | -3 | GLY | - | CLONING ARTIFACT | UNP Q15120 |
| F | -2 | MET | - | CLONING ARTIFACT | UNP Q15120 |
| F | -1 | ALA | - | CLONING ARTIFACT | UNP Q15120 |
| F | 0 | ARG | - | CLONING ARTIFACT | UNP Q15120 |
| F | 1 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| F | 2 | GLU | - | CLONING ARTIFACT | UNP Q15120 |
| F | 3 | ASN | - | CLONING ARTIFACT | UNP Q15120 |
| F | 4 | LEU | - | CLONING ARTIFACT | UNP Q15120 |
| F | 5 | TYR | - | CLONING ARTIFACT | UNP Q15120 |
| F | 6 | PHE | - | CLONING ARTIFACT | UNP Q15120 |
| F | 7 | GLN | - | CLONING ARTIFACT | UNP Q15120 |
| F | 8 | GLY | - | CLONING ARTIFACT | UNP Q15120 |

- Molecule 2 is a protein called Dihydrolipoyllysine-residue acetyltransferase component of pyruvate dehydrogenase complex.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|-----|---|---------|---------|-------|
| 2 | C | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 602 | 384 | 94 | 121 | 3 | | | |
| 2 | G | 79 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 602 | 384 | 94 | 121 | 3 | | | |

There are 40 discrepancies between the modelled and reference sequences:

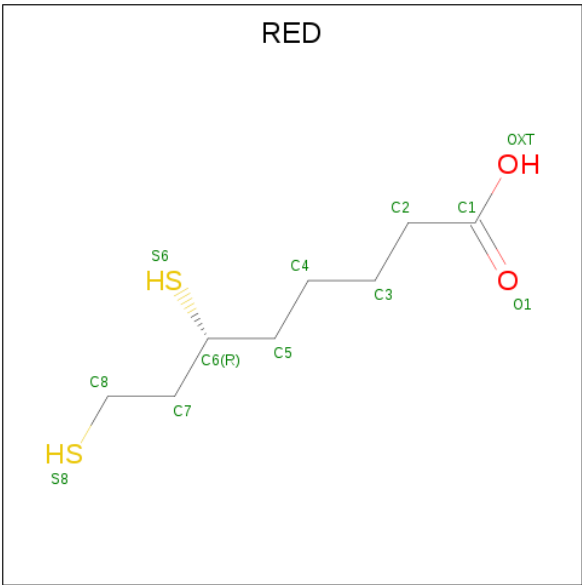
| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| C | 106 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| C | 107 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| C | 108 | SER | - | CLONING ARTIFACT | UNP P10515 |
| C | 109 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| C | 110 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| C | 111 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| C | 112 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| C | 113 | HIS | - | CLONING ARTIFACT | UNP P10515 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|------------|
| C | 114 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| C | 115 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| C | 116 | MET | - | CLONING ARTIFACT | UNP P10515 |
| C | 117 | ALA | - | CLONING ARTIFACT | UNP P10515 |
| C | 118 | ARG | - | CLONING ARTIFACT | UNP P10515 |
| C | 119 | LEU | - | CLONING ARTIFACT | UNP P10515 |
| C | 120 | GLU | - | CLONING ARTIFACT | UNP P10515 |
| C | 121 | ASN | - | CLONING ARTIFACT | UNP P10515 |
| C | 122 | LEU | - | CLONING ARTIFACT | UNP P10515 |
| C | 123 | TYR | - | CLONING ARTIFACT | UNP P10515 |
| C | 124 | PHE | - | CLONING ARTIFACT | UNP P10515 |
| C | 125 | GLN | - | CLONING ARTIFACT | UNP P10515 |
| G | 106 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| G | 107 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| G | 108 | SER | - | CLONING ARTIFACT | UNP P10515 |
| G | 109 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 110 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 111 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 112 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 113 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 114 | HIS | - | CLONING ARTIFACT | UNP P10515 |
| G | 115 | GLY | - | CLONING ARTIFACT | UNP P10515 |
| G | 116 | MET | - | CLONING ARTIFACT | UNP P10515 |
| G | 117 | ALA | - | CLONING ARTIFACT | UNP P10515 |
| G | 118 | ARG | - | CLONING ARTIFACT | UNP P10515 |
| G | 119 | LEU | - | CLONING ARTIFACT | UNP P10515 |
| G | 120 | GLU | - | CLONING ARTIFACT | UNP P10515 |
| G | 121 | ASN | - | CLONING ARTIFACT | UNP P10515 |
| G | 122 | LEU | - | CLONING ARTIFACT | UNP P10515 |
| G | 123 | TYR | - | CLONING ARTIFACT | UNP P10515 |
| G | 124 | PHE | - | CLONING ARTIFACT | UNP P10515 |
| G | 125 | GLN | - | CLONING ARTIFACT | UNP P10515 |

- Molecule 3 is DIHYDROLIPOIC ACID (three-letter code: RED) (formula: $C_8H_{16}O_2S_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3 | C | 1 | Total | C | O | S | 0 | 0 |
| | | | 11 | 8 | 1 | 2 | | |
| 3 | G | 1 | Total | C | O | S | 0 | 0 |
| | | | 11 | 8 | 1 | 2 | | |

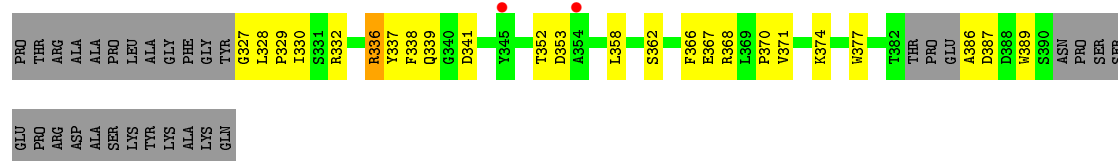
- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | A | 172 | Total | O | 0 | 0 |
| | | | 172 | 172 | | |
| 4 | B | 165 | Total | O | 0 | 0 |
| | | | 165 | 165 | | |
| 4 | C | 26 | Total | O | 0 | 0 |
| | | | 26 | 26 | | |
| 4 | E | 172 | Total | O | 0 | 0 |
| | | | 172 | 172 | | |
| 4 | F | 155 | Total | O | 0 | 0 |
| | | | 155 | 155 | | |
| 4 | G | 33 | Total | O | 0 | 0 |
| | | | 33 | 33 | | |

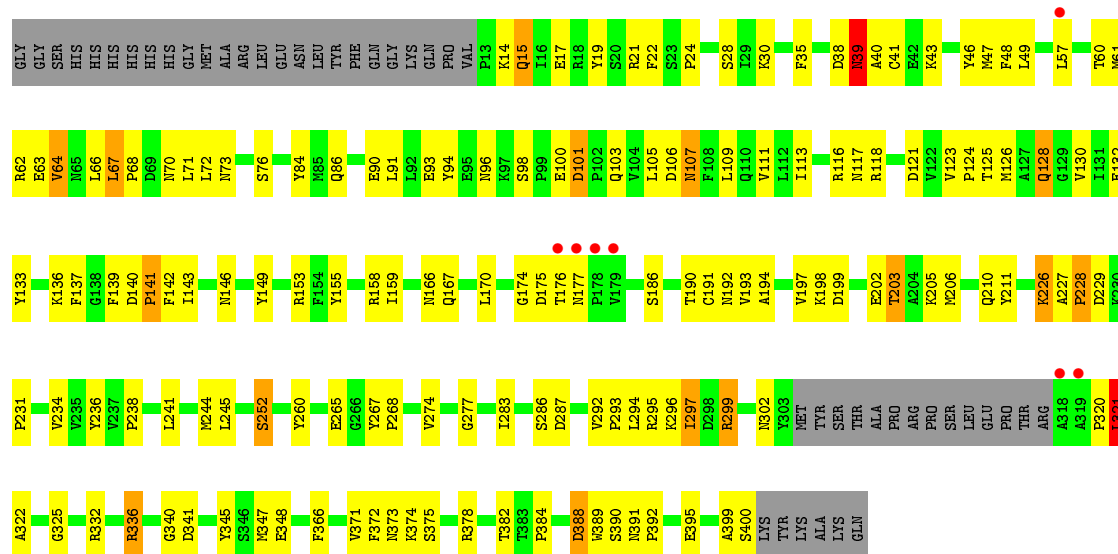
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- Chain A:
-
- 52% 32% 5% 11%
- 3%
- GLY GLY HIS HIS HIS HIS HIS MET ALA ARG LEU LEU ASN LEU TYR PHE GLN P13 P14 Q15 I16 S23 P24 S28 R39 A40 C41 Y46 R50 R51 E52 L53 P54 V55 R56 L57 M61 R62 S63 N64 R65 L66 L67 N70 L74 L72 N73 R74 P75 S76 Y84 R85 Q86 S87 F88 L89 E90 L91 L92 L93 E93 S98 P99 E100 D101 P102 P103 V104 L105 D106 N107 V111 L112 I113 N117 R118 D121 V122 V123 P124 T125 M126 A127 Q128 V130 Y133 F139 D140 P141 F142 I143 S144 T145 N146 Y149 R159 F154 Y155 R158 I159 R162 M163 Q167 T176 N177 P178 V179 H180 P181 K182 H183 S186 I187 D188 C191 N192 V193 A194 V197 K198 D199 A200 T203 M206 L300 E209 Q210 Y211 V214 E217 L218 E219 V220 E221 E222 K226 A227 P228 D229 Q233 V234 V235 Y236 V237 P238 L241 F242 E243 M244 L245 L248 F249 K250 R254 V257 R263 K264 E265 G266 Y267 K271 T272 K278 L281 K284 P293 L297 D298 R299 L300 F301 N302 Y303 MET TYR SER THR ALA PRO ARG PRO LEU GLU PRO THR ARG A318 A319 P320 L321 A322 G323 F324 G325 R336 D341 M347 E348 Y357 L358 L361 F366 V371 F372 N373 K374 S375 T382 T383 P384 D388 W389 S394 E395 F396 R397 A398 A399 S400 LYS TYR LYS ALA GLN

