



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E1Q
Title : Crystal Structure of Human Xanthine Oxidoreductase mutant, Glu803Val
Authors : Yamaguchi, Y.; Matsumura, T.; Ichida, K.; Okamoto, K.; Nishino, T.
Deposited on : 2006-10-27
Resolution : 2.60 Å(reported)

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

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

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

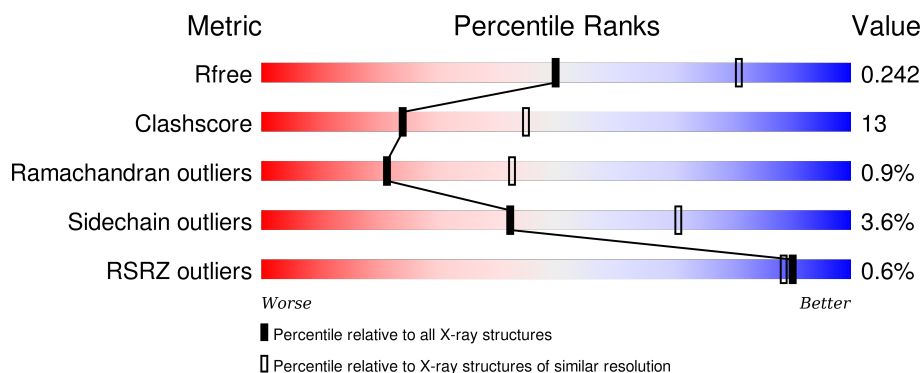
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 2328 (2.60-2.60) |
| Clashscore | 102246 | 2679 (2.60-2.60) |
| Ramachandran outliers | 100387 | 2635 (2.60-2.60) |
| Sidechain outliers | 100360 | 2635 (2.60-2.60) |
| RSRZ outliers | 91569 | 2334 (2.60-2.60) |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 1333 | <div> <div>%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div> |
| 1 | B | 1333 | <div> <div></div> <div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div> |
| 1 | C | 1333 | <div> <div>%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>..</div> </div> </div> |
| 1 | D | 1333 | <div> <div>%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3 | CA | A | 7002 | - | - | - | X |
| 3 | CA | B | 7004 | - | - | - | X |
| 3 | CA | C | 7006 | - | - | - | X |
| 3 | CA | D | 7008 | - | - | - | X |
| 7 | MOM | A | 2005 | - | - | X | - |
| 7 | MOM | B | 3005 | - | - | X | - |
| 7 | MOM | C | 4005 | - | - | X | - |
| 7 | MOM | D | 5005 | - | - | X | - |
| 8 | SAL | A | 2006 | - | - | - | X |
| 8 | SAL | B | 3006 | - | - | - | X |
| 8 | SAL | C | 4006 | - | - | - | X |
| 8 | SAL | D | 5006 | - | - | - | X |

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 41721 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.

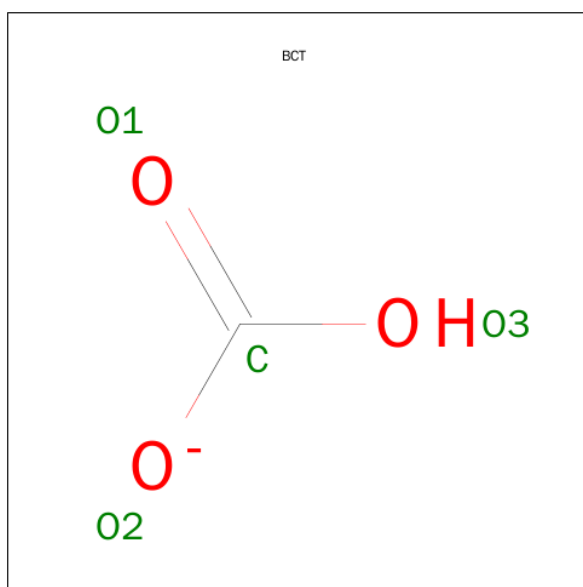
- Molecule 1 is a protein called Xanthine dehydrogenase/oxidase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1 | A | 1307 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10088 | 6394 | 1737 | 1891 | 66 | | | |
| 1 | B | 1307 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10088 | 6394 | 1737 | 1891 | 66 | | | |
| 1 | C | 1307 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10088 | 6394 | 1737 | 1891 | 66 | | | |
| 1 | D | 1307 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 10088 | 6394 | 1737 | 1891 | 66 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| A | 1 | MET | - | INITIATING METHIONINE | UNP P47989 |
| A | 803 | VAL | GLU | ENGINEERED | UNP P47989 |
| B | 1 | MET | - | INITIATING METHIONINE | UNP P47989 |
| B | 803 | VAL | GLU | ENGINEERED | UNP P47989 |
| C | 1 | MET | - | INITIATING METHIONINE | UNP P47989 |
| C | 803 | VAL | GLU | ENGINEERED | UNP P47989 |
| D | 1 | MET | - | INITIATING METHIONINE | UNP P47989 |
| D | 803 | VAL | GLU | ENGINEERED | UNP P47989 |