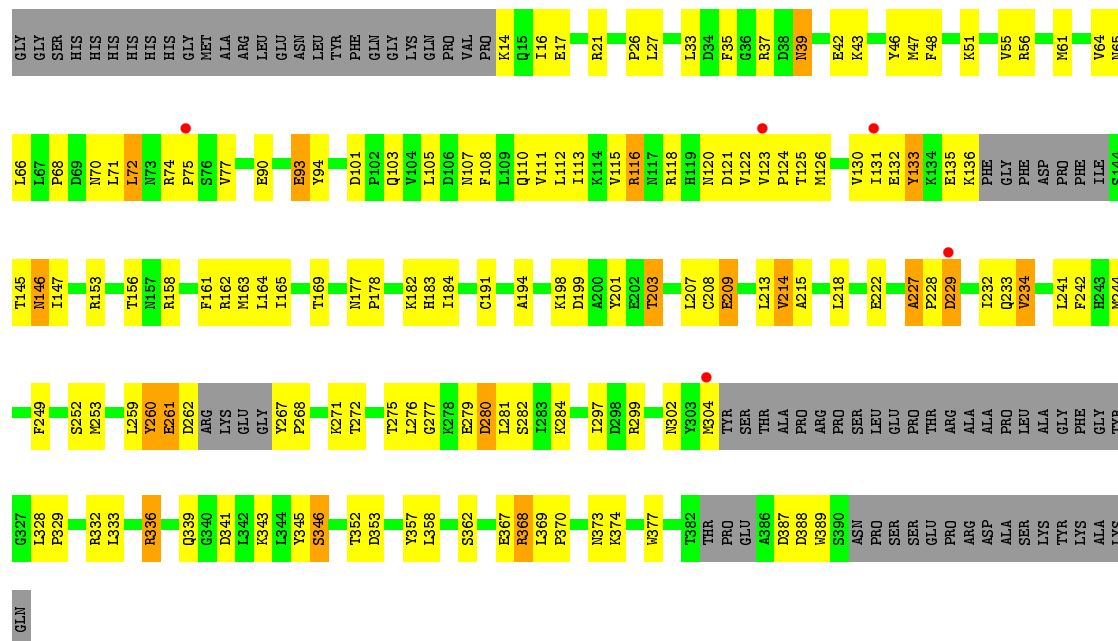
- [illegible]




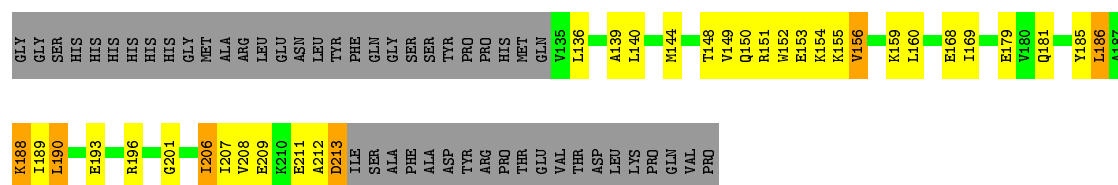
• Molecule 1: [Pyruvate dehydrogenase [lipamide]] kinase isozyme 3



• Molecule 1: [Pyruvate dehydrogenase [lipamide]] kinase isozyme 3



- Chain C: 



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 41 | Depositor |
| Cell constants a, b, c, α , β , γ | 96.16 Å 96.16 Å 222.98 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 2.50 29.43 – 2.50 | Depositor EDS |
| % Data completeness (in resolution range) | 92.9 (30.00-2.50) 93.0 (29.43-2.50) | Depositor EDS |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | 0.10 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.38 (at 2.51 Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.176 , 0.229 0.176 , 0.229 | Depositor DCC |
| R_{free} test set | 3746 reflections (5.79%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 42.8 | Xtriage |
| Anisotropy | 0.032 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 83.4 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$ | Xtriage |
| Estimated twinning fraction | 0.190 for h,-k,-l | Xtriage |
| F_o, F_c correlation | 0.95 | EDS |
| Total number of atoms | 13603 | wwPDB-VP |
| Average B, all atoms (Å ²) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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 | 0.69 | 0/3116 | 0.77 | 1/4222 (0.0%) |
| 1 | B | 0.68 | 0/2853 | 0.75 | 0/3858 |
| 1 | E | 0.69 | 0/3116 | 0.78 | 1/4222 (0.0%) |
| 1 | F | 0.68 | 0/2853 | 0.76 | 0/3858 |
| 2 | C | 0.57 | 0/610 | 0.77 | 0/827 |
| 2 | G | 0.59 | 0/610 | 0.78 | 0/827 |
| All | All | 0.68 | 0/13158 | 0.77 | 2/17814 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1 | A | 321 | LEU | N-CA-C | 7.43 | 131.07 | 111.00 |
| 1 | E | 321 | LEU | N-CA-C | 7.10 | 130.18 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 | 3038 | 0 | 3003 | 113 | 0 |
| 1 | B | 2789 | 0 | 2774 | 139 | 0 |
| 1 | E | 3038 | 0 | 3003 | 129 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | F | 2789 | 0 | 2774 | 125 | 0 |
| 2 | C | 602 | 0 | 618 | 35 | 0 |
| 2 | G | 602 | 0 | 618 | 33 | 0 |
| 3 | C | 11 | 0 | 15 | 0 | 0 |
| 3 | G | 11 | 0 | 15 | 2 | 0 |
| 4 | A | 172 | 0 | 0 | 31 | 0 |
| 4 | B | 165 | 0 | 0 | 22 | 0 |
| 4 | C | 26 | 0 | 0 | 7 | 0 |
| 4 | E | 172 | 0 | 0 | 25 | 0 |
| 4 | F | 155 | 0 | 0 | 23 | 0 |
| 4 | G | 33 | 0 | 0 | 6 | 0 |
| All | All | 13603 | 0 | 12820 | 541 | 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 21.

All (541) 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:211:TYR:HB3 | 1:A:321:LEU:HD21 | 1.47 | 0.94 |
| 2:C:182:GLU:HG3 | 4:C:924:HOH:O | 1.72 | 0.90 |
| 1:A:278:LYS:HD3 | 4:B:541:HOH:O | 1.72 | 0.89 |
| 1:E:14:LYS:HB2 | 4:E:492:HOH:O | 1.74 | 0.88 |
| 1:B:241:LEU:HA | 1:B:244:MET:HE3 | 1.54 | 0.86 |
| 1:F:343:LYS:HA | 4:F:475:HOH:O | 1.75 | 0.85 |
| 1:A:149:TYR:HA | 4:A:488:HOH:O | 1.76 | 0.83 |
| 1:A:395:GLU:HG2 | 4:A:531:HOH:O | 1.77 | 0.83 |
| 1:F:70:ASN:HB3 | 1:F:136:LYS:HE2 | 1.60 | 0.83 |
| 1:F:131:ILE:HG12 | 4:F:545:HOH:O | 1.80 | 0.81 |
| 1:E:399:ALA:HB1 | 1:F:35:PHE:HB2 | 1.62 | 0.80 |
| 1:F:125:THR:HB | 4:F:506:HOH:O | 1.79 | 0.80 |
| 1:F:68:PRO:HB2 | 4:F:496:HOH:O | 1.81 | 0.80 |
| 1:F:199:ASP:O | 1:F:203:THR:HG23 | 1.81 | 0.80 |
| 1:E:395:GLU:HG2 | 4:E:453:HOH:O | 1.80 | 0.80 |
| 1:B:24:PRO:HD2 | 1:B:371:VAL:HG22 | 1.64 | 0.79 |
| 1:A:167:GLN:HE22 | 1:A:186:SER:H | 1.31 | 0.78 |
| 1:B:70:ASN:HB3 | 1:B:136:LYS:HE2 | 1.65 | 0.78 |
| 1:E:211:TYR:HB3 | 1:E:321:LEU:HD21 | 1.66 | 0.78 |
| 1:A:15:GLN:HE21 | 1:A:15:GLN:HA | 1.49 | 0.78 |
| 1:B:203:THR:HG21 | 1:B:242:PHE:HZ | 1.49 | 0.77 |
| 1:A:70:ASN:HB2 | 1:A:133:TYR:HE2 | 1.47 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:373:ASN:HD21 | 1:F:388:ASP:HA | 1.51 | 0.76 |
| 1:A:14:LYS:HB2 | 4:A:462:HOH:O | 1.85 | 0.75 |
| 1:E:96:ASN:HB2 | 4:E:519:HOH:O | 1.86 | 0.75 |
| 2:G:190:LEU:HD11 | 2:G:206:ILE:HD11 | 1.68 | 0.75 |
| 1:F:120:ASN:HA | 4:F:503:HOH:O | 1.87 | 0.75 |
| 1:F:68:PRO:HB3 | 4:F:550:HOH:O | 1.86 | 0.74 |
| 1:A:254:ARG:HD2 | 4:A:432:HOH:O | 1.86 | 0.74 |
| 1:F:74:ARG:HD3 | 1:F:132:GLU:HB2 | 1.68 | 0.73 |
| 1:A:221:GLU:HG3 | 4:A:481:HOH:O | 1.87 | 0.73 |
| 2:G:208:VAL:HG21 | 2:G:213:ASP:HB2 | 1.68 | 0.73 |
| 1:F:368:ARG:O | 1:F:368:ARG:HG3 | 1.88 | 0.72 |
| 1:A:13:PRO:HB3 | 4:A:456:HOH:O | 1.88 | 0.72 |
| 2:C:190:LEU:HD11 | 2:C:206:ILE:HD11 | 1.71 | 0.72 |
| 1:B:134:LYS:HG3 | 4:B:515:HOH:O | 1.89 | 0.71 |
| 1:E:293:PRO:HA | 1:F:280:ASP:OD2 | 1.91 | 0.71 |
| 2:C:148:THR:HG23 | 2:C:196:ARG:HA | 1.70 | 0.71 |
| 1:E:126:MET:HE2 | 1:E:130:VAL:HG13 | 1.71 | 0.71 |
| 1:E:98:SER:OG | 1:E:100:GLU:HG2 | 1.91 | 0.71 |
| 1:B:330:ILE:HG12 | 4:B:434:HOH:O | 1.90 | 0.70 |
| 1:B:74:ARG:HD3 | 1:B:132:GLU:HB2 | 1.71 | 0.70 |
| 1:E:167:GLN:HE22 | 1:E:186:SER:H | 1.38 | 0.70 |
| 1:F:110:GLN:HG3 | 4:F:554:HOH:O | 1.92 | 0.69 |
| 1:F:336:ARG:HD3 | 1:F:341:ASP:OD1 | 1.92 | 0.69 |
| 1:B:298:ASP:HB2 | 4:B:436:HOH:O | 1.91 | 0.69 |
| 1:A:74:ARG:HB3 | 4:A:425:HOH:O | 1.92 | 0.69 |
| 1:E:62:ARG:O | 1:E:66:LEU:HD13 | 1.93 | 0.69 |
| 1:B:368:ARG:HG3 | 1:B:368:ARG:O | 1.92 | 0.69 |
| 1:A:72:LEU:HD12 | 4:A:577:HOH:O | 1.94 | 0.68 |
| 1:B:199:ASP:O | 1:B:203:THR:HG23 | 1.94 | 0.68 |
| 1:E:192:ASN:HB2 | 4:E:411:HOH:O | 1.94 | 0.68 |
| 2:G:151:ARG:HB3 | 2:G:168:GLU:HG3 | 1.74 | 0.68 |
| 1:A:39:ASN:ND2 | 1:A:41:CYS:HB2 | 2.09 | 0.68 |
| 1:F:68:PRO:HG3 | 4:F:435:HOH:O | 1.94 | 0.68 |
| 2:G:212:ALA:HA | 4:G:914:HOH:O | 1.93 | 0.68 |
| 1:E:211:TYR:HB3 | 1:E:321:LEU:CD2 | 2.22 | 0.68 |
| 1:B:332:ARG:O | 1:B:336:ARG:HG2 | 1.94 | 0.67 |
| 1:E:390:SER:HB2 | 1:F:26:PRO:HG3 | 1.75 | 0.67 |
| 1:F:281:LEU:HD23 | 1:F:358:LEU:HD12 | 1.75 | 0.67 |
| 1:A:397:ARG:NE | 2:C:172:ASP:OD2 | 2.27 | 0.67 |
| 1:B:28:SER:OG | 1:B:31:GLN:HG3 | 1.94 | 0.67 |
| 1:A:57:LEU:O | 1:A:61:MET:HG3 | 1.95 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:156:VAL:HA | 2:C:186:LEU:HB3 | 1.76 | 0.67 |
| 1:A:102:PRO:O | 1:A:106:ASP:HB2 | 1.95 | 0.67 |
| 1:F:101:ASP:OD2 | 1:F:103:GLN:HB3 | 1.95 | 0.67 |
| 4:A:420:HOH:O | 1:B:386:ALA:HB3 | 1.95 | 0.66 |
| 1:B:42:GLU:HG2 | 1:B:105:LEU:HD23 | 1.77 | 0.66 |
| 1:A:167:GLN:NE2 | 1:A:186:SER:H | 1.93 | 0.66 |
| 1:A:336:ARG:HD3 | 1:A:341:ASP:OD1 | 1.96 | 0.66 |
| 1:B:332:ARG:HD3 | 1:B:336:ARG:CZ | 2.26 | 0.66 |
| 1:B:158:ARG:HB2 | 4:B:499:HOH:O | 1.96 | 0.65 |
| 1:E:15:GLN:HA | 1:E:15:GLN:HE21 | 1.62 | 0.65 |
| 1:F:232:ILE:HG23 | 1:F:276:LEU:HD22 | 1.79 | 0.64 |
| 1:A:199:ASP:O | 1:A:203:THR:HG23 | 1.96 | 0.64 |
| 1:A:197:VAL:HA | 1:A:245:LEU:HD13 | 1.79 | 0.64 |
| 1:B:101:ASP:OD2 | 1:B:103:GLN:HB3 | 1.98 | 0.64 |
| 1:E:155:TYR:O | 1:E:159:ILE:HG13 | 1.98 | 0.64 |
| 1:F:21:ARG:HB2 | 1:F:21:ARG:HH11 | 1.62 | 0.64 |
| 2:C:208:VAL:HG21 | 2:C:213:ASP:HB2 | 1.80 | 0.63 |
| 1:E:321:LEU:HD11 | 4:E:484:HOH:O | 1.97 | 0.63 |
| 1:A:28:SER:HB3 | 1:A:366:PHE:CE1 | 2.33 | 0.63 |
| 1:E:226:LYS:HE2 | 1:E:277:GLY:O | 1.98 | 0.63 |
| 1:A:140:ASP:HB2 | 1:A:141:PRO:HD2 | 1.81 | 0.63 |
| 1:A:236:TYR:O | 1:A:238:PRO:HD3 | 1.98 | 0.63 |
| 1:A:62:ARG:O | 1:A:66:LEU:HD13 | 1.99 | 0.62 |
| 1:A:62:ARG:HG2 | 1:A:372:PHE:CE2 | 2.34 | 0.62 |
| 1:B:208:CYS:SG | 1:B:215:ALA:HB2 | 2.40 | 0.62 |
| 1:B:51:LYS:HE3 | 4:B:533:HOH:O | 1.98 | 0.62 |
| 1:E:64:VAL:O | 1:E:67:LEU:HD22 | 1.99 | 0.62 |
| 1:A:99:PRO:HD3 | 4:A:417:HOH:O | 1.99 | 0.62 |
| 1:F:234:VAL:HG23 | 4:F:479:HOH:O | 1.98 | 0.62 |
| 1:F:74:ARG:HA | 1:F:74:ARG:CZ | 2.29 | 0.62 |
| 1:A:382:THR:HB | 4:A:501:HOH:O | 2.00 | 0.62 |
| 1:E:60:THR:O | 1:E:64:VAL:HG12 | 1.99 | 0.62 |
| 1:F:271:LYS:HE2 | 4:F:446:HOH:O | 2.00 | 0.62 |
| 1:E:336:ARG:HD3 | 1:E:341:ASP:OD1 | 2.00 | 0.61 |
| 1:E:336:ARG:HA | 1:E:340:GLY:O | 2.01 | 0.61 |
| 1:E:35:PHE:HD1 | 4:E:469:HOH:O | 1.84 | 0.61 |
| 1:B:61:MET:HA | 1:B:64:VAL:HG12 | 1.82 | 0.61 |
| 2:G:181:GLN:NE2 | 2:G:181:GLN:HA | 2.14 | 0.61 |
| 1:E:206:MET:O | 1:E:210:GLN:HG2 | 2.00 | 0.61 |
| 1:A:126:MET:HE2 | 1:A:130:VAL:HG13 | 1.82 | 0.60 |
| 1:F:61:MET:HA | 1:F:64:VAL:HG12 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:384:PRO:HA | 4:E:483:HOH:O | 2.00 | 0.60 |
| 1:F:74:ARG:HD3 | 1:F:132:GLU:CB | 2.32 | 0.60 |
| 1:F:162:ARG:HD3 | 4:F:503:HOH:O | 2.01 | 0.60 |
| 1:B:192:ASN:HD21 | 1:B:233:GLN:HE21 | 1.49 | 0.60 |
| 1:A:145:THR:HG21 | 4:A:530:HOH:O | 2.01 | 0.60 |
| 1:E:48:PHE:HD2 | 1:E:49:LEU:HD23 | 1.67 | 0.60 |
| 1:B:146:ASN:H | 1:B:147:ILE:HD12 | 1.67 | 0.59 |
| 1:E:62:ARG:HG2 | 1:E:372:PHE:CE2 | 2.37 | 0.59 |
| 1:A:180:HIS:HB2 | 4:A:447:HOH:O | 2.02 | 0.59 |
| 1:A:158:ARG:HH22 | 1:A:162:ARG:HH21 | 1.50 | 0.59 |
| 1:A:302:ASN:HB3 | 4:A:450:HOH:O | 2.00 | 0.59 |
| 2:C:154:LYS:HA | 4:C:903:HOH:O | 2.02 | 0.59 |
| 2:G:151:ARG:H | 2:G:168:GLU:HB2 | 1.67 | 0.59 |
| 1:E:143:ILE:O | 1:E:146:ASN:HB2 | 2.01 | 0.59 |
| 1:F:74:ARG:HB3 | 1:F:132:GLU:OE1 | 2.02 | 0.59 |
| 1:A:14:LYS:HG2 | 4:A:438:HOH:O | 2.03 | 0.59 |
| 1:F:213:LEU:O | 1:F:214:VAL:HG23 | 2.02 | 0.59 |
| 1:F:203:THR:HG21 | 1:F:242:PHE:HZ | 1.68 | 0.58 |
| 1:E:30:LYS:HE3 | 4:E:553:HOH:O | 2.02 | 0.58 |
| 1:A:86:GLN:O | 1:A:90:GLU:HG3 | 2.04 | 0.58 |
| 1:A:24:PRO:HD2 | 1:A:371:VAL:HG22 | 1.85 | 0.58 |
| 1:B:147:ILE:H | 1:B:147:ILE:HD12 | 1.69 | 0.58 |
| 1:A:293:PRO:HD3 | 1:A:348:GLU:OE2 | 2.03 | 0.58 |
| 1:F:70:ASN:CB | 1:F:136:LYS:HE2 | 2.31 | 0.58 |
| 1:E:227:ALA:O | 1:E:229:ASP:N | 2.34 | 0.57 |
| 1:B:241:LEU:HA | 1:B:244:MET:CE | 2.30 | 0.57 |
| 1:E:35:PHE:HB2 | 4:E:469:HOH:O | 2.04 | 0.57 |
| 2:G:151:ARG:N | 2:G:168:GLU:HB2 | 2.20 | 0.57 |
| 1:B:213:LEU:HB2 | 4:B:428:HOH:O | 2.04 | 0.57 |
| 1:E:123:VAL:HB | 1:E:124:PRO:HD3 | 1.87 | 0.57 |
| 1:E:136:LYS:HE2 | 4:E:568:HOH:O | 2.05 | 0.56 |
| 1:E:24:PRO:HD2 | 1:E:371:VAL:HG22 | 1.87 | 0.56 |
| 1:A:176:THR:O | 1:A:178:PRO:HD3 | 2.04 | 0.56 |
| 1:E:17:GLU:O | 1:E:21:ARG:HG3 | 2.05 | 0.56 |
| 1:B:374:LYS:HB2 | 2:C:179:GLU:OE2 | 2.05 | 0.56 |
| 1:A:227:ALA:O | 1:A:229:ASP:N | 2.38 | 0.56 |
| 1:E:137:PHE:HB3 | 4:E:516:HOH:O | 2.05 | 0.56 |
| 1:F:121:ASP:HB2 | 4:F:542:HOH:O | 2.06 | 0.56 |
| 1:F:332:ARG:HD3 | 1:F:336:ARG:CZ | 2.36 | 0.56 |
| 2:C:138:PRO:HG2 | 2:C:140:LEU:CD1 | 2.35 | 0.56 |
| 1:A:144:SER:HB2 | 4:A:496:HOH:O | 2.06 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:69:ASP:O | 1:B:73:ASN:HB2 | 2.05 | 0.56 |
| 1:E:109:LEU:O | 1:E:113:ILE:HD13 | 2.06 | 0.56 |
| 1:A:123:VAL:HB | 1:A:124:PRO:HD3 | 1.87 | 0.56 |
| 1:A:142:PHE:CD2 | 1:A:384:PRO:HG3 | 2.40 | 0.56 |
| 1:F:51:LYS:HE3 | 4:F:427:HOH:O | 2.06 | 0.56 |
| 2:G:188:LYS:O | 2:G:206:ILE:HD12 | 2.06 | 0.56 |
| 1:E:106:ASP:HB2 | 4:E:548:HOH:O | 2.06 | 0.56 |
| 1:A:62:ARG:HG2 | 1:A:372:PHE:CD2 | 2.41 | 0.56 |
| 1:E:231:PRO:HB3 | 4:E:558:HOH:O | 2.05 | 0.56 |
| 1:B:107:ASN:O | 1:B:111:VAL:HG23 | 2.07 | 0.56 |
| 1:F:27:LEU:HD21 | 3:G:901:RED:H32 | 1.87 | 0.55 |
| 1:A:244:MET:O | 1:A:248:LEU:HG | 2.06 | 0.55 |
| 1:A:139:PHE:HD1 | 4:A:483:HOH:O | 1.89 | 0.55 |
| 1:A:217:GLU:HG2 | 4:A:439:HOH:O | 2.06 | 0.55 |
| 1:B:118:ARG:HB3 | 1:B:119:HIS:ND1 | 2.22 | 0.55 |
| 1:F:124:PRO:HG3 | 4:F:438:HOH:O | 2.05 | 0.55 |
| 1:B:260:TYR:CE2 | 1:B:268:PRO:HG2 | 2.41 | 0.55 |
| 1:E:241:LEU:HA | 1:E:244:MET:CE | 2.36 | 0.55 |
| 1:B:75:PRO:HD2 | 1:B:132:GLU:OE1 | 2.06 | 0.55 |
| 1:E:197:VAL:HA | 1:E:245:LEU:HD13 | 1.87 | 0.55 |
| 2:G:151:ARG:HG2 | 2:G:153:GLU:OE2 | 2.07 | 0.55 |
| 1:B:228:PRO:HA | 4:B:447:HOH:O | 2.07 | 0.55 |
| 1:B:236:TYR:O | 1:B:238:PRO:HD3 | 2.06 | 0.55 |
| 1:B:74:ARG:HD3 | 1:B:132:GLU:CB | 2.37 | 0.55 |
| 1:E:389:TRP:CZ3 | 1:F:370:PRO:HG3 | 2.42 | 0.55 |
| 1:E:28:SER:HA | 1:E:366:PHE:HA | 1.88 | 0.55 |
| 1:F:90:GLU:O | 1:F:93:GLU:HG3 | 2.07 | 0.55 |
| 1:F:21:ARG:NH1 | 1:F:21:ARG:HB2 | 2.21 | 0.55 |
| 1:A:62:ARG:O | 1:A:65:ASN:HB3 | 2.07 | 0.54 |
| 1:B:93:GLU:O | 1:B:97:LYS:HE3 | 2.08 | 0.54 |
| 1:F:116:ARG:HH11 | 1:F:116:ARG:HG3 | 1.72 | 0.54 |
| 1:B:181:PRO:HD2 | 4:B:410:HOH:O | 2.07 | 0.54 |
| 1:B:281:LEU:HD23 | 1:B:358:LEU:HD12 | 1.89 | 0.54 |
| 1:B:257:VAL:HA | 1:B:267:TYR:CE1 | 2.41 | 0.54 |
| 1:E:63:GLU:HG2 | 1:E:372:PHE:HD1 | 1.71 | 0.54 |