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

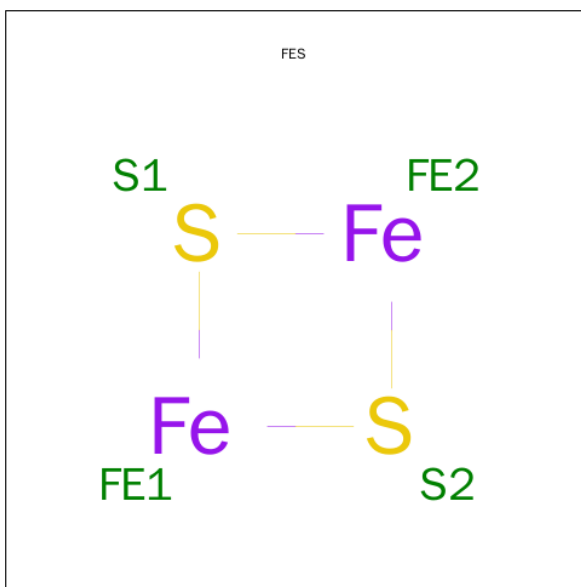


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 2 | A | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 2 | B | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3 | | |
| 2 | C | 1 | Total | C | O | 0 | 0 |
| | | | 4 | 1 | 3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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

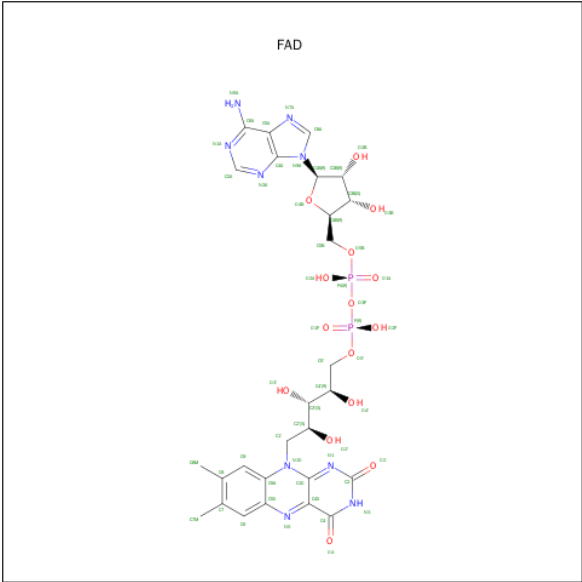
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 3 | B | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | A | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | D | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |
| 3 | C | 2 | Total | Ca | 0 | 0 |
| | | | 2 | 2 | | |

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



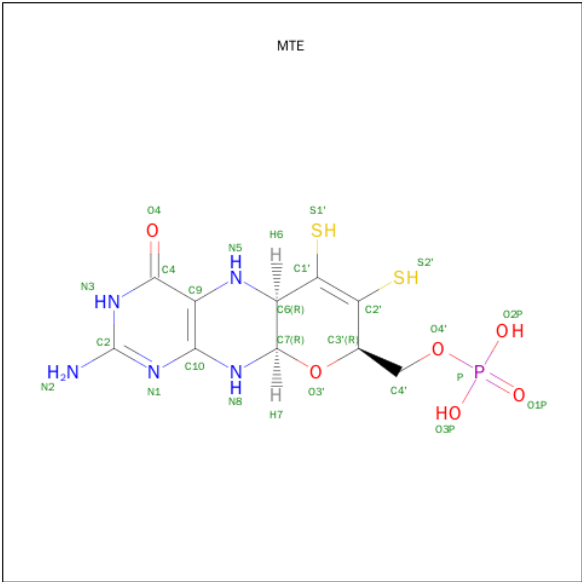
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4 | A | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | A | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | B | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | C | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |
| 4 | D | 1 | Total | Fe | S | 0 | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