| 1:F:16:ILE:HD12 | 4:F:415:HOH:O | 2.06 | 0.54 |
| 2:G:156:VAL:HA | 2:G:186:LEU:HB3 | 1.89 | 0.54 |
| 1:B:19:TYR:HA | 1:B:22:PHE:HD1 | 1.71 | 0.54 |
| 1:F:103:GLN:OE1 | 1:F:103:GLN:HA | 2.07 | 0.54 |
| 1:A:13:PRO:HA | 1:A:16:ILE:HB | 1.90 | 0.54 |
| 1:B:158:ARG:CB | 4:B:499:HOH:O | 2.55 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:241:LEU:HA | 1:F:244:MET:CE | 2.38 | 0.54 |
| 2:G:148:THR:HG23 | 2:G:196:ARG:HA | 1.88 | 0.54 |
| 1:A:46:TYR:HD2 | 1:A:99:PRO:HB3 | 1.72 | 0.53 |
| 1:E:123:VAL:HG13 | 1:E:155:TYR:CE1 | 2.43 | 0.53 |
| 1:E:67:LEU:HG | 1:E:71:LEU:HD23 | 1.90 | 0.53 |
| 1:B:192:ASN:HD21 | 1:B:233:GLN:NE2 | 2.05 | 0.53 |
| 1:B:82:SER:O | 1:B:85:MET:HB3 | 2.08 | 0.53 |
| 1:A:84:TYR:HE1 | 1:A:122:VAL:HG21 | 1.73 | 0.53 |
| 1:B:27:LEU:O | 1:B:367:GLU:HG3 | 2.09 | 0.53 |
| 1:E:274:VAL:HG22 | 1:E:283:ILE:HG23 | 1.89 | 0.53 |
| 1:F:108:PHE:CE2 | 1:F:112:LEU:HD11 | 2.44 | 0.53 |
| 1:F:27:LEU:O | 1:F:367:GLU:HG3 | 2.08 | 0.53 |
| 1:E:86:GLN:O | 1:E:90:GLU:HG3 | 2.07 | 0.53 |
| 1:F:14:LYS:N | 4:F:415:HOH:O | 2.41 | 0.53 |
| 2:G:185:TYR:CE1 | 2:G:211:GLU:HB3 | 2.43 | 0.53 |
| 1:B:192:ASN:ND2 | 1:B:233:GLN:HE21 | 2.07 | 0.53 |
| 1:F:147:ILE:H | 1:F:147:ILE:HD12 | 1.74 | 0.53 |
| 1:E:389:TRP:CZ2 | 1:F:153:ARG:HG2 | 2.44 | 0.53 |
| 1:E:48:PHE:CD2 | 1:E:49:LEU:HD23 | 2.43 | 0.53 |
| 1:B:158:ARG:HA | 1:B:161:PHE:CD1 | 2.44 | 0.53 |
| 1:F:135:GLU:O | 1:F:136:LYS:HB2 | 2.08 | 0.53 |
| 1:E:126:MET:CE | 1:E:130:VAL:HG13 | 2.38 | 0.53 |
| 1:E:60:THR:HG21 | 1:E:84:TYR:HE2 | 1.74 | 0.53 |
| 1:F:208:CYS:SG | 1:F:215:ALA:HB2 | 2.49 | 0.53 |
| 2:C:210:LYS:HA | 4:C:916:HOH:O | 2.09 | 0.52 |
| 1:F:272:THR:HA | 1:F:284:LYS:O | 2.09 | 0.52 |
| 1:E:193:VAL:O | 1:E:197:VAL:HG23 | 2.08 | 0.52 |
| 1:E:295:ARG:HD3 | 4:F:504:HOH:O | 2.09 | 0.52 |
| 1:F:123:VAL:HG11 | 4:F:473:HOH:O | 2.08 | 0.52 |
| 1:F:299:ARG:HD2 | 1:F:304:MET:CE | 2.40 | 0.52 |
| 2:C:155:LYS:HB2 | 2:C:158:GLU:HG3 | 1.91 | 0.52 |
| 1:B:339:GLN:NE2 | 1:B:368:ARG:HB3 | 2.24 | 0.52 |
| 1:E:389:TRP:HZ3 | 1:F:156:THR:HG21 | 1.75 | 0.52 |
| 1:E:15:GLN:CA | 1:E:15:GLN:HE21 | 2.21 | 0.52 |
| 1:E:17:GLU:OE2 | 1:E:21:ARG:HD2 | 2.10 | 0.52 |
| 1:A:361:LEU:HD13 | 4:A:470:HOH:O | 2.10 | 0.52 |
| 1:F:297:ILE:HD11 | 1:F:346:SER:HB2 | 1.90 | 0.52 |
| 1:E:194:ALA:O | 1:E:198:LYS:HG3 | 2.09 | 0.52 |
| 1:F:61:MET:O | 1:F:64:VAL:HG12 | 2.10 | 0.52 |
| 2:G:155:LYS:HB3 | 4:G:927:HOH:O | 2.08 | 0.52 |
| 1:E:117:ASN:ND2 | 4:E:507:HOH:O | 2.43 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:43:LYS:O | 1:F:47:MET:HG2 | 2.10 | 0.51 |
| 1:F:72:LEU:HA | 1:F:77:VAL:HG11 | 1.92 | 0.51 |
| 2:G:207:ILE:HG22 | 2:G:208:VAL:N | 2.25 | 0.51 |
| 1:A:271:LYS:HE3 | 4:A:431:HOH:O | 2.11 | 0.51 |
| 1:B:260:TYR:CZ | 1:B:268:PRO:HG2 | 2.45 | 0.51 |
| 1:F:56:ARG:NH1 | 1:F:164:LEU:HD11 | 2.26 | 0.51 |
| 1:F:75:PRO:HD2 | 1:F:132:GLU:OE1 | 2.10 | 0.51 |
| 1:B:163:MET:CE | 1:B:163:MET:HA | 2.41 | 0.51 |
| 1:E:39:ASN:HD21 | 1:E:41:CYS:HB3 | 1.75 | 0.51 |
| 1:E:68:PRO:CB | 4:E:563:HOH:O | 2.59 | 0.51 |
| 1:B:107:ASN:ND2 | 4:B:570:HOH:O | 2.42 | 0.51 |
| 1:B:336:ARG:HD3 | 1:B:341:ASP:OD1 | 2.11 | 0.51 |
| 2:C:170:GLU:HG3 | 2:C:175:THR:OG1 | 2.10 | 0.51 |
| 1:B:21:ARG:NH1 | 1:B:21:ARG:HB2 | 2.26 | 0.51 |
| 1:B:112:LEU:HB3 | 1:B:165:ILE:HG23 | 1.93 | 0.51 |
| 1:B:153:ARG:HB3 | 1:B:370:PRO:HB3 | 1.93 | 0.51 |
| 1:E:140:ASP:HB2 | 1:E:141:PRO:HD2 | 1.93 | 0.51 |
| 1:E:153:ARG:HG2 | 1:F:389:TRP:CZ2 | 2.46 | 0.51 |
| 1:E:15:GLN:HA | 1:E:15:GLN:NE2 | 2.25 | 0.51 |
| 1:F:165:ILE:O | 1:F:169:THR:HG23 | 2.11 | 0.51 |
| 1:B:213:LEU:O | 1:B:214:VAL:HG23 | 2.10 | 0.50 |
| 1:E:202:GLU:O | 1:E:205:LYS:HB3 | 2.11 | 0.50 |
| 1:F:373:ASN:HB2 | 2:G:179:GLU:OE1 | 2.11 | 0.50 |
| 1:A:64:VAL:O | 1:A:67:LEU:HD22 | 2.10 | 0.50 |
| 1:B:199:ASP:O | 1:B:203:THR:CG2 | 2.59 | 0.50 |
| 2:C:154:LYS:HG2 | 2:C:160:LEU:CD2 | 2.41 | 0.50 |
| 1:A:140:ASP:OD2 | 1:A:143:ILE:HB | 2.11 | 0.50 |
| 1:A:398:ASP:HA | 4:A:548:HOH:O | 2.11 | 0.50 |
| 2:G:139:ALA:HA | 2:G:144:MET:SD | 2.51 | 0.50 |
| 1:A:85:MET:O | 1:A:88:PHE:HB3 | 2.12 | 0.50 |
| 1:B:33:LEU:HD12 | 1:B:184:ILE:HG13 | 1.94 | 0.50 |
| 2:G:159:LYS:HE3 | 4:G:904:HOH:O | 2.12 | 0.50 |
| 1:B:222:GLU:HB3 | 1:B:232:ILE:HD12 | 1.94 | 0.49 |
| 2:C:153:GLU:HG3 | 2:C:165:LEU:HD21 | 1.93 | 0.49 |
| 1:E:140:ASP:OD2 | 1:E:143:ILE:HB | 2.12 | 0.49 |
| 1:E:345:TYR:CZ | 1:F:345:TYR:HB3 | 2.47 | 0.49 |
| 1:B:115:VAL:HG12 | 1:B:118:ARG:NH2 | 2.27 | 0.49 |
| 1:B:221:GLU:HA | 1:B:221:GLU:OE2 | 2.12 | 0.49 |
| 1:F:374:LYS:O | 1:F:377:TRP:HB3 | 2.12 | 0.49 |
| 1:B:286:SER:HB3 | 1:B:353:ASP:OD1 | 2.12 | 0.49 |
| 1:B:338:PHE:HB2 | 4:B:409:HOH:O | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:147:ILE:N | 1:F:147:ILE:HD12 | 2.28 | 0.49 |
| 1:E:107:ASN:O | 1:E:111:VAL:HG23 | 2.13 | 0.49 |
| 1:E:322:ALA:CB | 4:E:525:HOH:O | 2.60 | 0.49 |
| 1:E:70:ASN:HB2 | 4:E:563:HOH:O | 2.11 | 0.49 |
| 1:F:51:LYS:O | 1:F:55:VAL:HG23 | 2.13 | 0.49 |
| 1:A:163:MET:HE1 | 1:A:237:VAL:HG21 | 1.94 | 0.49 |
| 1:A:67:LEU:HG | 1:A:71:LEU:HD23 | 1.93 | 0.49 |
| 1:B:162:ARG:NH2 | 4:B:499:HOH:O | 2.42 | 0.49 |
| 1:B:132:GLU:C | 1:B:134:LYS:H | 2.16 | 0.49 |
| 1:B:135:GLU:O | 1:B:136:LYS:HB2 | 2.13 | 0.49 |
| 1:B:271:LYS:HG3 | 4:B:424:HOH:O | 2.12 | 0.49 |
| 1:A:121:ASP:C | 1:A:124:PRO:HD2 | 2.33 | 0.49 |
| 1:B:208:CYS:O | 1:B:210:GLN:N | 2.46 | 0.49 |
| 1:B:28:SER:H | 1:B:31:GLN:HE21 | 1.60 | 0.48 |
| 1:F:227:ALA:O | 1:F:229:ASP:N | 2.45 | 0.48 |
| 1:E:137:PHE:HD2 | 4:E:516:HOH:O | 1.95 | 0.48 |
| 1:F:339:GLN:NE2 | 1:F:368:ARG:HB3 | 2.29 | 0.48 |
| 1:B:221:GLU:O | 1:B:273:LEU:HD12 | 2.13 | 0.48 |
| 1:E:142:PHE:CD2 | 1:E:384:PRO:HG3 | 2.49 | 0.48 |
| 1:E:39:ASN:HD22 | 1:E:39:ASN:C | 2.17 | 0.48 |
| 1:A:347:MET:HE1 | 1:B:275:THR:HG23 | 1.96 | 0.48 |
| 1:B:121:ASP:OD1 | 1:B:162:ARG:NH2 | 2.47 | 0.48 |
| 1:B:257:VAL:HG22 | 1:B:267:TYR:CZ | 2.49 | 0.48 |
| 1:B:28:SER:HA | 1:B:366:PHE:HA | 1.95 | 0.48 |
| 1:B:297:ILE:O | 1:B:300:LEU:HB2 | 2.13 | 0.48 |
| 1:F:42:GLU:HG2 | 1:F:105:LEU:HD23 | 1.96 | 0.48 |
| 1:B:250:LYS:HE2 | 1:B:251:ASN:ND2 | 2.28 | 0.48 |
| 1:F:135:GLU:O | 1:F:136:LYS:CB | 2.61 | 0.48 |
| 1:F:46:TYR:OH | 1:F:94:TYR:HB3 | 2.14 | 0.48 |
| 1:A:90:GLU:CD | 1:A:118:ARG:HH12 | 2.16 | 0.48 |
| 1:B:74:ARG:HB3 | 1:B:132:GLU:OE1 | 2.14 | 0.48 |
| 1:B:135:GLU:O | 1:B:136:LYS:CB | 2.62 | 0.48 |
| 1:B:136:LYS:HB3 | 1:B:136:LYS:NZ | 2.28 | 0.48 |
| 2:C:137:LEU:HD12 | 2:C:138:PRO:HD2 | 1.95 | 0.48 |
| 4:A:519:HOH:O | 1:B:295:ARG:HG3 | 2.14 | 0.48 |
| 1:B:43:LYS:O | 1:B:47:MET:HG2 | 2.14 | 0.48 |
| 1:F:94:TYR:N | 1:F:94:TYR:CD1 | 2.82 | 0.47 |
| 1:E:241:LEU:HA | 1:E:244:MET:HE3 | 1.96 | 0.47 |
| 1:E:373:ASN:OD1 | 1:E:375:SER:HB3 | 2.14 | 0.47 |
| 2:C:138:PRO:O | 2:C:144:MET:HE1 | 2.14 | 0.47 |
| 1:F:241:LEU:HA | 1:F:244:MET:HE3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:375:SER:HB3 | 1:F:388:ASP:HB3 | 1.96 | 0.47 |
| 1:A:107:ASN:O | 1:A:111:VAL:HG23 | 2.13 | 0.47 |
| 1:A:399:ALA:O | 1:A:400:SER:CB | 2.61 | 0.47 |
| 1:E:299:ARG:HA | 1:E:302:ASN:ND2 | 2.28 | 0.47 |
| 1:F:146:ASN:ND2 | 4:F:435:HOH:O | 2.46 | 0.47 |
| 1:F:37:ARG:HB2 | 1:F:184:ILE:HD12 | 1.96 | 0.47 |
| 1:A:15:GLN:HG3 | 1:A:92:LEU:HD21 | 1.97 | 0.47 |
| 1:A:193:VAL:O | 1:A:197:VAL:HG23 | 2.15 | 0.47 |
| 1:E:132:GLU:O | 1:E:132:GLU:HG2 | 2.14 | 0.47 |
| 2:G:136:LEU:HD22 | 2:G:201:GLY:O | 2.14 | 0.47 |
| 1:A:191:CYS:O | 1:A:233:GLN:HA | 2.14 | 0.47 |
| 1:F:177:ASN:N | 1:F:178:PRO:HD3 | 2.29 | 0.47 |
| 2:C:190:LEU:HD22 | 2:C:205:CYS:HA | 1.97 | 0.47 |
| 1:F:27:LEU:HD11 | 1:F:48:PHE:CZ | 2.50 | 0.47 |
| 1:A:297:ILE:HG22 | 1:A:298:ASP:OD1 | 2.15 | 0.47 |
| 1:B:128:GLN:HA | 1:B:131:ILE:HD12 | 1.97 | 0.47 |
| 1:E:391:ASN:HA | 1:E:392:PRO:HD3 | 1.63 | 0.47 |
| 1:E:388:ASP:HB3 | 1:E:389:TRP:CD1 | 2.49 | 0.47 |
| 1:F:107:ASN:O | 1:F:111:VAL:HG23 | 2.15 | 0.47 |
| 1:A:121:ASP:HB3 | 4:A:553:HOH:O | 2.15 | 0.47 |
| 1:A:241:LEU:HD13 | 1:A:358:LEU:HD11 | 1.97 | 0.46 |
| 1:A:264:LYS:CD | 4:A:514:HOH:O | 2.63 | 0.46 |
| 1:A:264:LYS:HD2 | 4:A:514:HOH:O | 2.14 | 0.46 |
| 1:A:153:ARG:HG2 | 1:B:389:TRP:CZ2 | 2.50 | 0.46 |
| 1:A:146:ASN:O | 1:A:149:TYR:HB3 | 2.15 | 0.46 |
| 1:A:28:SER:HA | 1:A:366:PHE:HA | 1.98 | 0.46 |
| 1:F:146:ASN:H | 1:F:147:ILE:HD12 | 1.79 | 0.46 |
| 1:B:328:LEU:N | 1:B:329:PRO:CD | 2.79 | 0.46 |
| 2:C:151:ARG:HA | 2:C:193:GLU:HG2 | 1.96 | 0.46 |
| 1:E:40:ALA:HB3 | 4:E:530:HOH:O | 2.15 | 0.46 |
| 1:E:57:LEU:O | 1:E:61:MET:HG3 | 2.15 | 0.46 |
| 2:G:181:GLN:CA | 2:G:181:GLN:HE21 | 2.27 | 0.46 |
| 1:A:88:PHE:CE2 | 1:A:92:LEU:HD22 | 2.50 | 0.46 |
| 1:B:86:GLN:NE2 | 1:B:118:ARG:HD3 | 2.30 | 0.46 |
| 1:E:43:LYS:HB2 | 4:E:512:HOH:O | 2.14 | 0.46 |
| 1:F:260:TYR:CE2 | 1:F:268:PRO:HG2 | 2.50 | 0.46 |
| 1:F:332:ARG:HD3 | 1:F:336:ARG:NH1 | 2.30 | 0.46 |
| 1:A:373:ASN:OD1 | 1:A:375:SER:HB3 | 2.16 | 0.46 |
| 1:F:262:ASP:HA | 4:F:425:HOH:O | 2.14 | 0.46 |
| 2:G:207:ILE:HG22 | 2:G:208:VAL:H | 1.80 | 0.46 |
| 1:B:109:LEU:O | 1:B:109:LEU:HG | 2.14 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:146:ASN:O | 1:E:149:TYR:HB3 | 2.16 | 0.46 |
| 4:C:921:HOH:O | 1:E:205:LYS:NZ | 2.48 | 0.46 |
| 1:E:348:GLU:HG2 | 1:F:277:GLY:HA3 | 1.96 | 0.46 |
| 1:E:62:ARG:HG2 | 1:E:372:PHE:CD2 | 2.50 | 0.46 |
| 1:F:194:ALA:O | 1:F:198:LYS:HG3 | 2.15 | 0.46 |
| 1:B:33:LEU:CD1 | 1:B:184:ILE:HG13 | 2.45 | 0.46 |
| 1:E:241:LEU:HA | 1:E:244:MET:HE2 | 1.97 | 0.46 |
| 1:A:257:VAL:HA | 1:A:267:TYR:CE1 | 2.51 | 0.46 |
| 1:B:216:PRO:HA | 4:B:422:HOH:O | 2.16 | 0.46 |
| 1:E:294:LEU:HD22 | 1:F:357:TYR:CG | 2.51 | 0.46 |