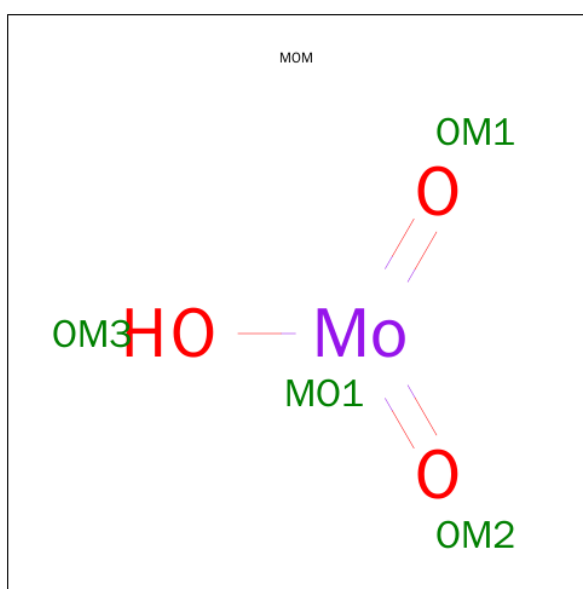
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|---------|
| 5 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 5 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 5 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |
| 5 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 53 | 27 | 9 | 15 | 2 | | |

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P₂).



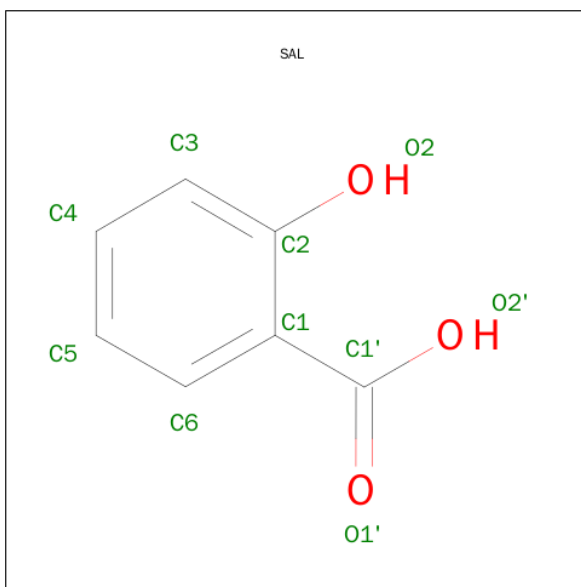
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---|---------|---------|
| 6 | A | 1 | Total | C | N | O | P | S | |
| | | | 24 | 10 | 5 | 6 | 1 | 2 | |
| 6 | B | 1 | Total | C | N | O | P | S | |
| | | | 24 | 10 | 5 | 6 | 1 | 2 | |
| 6 | C | 1 | Total | C | N | O | P | S | |
| | | | 24 | 10 | 5 | 6 | 1 | 2 | |
| 6 | D | 1 | Total | C | N | O | P | S | |
| | | | 24 | 10 | 5 | 6 | 1 | 2 | |

- Molecule 7 is HYDROXY(DIOXO)MOLYBDENUM (three-letter code: MOM) (formula: HMoO_3).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 7 | A | 1 | Total | Mo | O | | |
| | | | 4 | 1 | 3 | 0 | 0 |
| 7 | B | 1 | Total | Mo | O | | |
| | | | 4 | 1 | 3 | 0 | 0 |
| 7 | C | 1 | Total | Mo | O | | |
| | | | 4 | 1 | 3 | 0 | 0 |
| 7 | D | 1 | Total | Mo | O | | |
| | | | 4 | 1 | 3 | 0 | 0 |

- Molecule 8 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $\text{C}_7\text{H}_6\text{O}_3$).

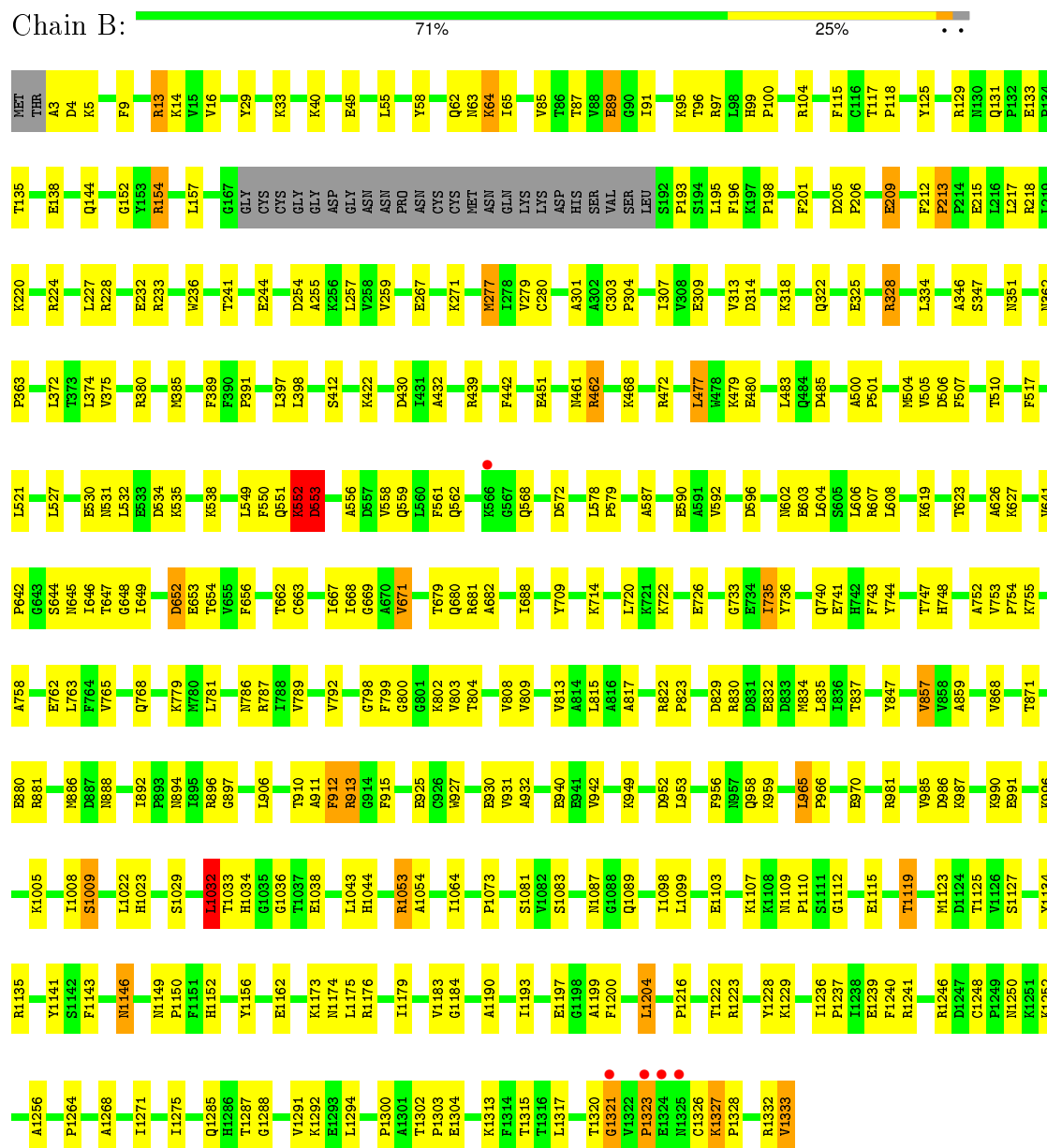


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8 | A | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 8 | B | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 8 | C | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |
| 8 | D | 1 | Total | C | O | 0 | 0 |
| | | | 10 | 7 | 3 | | |

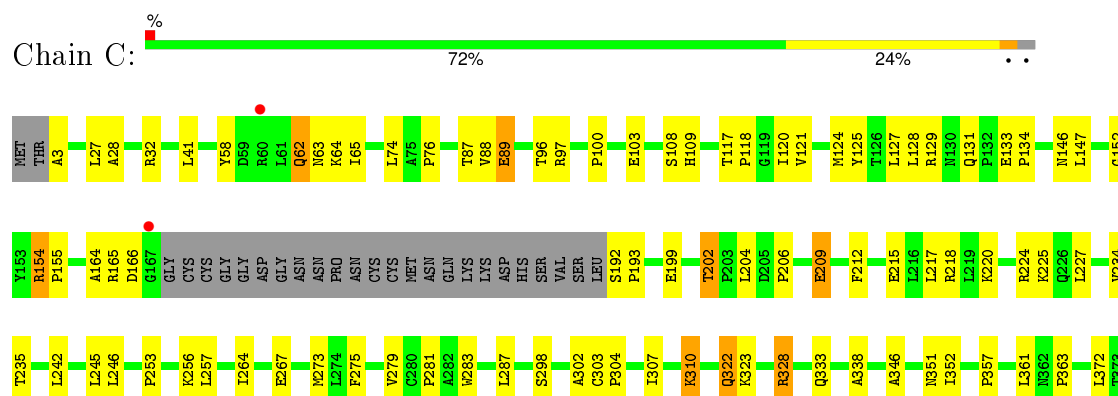
- Molecule 9 is water.