| 1:F:122:VAL:O | 1:F:124:PRO:HD3 | 2.15 | 0.46 |
| 1:E:390:SER:HB3 | 1:F:369:LEU:HB2 | 1.98 | 0.46 |
| 2:G:168:GLU:O | 2:G:169:ILE:HD13 | 2.16 | 0.46 |
| 1:A:234:VAL:HG22 | 1:A:235:VAL:H | 1.80 | 0.45 |
| 1:A:200:ALA:HA | 1:A:242:PHE:CE1 | 2.51 | 0.45 |
| 1:E:142:PHE:CG | 1:E:384:PRO:HG3 | 2.52 | 0.45 |
| 1:F:249:PHE:O | 1:F:253:MET:HG3 | 2.15 | 0.45 |
| 2:G:156:VAL:N | 4:G:927:HOH:O | 2.49 | 0.45 |
| 2:G:188:LYS:HG2 | 2:G:206:ILE:CD1 | 2.45 | 0.45 |
| 1:B:70:ASN:CB | 1:B:136:LYS:HE2 | 2.41 | 0.45 |
| 1:B:203:THR:HG21 | 1:B:242:PHE:CZ | 2.39 | 0.45 |
| 2:G:181:GLN:CA | 2:G:181:GLN:NE2 | 2.77 | 0.45 |
| 1:A:321:LEU:O | 1:A:322:ALA:HB2 | 2.15 | 0.45 |
| 1:F:71:LEU:HD12 | 1:F:74:ARG:HG3 | 1.98 | 0.45 |
| 1:A:347:MET:HE2 | 1:B:273:LEU:HD23 | 1.98 | 0.45 |
| 1:A:70:ASN:O | 1:A:74:ARG:NH1 | 2.49 | 0.45 |
| 1:B:327:GLY:N | 4:B:434:HOH:O | 2.48 | 0.45 |
| 1:A:397:ARG:HB2 | 2:C:172:ASP:OD2 | 2.16 | 0.45 |
| 1:E:378:ARG:O | 1:E:382:THR:HG23 | 2.17 | 0.45 |
| 1:E:295:ARG:CZ | 1:F:279:GLU:OE1 | 2.65 | 0.45 |
| 1:B:299:ARG:HG2 | 4:B:529:HOH:O | 2.16 | 0.45 |
| 1:B:39:ASN:ND2 | 1:B:41:CYS:HB2 | 2.32 | 0.45 |
| 1:E:236:TYR:O | 1:E:238:PRO:HD3 | 2.17 | 0.45 |
| 1:E:41:CYS:SG | 1:E:43:LYS:HB2 | 2.57 | 0.45 |
| 1:F:215:ALA:HB1 | 1:F:253:MET:HE2 | 1.99 | 0.45 |
| 1:F:332:ARG:O | 1:F:336:ARG:CG | 2.64 | 0.45 |
| 1:B:194:ALA:O | 1:B:197:VAL:HB | 2.16 | 0.45 |
| 1:B:21:ARG:HH11 | 1:B:21:ARG:HB2 | 1.82 | 0.45 |
| 1:F:111:VAL:O | 1:F:115:VAL:HG13 | 2.17 | 0.45 |
| 1:E:390:SER:CB | 1:F:26:PRO:HG3 | 2.45 | 0.45 |
| 1:A:145:THR:CG2 | 4:A:530:HOH:O | 2.62 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:146:ASN:N | 1:B:147:ILE:HD12 | 2.32 | 0.45 |
| 1:B:42:GLU:HB2 | 1:B:172:PHE:CD1 | 2.52 | 0.45 |
| 1:B:64:VAL:O | 1:B:67:LEU:HB2 | 2.17 | 0.45 |
| 1:E:252:SER:HB3 | 1:E:287:ASP:HB3 | 1.99 | 0.45 |
| 1:E:296:LYS:HA | 1:E:299:ARG:HD3 | 1.99 | 0.45 |
| 1:F:153:ARG:HB3 | 1:F:370:PRO:HB3 | 1.99 | 0.45 |
| 1:A:74:ARG:HA | 1:A:74:ARG:NE | 2.32 | 0.44 |
| 1:E:101:ASP:OD2 | 1:E:101:ASP:N | 2.48 | 0.44 |
| 1:E:190:THR:HG23 | 4:E:437:HOH:O | 2.16 | 0.44 |
| 1:E:399:ALA:O | 1:E:400:SER:CB | 2.65 | 0.44 |
| 1:F:328:LEU:N | 1:F:329:PRO:CD | 2.80 | 0.44 |
| 1:F:357:TYR:O | 1:F:358:LEU:HD23 | 2.17 | 0.44 |
| 1:F:65:ASN:HA | 1:F:72:LEU:HD11 | 1.99 | 0.44 |
| 1:A:388:ASP:HB3 | 1:A:389:TRP:CD1 | 2.52 | 0.44 |
| 1:E:399:ALA:HB1 | 1:F:35:PHE:CB | 2.40 | 0.44 |
| 1:E:399:ALA:CB | 1:F:35:PHE:HB2 | 2.40 | 0.44 |
| 1:A:293:PRO:HA | 1:B:280:ASP:OD2 | 2.17 | 0.44 |
| 1:B:207:LEU:HD12 | 1:B:246:PHE:HZ | 1.82 | 0.44 |
| 1:F:182:LYS:HE3 | 4:F:459:HOH:O | 2.17 | 0.44 |
| 2:G:156:VAL:CG1 | 4:G:927:HOH:O | 2.65 | 0.44 |
| 1:A:46:TYR:CD2 | 1:A:99:PRO:HB3 | 2.51 | 0.44 |
| 1:E:121:ASP:C | 1:E:124:PRO:HD2 | 2.37 | 0.44 |
| 1:E:19:TYR:O | 1:E:22:PHE:HB2 | 2.17 | 0.44 |
| 1:F:74:ARG:HA | 1:F:74:ARG:NE | 2.33 | 0.44 |
| 2:G:151:ARG:HA | 2:G:193:GLU:HG2 | 1.98 | 0.44 |
| 1:F:27:LEU:HD13 | 3:G:901:RED:S6 | 2.57 | 0.44 |
| 2:G:206:ILE:HD12 | 2:G:206:ILE:H | 1.82 | 0.44 |
| 2:C:155:LYS:O | 2:C:158:GLU:HG3 | 2.18 | 0.44 |
| 2:C:152:TRP:CZ2 | 2:C:189:ILE:HG23 | 2.53 | 0.44 |
| 2:G:152:TRP:CZ2 | 2:G:189:ILE:HG23 | 2.53 | 0.44 |
| 2:G:154:LYS:HG2 | 2:G:160:LEU:CD2 | 2.48 | 0.44 |
| 1:B:221:GLU:O | 1:B:273:LEU:HA | 2.17 | 0.44 |
| 1:E:292:VAL:HB | 1:E:297:ILE:CD1 | 2.48 | 0.44 |
| 1:F:329:PRO:O | 1:F:333:LEU:HG | 2.17 | 0.44 |
| 2:G:185:TYR:CZ | 2:G:211:GLU:HB3 | 2.53 | 0.44 |
| 1:E:43:LYS:O | 1:E:47:MET:HG2 | 2.18 | 0.44 |
| 1:A:15:GLN:CA | 1:A:15:GLN:HE21 | 2.26 | 0.43 |
| 1:A:194:ALA:HB2 | 1:A:222:GLU:OE2 | 2.18 | 0.43 |
| 1:A:389:TRP:CZ2 | 1:B:153:ARG:HG2 | 2.53 | 0.43 |
| 1:E:347:MET:CE | 1:F:275:THR:HG23 | 2.47 | 0.43 |
| 1:E:46:TYR:OH | 1:E:94:TYR:HB3 | 2.17 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:F:339:GLN:NE2 | 4:F:511:HOH:O | 2.50 | 0.43 |
| 2:G:151:ARG:HB3 | 2:G:168:GLU:CG | 2.46 | 0.43 |
| 2:C:184:GLY:HA3 | 2:C:207:ILE:CG2 | 2.48 | 0.43 |
| 1:F:33:LEU:HD12 | 1:F:184:ILE:HG13 | 1.99 | 0.43 |
| 1:B:191:CYS:HB3 | 1:B:234:VAL:O | 2.17 | 0.43 |
| 2:C:148:THR:HG21 | 2:C:196:ARG:HG2 | 1.99 | 0.43 |
| 2:C:188:LYS:O | 2:C:205:CYS:HB2 | 2.19 | 0.43 |
| 2:C:206:ILE:HG22 | 4:C:913:HOH:O | 2.18 | 0.43 |
| 1:B:155:TYR:HA | 1:B:158:ARG:HG3 | 2.01 | 0.43 |
| 1:B:332:ARG:HD3 | 1:B:336:ARG:NE | 2.33 | 0.43 |
| 1:A:297:ILE:O | 1:A:300:LEU:HB2 | 2.18 | 0.43 |
| 1:A:51:LYS:O | 1:A:55:VAL:HG23 | 2.19 | 0.43 |
| 1:A:98:SER:O | 1:A:104:VAL:HG21 | 2.19 | 0.43 |
| 2:C:136:LEU:HD13 | 4:C:923:HOH:O | 2.19 | 0.43 |
| 2:C:151:ARG:HB3 | 2:C:168:GLU:HG3 | 2.01 | 0.43 |
| 1:E:106:ASP:CB | 4:E:548:HOH:O | 2.66 | 0.43 |
| 1:F:90:GLU:OE1 | 1:F:118:ARG:NH2 | 2.52 | 0.43 |
| 1:F:328:LEU:HD12 | 1:F:328:LEU:HA | 1.79 | 0.43 |
| 1:A:234:VAL:HG22 | 1:A:235:VAL:N | 2.34 | 0.43 |
| 1:B:374:LYS:O | 1:B:377:TRP:HB3 | 2.19 | 0.43 |
| 2:G:156:VAL:HG13 | 4:G:927:HOH:O | 2.18 | 0.43 |
| 1:A:250:LYS:HZ3 | 1:A:325:GLY:H | 1.66 | 0.42 |
| 1:B:28:SER:HB3 | 1:B:366:PHE:CD1 | 2.53 | 0.42 |
| 1:F:222:GLU:HB3 | 1:F:232:ILE:HD12 | 2.01 | 0.42 |
| 1:B:103:GLN:HA | 1:B:103:GLN:OE1 | 2.19 | 0.42 |
| 1:B:256:THR:CG2 | 1:B:268:PRO:HD2 | 2.49 | 0.42 |
| 1:E:68:PRO:HB2 | 4:E:563:HOH:O | 2.19 | 0.42 |
| 1:A:192:ASN:HB2 | 4:A:412:HOH:O | 2.18 | 0.42 |
| 1:A:394:SER:C | 1:A:395:GLU:HG3 | 2.39 | 0.42 |
| 1:A:218:LEU:HG | 1:A:219:GLU:N | 2.33 | 0.42 |
| 1:A:76:SER:OG | 1:A:128:GLN:HG3 | 2.19 | 0.42 |
| 2:C:151:ARG:NE | 2:C:153:GLU:OE2 | 2.46 | 0.42 |
| 1:F:131:ILE:C | 1:F:133:TYR:N | 2.71 | 0.42 |
| 1:F:158:ARG:HA | 1:F:161:PHE:CD1 | 2.54 | 0.42 |
| 1:E:345:TYR:OH | 1:F:345:TYR:HB3 | 2.20 | 0.42 |
| 1:B:19:TYR:HA | 1:B:22:PHE:CD1 | 2.53 | 0.42 |
| 1:A:113:ILE:O | 1:A:117:ASN:ND2 | 2.52 | 0.42 |
| 1:A:126:MET:CE | 1:A:130:VAL:HG13 | 2.48 | 0.42 |
| 1:E:125:THR:O | 1:E:128:GLN:HB3 | 2.19 | 0.42 |
| 1:E:158:ARG:HD2 | 4:E:421:HOH:O | 2.19 | 0.42 |
| 1:E:191:CYS:HB3 | 1:E:234:VAL:O | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:63:GLU:HG2 | 1:E:372:PHE:CD1 | 2.53 | 0.42 |
| 1:A:272:THR:HA | 1:A:284:LYS:O | 2.19 | 0.42 |
| 1:B:267:TYR:HA | 1:B:268:PRO:HD3 | 1.88 | 0.42 |
| 2:C:191:VAL:HG11 | 2:C:198:VAL:HG21 | 2.02 | 0.42 |
| 1:F:113:ILE:HG23 | 4:F:426:HOH:O | 2.19 | 0.42 |
| 1:A:188:ASP:HB2 | 1:A:238:PRO:CG | 2.49 | 0.42 |
| 1:B:126:MET:O | 1:B:130:VAL:HG23 | 2.19 | 0.42 |
| 1:B:256:THR:HG23 | 1:B:268:PRO:HD2 | 2.02 | 0.42 |
| 1:B:71:LEU:HD12 | 1:B:74:ARG:HG3 | 2.02 | 0.42 |
| 1:B:181:PRO:HB2 | 4:B:555:HOH:O | 2.19 | 0.41 |
| 1:B:61:MET:SD | 1:B:84:TYR:HB3 | 2.59 | 0.41 |
| 1:B:84:TYR:OH | 1:B:158:ARG:HD2 | 2.19 | 0.41 |
| 1:E:98:SER:HG | 1:E:100:GLU:HG2 | 1.82 | 0.41 |
| 1:E:90:GLU:CD | 1:E:118:ARG:HH12 | 2.23 | 0.41 |
| 1:A:155:TYR:O | 1:A:159:ILE:HG13 | 2.20 | 0.41 |
| 1:A:179:VAL:O | 1:A:181:PRO:HD3 | 2.20 | 0.41 |
| 1:A:50:ARG:CZ | 4:A:417:HOH:O | 2.67 | 0.41 |
| 1:B:262:ASP:C | 4:B:470:HOH:O | 2.57 | 0.41 |
| 1:B:337:TYR:OH | 1:B:367:GLU:OE2 | 2.36 | 0.41 |
| 1:B:51:LYS:HB2 | 4:B:457:HOH:O | 2.20 | 0.41 |
| 1:E:70:ASN:HB2 | 1:E:133:TYR:HE2 | 1.84 | 0.41 |
| 1:E:347:MET:HE2 | 1:F:275:THR:HG23 | 2.02 | 0.41 |
| 1:B:26:PRO:HD2 | 2:C:174:ALA:HB2 | 2.01 | 0.41 |
| 1:F:259:LEU:O | 1:F:261:GLU:N | 2.49 | 0.41 |
| 1:B:42:GLU:HG2 | 1:B:105:LEU:CD2 | 2.46 | 0.41 |
| 1:B:65:ASN:HA | 1:B:72:LEU:HD11 | 2.02 | 0.41 |
| 1:B:22:PHE:HA | 2:C:140:LEU:O | 2.20 | 0.41 |
| 2:C:206:ILE:H | 2:C:206:ILE:HD12 | 1.85 | 0.41 |
| 1:F:201:TYR:CG | 1:F:218:LEU:HD22 | 2.55 | 0.41 |
| 1:B:243:HIS:CE1 | 4:B:417:HOH:O | 2.73 | 0.41 |
| 1:B:26:PRO:CD | 2:C:174:ALA:HB2 | 2.51 | 0.41 |
| 1:E:76:SER:OG | 1:E:128:GLN:HG3 | 2.20 | 0.41 |
| 1:E:166:ASN:O | 1:E:170:LEU:HG | 2.21 | 0.41 |
| 1:E:267:TYR:HA | 1:E:268:PRO:HD3 | 1.85 | 0.41 |
| 1:A:357:TYR:CG | 1:B:294:LEU:HD22 | 2.55 | 0.41 |
| 1:B:227:ALA:O | 1:B:229:ASP:N | 2.54 | 0.41 |
| 1:B:336:ARG:O | 1:B:368:ARG:HG2 | 2.20 | 0.41 |
| 1:B:61:MET:HA | 1:B:64:VAL:CG1 | 2.49 | 0.41 |
| 1:E:14:LYS:CD | 4:E:485:HOH:O | 2.68 | 0.41 |
| 1:E:260:TYR:CE2 | 1:E:268:PRO:HG2 | 2.56 | 0.41 |
| 1:A:233:GLN:NE2 | 4:A:412:HOH:O | 2.49 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:86:GLN:HE21 | 1:B:118:ARG:NH1 | 2.18 | 0.41 |
| 1:F:191:CYS:O | 1:F:233:GLN:HA | 2.21 | 0.41 |
| 1:A:13:PRO:CB | 4:A:456:HOH:O | 2.58 | 0.41 |
| 1:A:73:ASN:HA | 1:A:73:ASN:HD22 | 1.73 | 0.41 |
| 1:B:133:TYR:HB3 | 4:B:444:HOH:O | 2.21 | 0.41 |
| 1:E:39:ASN:ND2 | 1:E:41:CYS:HB3 | 2.35 | 0.41 |
| 1:A:206:MET:HG2 | 4:A:446:HOH:O | 2.20 | 0.41 |
| 1:A:53:LEU:N | 1:A:54:PRO:HD2 | 2.36 | 0.41 |
| 1:E:91:LEU:C | 1:E:93:GLU:H | 2.25 | 0.41 |
| 1:F:233:GLN:O | 1:F:234:VAL:HB | 2.20 | 0.41 |
| 1:F:352:THR:HG22 | 1:F:353:ASP:N | 2.35 | 0.41 |
| 1:B:115:VAL:HG12 | 1:B:118:ARG:HH21 | 1.86 | 0.40 |
| 1:B:145:THR:HA | 1:B:147:ILE:HD13 | 2.03 | 0.40 |
| 1:B:352:THR:HG22 | 1:B:353:ASP:N | 2.36 | 0.40 |
| 1:F:201:TYR:HE1 | 1:F:253:MET:HE3 | 1.86 | 0.40 |
| 1:F:267:TYR:HA | 1:F:268:PRO:HD3 | 1.85 | 0.40 |
| 1:B:332:ARG:O | 1:B:336:ARG:CG | 2.67 | 0.40 |
| 1:B:53:LEU:HA | 1:B:53:LEU:HD23 | 1.81 | 0.40 |
| 2:C:136:LEU:CD1 | 4:C:923:HOH:O | 2.69 | 0.40 |
| 1:F:126:MET:O | 1:F:130:VAL:HG23 | 2.21 | 0.40 |
| 1:B:94:TYR:N | 1:B:94:TYR:CD1 | 2.89 | 0.40 |
| 1:E:199:ASP:O | 1:E:203:THR:HG23 | 2.21 | 0.40 |
| 2:G:150:GLN:HB3 | 2:G:168:GLU:HB3 | 2.03 | 0.40 |
| 1:B:147:ILE:N | 1:B:147:ILE:HD12 | 2.36 | 0.40 |
| 2:C:138:PRO:HG2 | 2:C:140:LEU:HD11 | 2.04 | 0.40 |
| 1:B:61:MET:O | 1:B:64:VAL:HG12 | 2.21 | 0.40 |
| 1:E:61:MET:SD | 1:E:84:TYR:HB3 | 2.61 | 0.40 |

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 370/419 (88%) | 327 (88%) | 36 (10%) | 7 (2%) | 8 | 13 |
| 1 | B | 331/419 (79%) | 300 (91%) | 24 (7%) | 7 (2%) | 7 | 11 |
| 1 | E | 370/419 (88%) | 329 (89%) | 32 (9%) | 9 (2%) | 6 | 9 |
| 1 | F | 331/419 (79%) | 303 (92%) | 20 (6%) | 8 (2%) | 6 | 9 |
| 2 | C | 77/128 (60%) | 65 (84%) | 9 (12%) | 3 (4%) | 3 | 4 |
| 2 | G | 77/128 (60%) | 64 (83%) | 10 (13%) | 3 (4%) | 3 | 4 |
| All | All | 1556/1932 (80%) | 1388 (89%) | 131 (8%) | 37 (2%) | 6 | 9 |

All (37) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 228 | PRO |
| 1 | A | 320 | PRO |
| 1 | B | 209 | GLU |
| 1 | B | 214 | VAL |
| 2 | C | 209 | GLU |
| 1 | E | 228 | PRO |
| 1 | E | 320 | PRO |
| 1 | F | 214 | VAL |
| 1 | F | 228 | PRO |
| 2 | G | 209 | GLU |
| 1 | A | 141 | PRO |
| 1 | B | 228 | PRO |
| 1 | B | 261 | GLU |
| 2 | C | 162 | GLU |
| 1 | E | 141 | PRO |
| 1 | E | 176 | THR |
| 1 | E | 325 | GLY |
| 1 | F | 39 | ASN |
| 1 | F | 261 | GLU |
| 1 | A | 300 | LEU |
| 1 | A | 322 | ALA |
| 1 | B | 39 | ASN |
| 1 | E | 39 | ASN |
| 1 | E | 175 | ASP |
| 1 | F | 209 | GLU |
| 1 | B | 260 | TYR |
| 1 | E | 174 | GLY |
| 1 | A | 176 | THR |
| 1 | A | 325 | GLY |
| 1 | B | 227 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 156 | VAL |
| 1 | E | 321 | LEU |
| 1 | F | 234 | VAL |
| 1 | F | 260 | TYR |
| 2 | G | 149 | VAL |
| 1 | F | 227 | ALA |
| 2 | G | 156 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1 | A | 336/374 (90%) | 305 (91%) | 31 (9%) | 9 | 18 |
| 1 | B | 311/374 (83%) | 285 (92%) | 26 (8%) | 11 | 21 |
| 1 | E | 336/374 (90%) | 308 (92%) | 28 (8%) | 11 | 22 |
| 1 | F | 311/374 (83%) | 287 (92%) | 24 (8%) | 13 | 25 |
| 2 | C | 67/109 (62%) | 60 (90%) | 7 (10%) | 7 | 13 |
| 2 | G | 67/109 (62%) | 61 (91%) | 6 (9%) | 9 | 19 |
| All | All | 1428/1714 (83%) | 1306 (92%) | 122 (8%) | 10 | 21 |