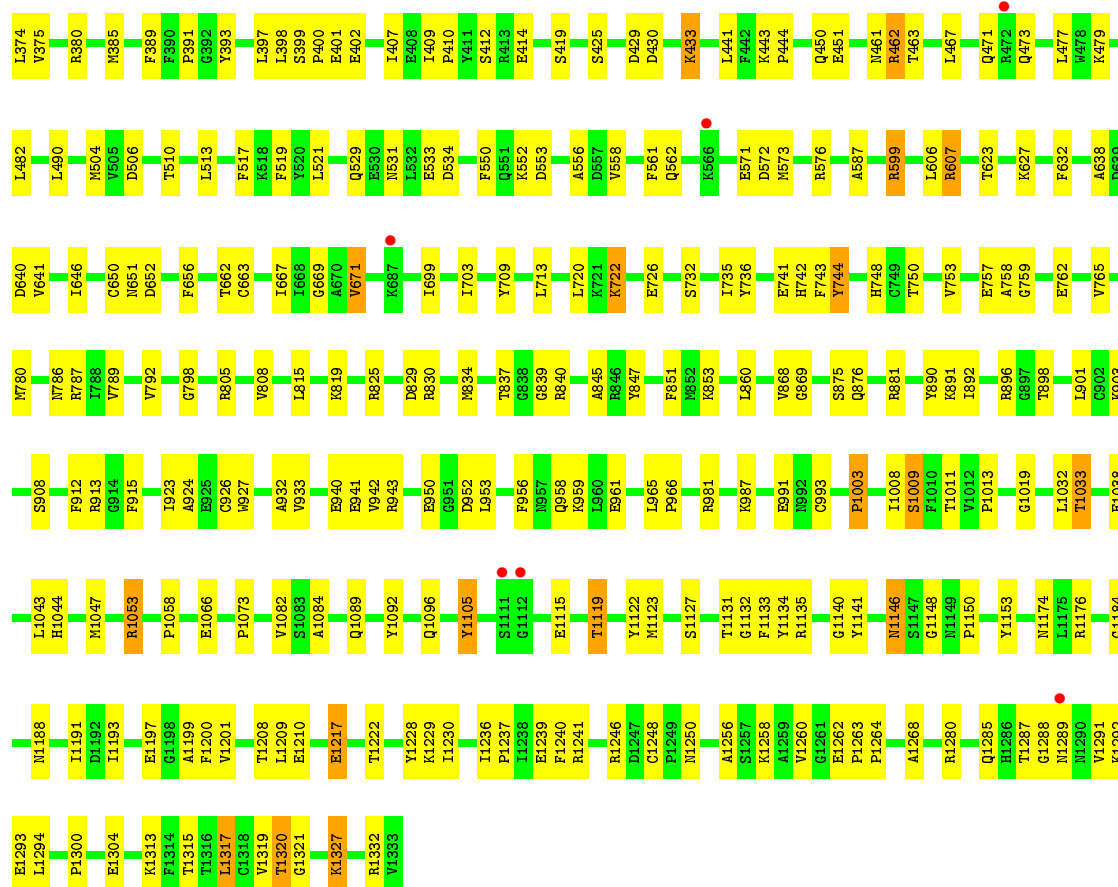
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 9 | A | 234 | Total | O | 0 | 0 |
| | | | 234 | 234 | | |
| 9 | B | 245 | Total | O | 0 | 0 |
| | | | 245 | 245 | | |
| 9 | C | 237 | Total | O | 0 | 0 |
| | | | 237 | 237 | | |
| 9 | D | 233 | Total | O | 0 | 0 |
| | | | 233 | 233 | | |