All (122) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 15 | GLN |
| 1 | A | 23 | SER |
| 1 | A | 39 | ASN |
| 1 | A | 64 | VAL |
| 1 | A | 66 | LEU |
| 1 | A | 67 | LEU |
| 1 | A | 72 | LEU |
| 1 | A | 93 | GLU |
| 1 | A | 101 | ASP |
| 1 | A | 103 | GLN |
| 1 | A | 105 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 128 | GLN |
| 1 | A | 139 | PHE |
| 1 | A | 177 | ASN |
| 1 | A | 183 | HIS |
| 1 | A | 186 | SER |
| 1 | A | 203 | THR |
| 1 | A | 209 | GLU |
| 1 | A | 214 | VAL |
| 1 | A | 226 | LYS |
| 1 | A | 228 | PRO |
| 1 | A | 229 | ASP |
| 1 | A | 263 | ARG |
| 1 | A | 265 | GLU |
| 1 | A | 281 | LEU |
| 1 | A | 297 | ILE |
| 1 | A | 298 | ASP |
| 1 | A | 320 | PRO |
| 1 | A | 321 | LEU |
| 1 | A | 336 | ARG |
| 1 | A | 388 | ASP |
| 1 | B | 17 | GLU |
| 1 | B | 39 | ASN |
| 1 | B | 66 | LEU |
| 1 | B | 67 | LEU |
| 1 | B | 70 | ASN |
| 1 | B | 72 | LEU |
| 1 | B | 73 | ASN |
| 1 | B | 93 | GLU |
| 1 | B | 128 | GLN |
| 1 | B | 133 | TYR |
| 1 | B | 145 | THR |
| 1 | B | 146 | ASN |
| 1 | B | 148 | GLN |
| 1 | B | 158 | ARG |
| 1 | B | 163 | MET |
| 1 | B | 182 | LYS |
| 1 | B | 183 | HIS |
| 1 | B | 203 | THR |
| 1 | B | 209 | GLU |
| 1 | B | 229 | ASP |
| 1 | B | 252 | SER |
| 1 | B | 286 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 302 | ASN |
| 1 | B | 336 | ARG |
| 1 | B | 362 | SER |
| 1 | B | 387 | ASP |
| 2 | C | 140 | LEU |
| 2 | C | 171 | THR |
| 2 | C | 186 | LEU |
| 2 | C | 188 | LYS |
| 2 | C | 190 | LEU |
| 2 | C | 206 | ILE |
| 2 | C | 213 | ASP |
| 1 | E | 15 | GLN |
| 1 | E | 38 | ASP |
| 1 | E | 39 | ASN |
| 1 | E | 64 | VAL |
| 1 | E | 67 | LEU |
| 1 | E | 72 | LEU |
| 1 | E | 73 | ASN |
| 1 | E | 101 | ASP |
| 1 | E | 103 | GLN |
| 1 | E | 105 | LEU |
| 1 | E | 107 | ASN |
| 1 | E | 116 | ARG |
| 1 | E | 128 | GLN |
| 1 | E | 139 | PHE |
| 1 | E | 177 | ASN |
| 1 | E | 203 | THR |
| 1 | E | 226 | LYS |
| 1 | E | 228 | PRO |
| 1 | E | 252 | SER |
| 1 | E | 265 | GLU |
| 1 | E | 286 | SER |
| 1 | E | 297 | ILE |
| 1 | E | 299 | ARG |
| 1 | E | 321 | LEU |
| 1 | E | 332 | ARG |
| 1 | E | 336 | ARG |
| 1 | E | 374 | LYS |
| 1 | E | 388 | ASP |
| 1 | F | 17 | GLU |
| 1 | F | 39 | ASN |
| 1 | F | 66 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | F | 72 | LEU |
| 1 | F | 93 | GLU |
| 1 | F | 116 | ARG |
| 1 | F | 133 | TYR |
| 1 | F | 145 | THR |
| 1 | F | 146 | ASN |
| 1 | F | 163 | MET |
| 1 | F | 183 | HIS |
| 1 | F | 203 | THR |
| 1 | F | 207 | LEU |
| 1 | F | 209 | GLU |
| 1 | F | 229 | ASP |
| 1 | F | 252 | SER |
| 1 | F | 280 | ASP |
| 1 | F | 282 | SER |
| 1 | F | 302 | ASN |
| 1 | F | 336 | ARG |
| 1 | F | 346 | SER |
| 1 | F | 362 | SER |
| 1 | F | 368 | ARG |
| 1 | F | 387 | ASP |
| 2 | G | 140 | LEU |
| 2 | G | 186 | LEU |
| 2 | G | 188 | LYS |
| 2 | G | 190 | LEU |
| 2 | G | 206 | ILE |
| 2 | G | 213 | ASP |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 15 | GLN |
| 1 | A | 39 | ASN |
| 1 | A | 70 | ASN |
| 1 | A | 73 | ASN |
| 1 | A | 103 | GLN |
| 1 | A | 107 | ASN |
| 1 | A | 117 | ASN |
| 1 | A | 128 | GLN |
| 1 | A | 157 | ASN |
| 1 | A | 167 | GLN |
| 1 | A | 177 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 192 | ASN |
| 1 | A | 240 | HIS |
| 1 | B | 31 | GLN |
| 1 | B | 39 | ASN |
| 1 | B | 86 | GLN |
| 1 | B | 107 | ASN |
| 1 | B | 128 | GLN |
| 1 | B | 192 | ASN |
| 1 | B | 243 | HIS |
| 1 | B | 251 | ASN |
| 1 | B | 339 | GLN |
| 2 | C | 181 | GLN |
| 1 | E | 15 | GLN |
| 1 | E | 39 | ASN |
| 1 | E | 70 | ASN |
| 1 | E | 73 | ASN |
| 1 | E | 103 | GLN |
| 1 | E | 107 | ASN |
| 1 | E | 128 | GLN |
| 1 | E | 157 | ASN |
| 1 | E | 167 | GLN |
| 1 | E | 177 | ASN |
| 1 | E | 192 | ASN |
| 1 | E | 210 | GLN |
| 1 | E | 233 | GLN |
| 1 | E | 240 | HIS |
| 1 | E | 302 | ASN |
| 1 | F | 39 | ASN |
| 1 | F | 86 | GLN |
| 1 | F | 107 | ASN |
| 1 | F | 119 | HIS |
| 1 | F | 128 | GLN |
| 1 | F | 146 | ASN |
| 1 | F | 157 | ASN |
| 1 | F | 243 | HIS |
| 1 | F | 251 | ASN |
| 1 | F | 302 | ASN |
| 1 | F | 339 | GLN |
| 1 | F | 379 | HIS |
| 2 | G | 181 | 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 ⓘ

2 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 | $\# Z > 2$ |
| 3 | RED | C | 900 | 2 | 9,10,11 | 1.41 | 1 (11%) | 6,10,12 | 3.61 | 1 (16%) |
| 3 | RED | G | 901 | 2 | 9,10,11 | 1.20 | 1 (11%) | 6,10,12 | 4.02 | 1 (16%) |

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 | RED | C | 900 | 2 | - | 4/7/9/10 | - |
| 3 | RED | G | 901 | 2 | - | 4/7/9/10 | - |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | C | 900 | RED | C7-C8 | 3.26 | 1.56 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3 | G | 901 | RED | C7-C8 | 2.64 | 1.56 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3 | G | 901 | RED | C7-C8-S8 | -9.74 | 103.59 | 113.74 |
| 3 | C | 900 | RED | C7-C8-S8 | -8.70 | 104.67 | 113.74 |

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | C | 900 | RED | C1-C2-C3-C4 |
| 3 | C | 900 | RED | C5-C6-C7-C8 |
| 3 | C | 900 | RED | C6-C7-C8-S8 |
| 3 | G | 901 | RED | C1-C2-C3-C4 |
| 3 | G | 901 | RED | C5-C6-C7-C8 |
| 3 | G | 901 | RED | C6-C7-C8-S8 |
| 3 | C | 900 | RED | C2-C3-C4-C5 |
| 3 | G | 901 | RED | C2-C3-C4-C5 |

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3 | G | 901 | RED | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 374/419 (89%) | -0.06 | 13 (3%) 44 47 | 23, 51, 83, 96 | 0 |
| 1 | B | 341/419 (81%) | -0.07 | 9 (2%) 56 59 | 27, 49, 70, 94 | 0 |
| 1 | E | 374/419 (89%) | -0.13 | 7 (1%) 66 69 | 24, 49, 77, 99 | 0 |
| 1 | F | 341/419 (81%) | -0.17 | 5 (1%) 73 75 | 23, 46, 74, 85 | 0 |
| 2 | C | 79/128 (61%) | -0.28 | 2 (2%) 57 61 | 42, 55, 79, 89 | 0 |
| 2 | G | 79/128 (61%) | -0.37 | 0 100 100 | 39, 56, 71, 77 | 0 |
| All | All | 1588/1932 (82%) | -0.13 | 36 (2%) 60 63 | 23, 51, 76, 99 | 0 |

All (36) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | E | 176 | THR | 4.8 |
| 1 | A | 176 | THR | 4.6 |
| 1 | A | 318 | ALA | 4.4 |
| 1 | B | 131 | ILE | 3.7 |
| 1 | B | 144 | SER | 3.7 |
| 1 | A | 177 | ASN | 3.7 |
| 1 | A | 319 | ALA | 3.5 |
| 1 | B | 123 | VAL | 3.5 |
| 1 | F | 131 | ILE | 2.9 |
| 1 | B | 145 | THR | 2.8 |
| 1 | F | 123 | VAL | 2.8 |
| 1 | E | 318 | ALA | 2.8 |
| 1 | E | 179 | VAL | 2.7 |
| 1 | B | 229 | ASP | 2.6 |
| 1 | A | 320 | PRO | 2.5 |
| 1 | A | 178 | PRO | 2.5 |
| 1 | E | 177 | ASN | 2.5 |
| 1 | E | 178 | PRO | 2.4 |
| 1 | A | 102 | PRO | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 262 | ASP | 2.4 |
| 1 | B | 345 | TYR | 2.3 |
| 1 | E | 57 | LEU | 2.3 |
| 1 | A | 181 | PRO | 2.2 |
| 2 | C | 210 | LYS | 2.2 |
| 1 | A | 103 | GLN | 2.2 |
| 1 | F | 229 | ASP | 2.2 |
| 1 | A | 229 | ASP | 2.1 |
| 1 | F | 304 | MET | 2.1 |
| 1 | E | 319 | ALA | 2.1 |
| 1 | A | 179 | VAL | 2.1 |
| 1 | F | 75 | PRO | 2.1 |
| 2 | C | 208 | VAL | 2.1 |
| 1 | A | 139 | PHE | 2.1 |
| 1 | A | 324 | PHE | 2.1 |
| 1 | B | 133 | TYR | 2.0 |
| 1 | B | 354 | ALA | 2.0 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3 | RED | C | 900 | 11/12 | 0.85 | 0.22 | 63,64,67,69 | 0 |
| 3 | RED | G | 901 | 11/12 | 0.95 | 0.14 | 39,46,54,55 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.