• Molecule 1: Xanthine dehydrogenase/oxidase

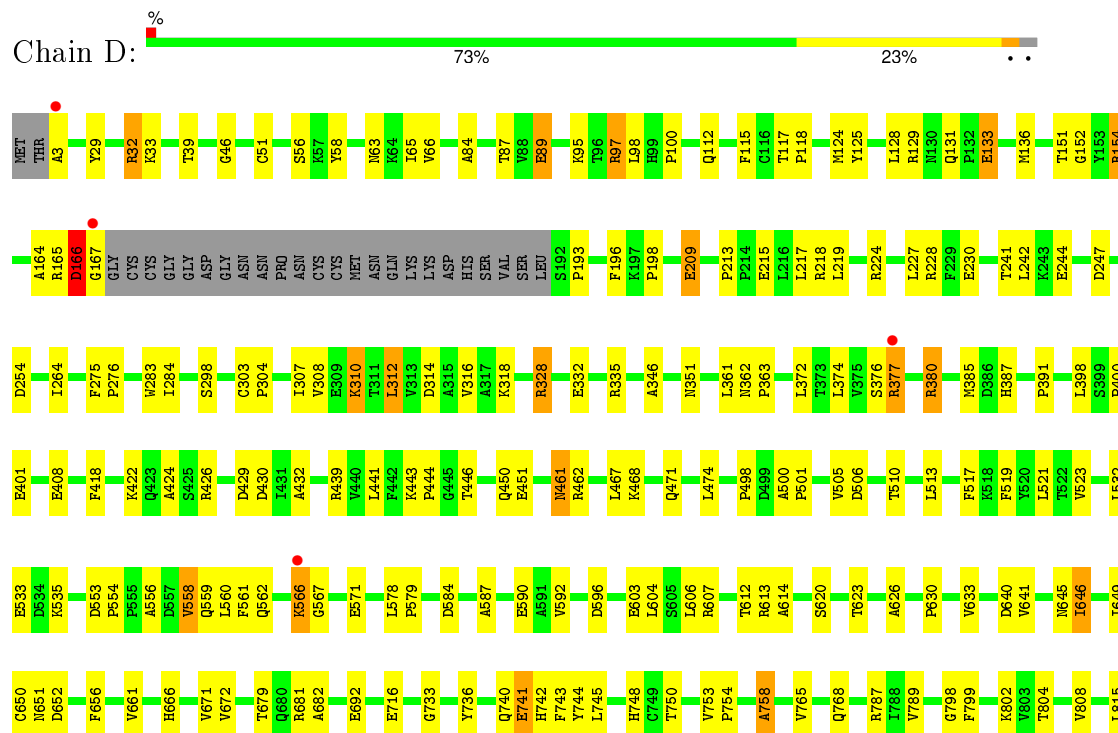


• Molecule 1: Xanthine dehydrogenase/oxidase





• Molecule 1: Xanthine dehydrogenase/oxidase



| | | | |
|-------|-------|-------|------|
| F1240 | K1106 | D952 | A816 |
| R1241 | K1107 | F956 | A817 |
| V1242 | K1108 | K1109 | W818 |
| S1243 | G1112 | P966 | W819 |
| R1246 | E1115 | E970 | R822 |
| N1250 | D1116 | E971 | P823 |
| K1251 | W1117 | Y978 | R830 |
| K1252 | V1118 | K982 | W834 |
| A1253 | T1119 | N989 | W837 |
| I1254 | M1123 | K996 | W841 |
| Y1255 | S1127 | R997 | R847 |
| A1256 | T1131 | G998 | W857 |
| S1257 | F1132 | L999 | L860 |
| E1262 | F1133 | G1000 | E861 |
| P1263 | Y1134 | I1001 | |
| P1264 | R1135 | I1002 | |
| L1265 | Y1141 | P1003 | W867 |
| | S1142 | I1008 | W868 |
| I1271 | F1143 | S1009 | D873 |
| D1277 | N1146 | L1021 | L878 |
| R1283 | P1150 | L1022 | W879 |
| H1286 | Y1163 | S1029 | E880 |
| T1287 | N1174 | H1034 | R881 |
| G1288 | I1193 | G1035 | R896 |
| N1289 | E1197 | T1037 | C902 |
| N1290 | G1198 | E1038 | N906 |
| V1291 | A1199 | M1039 | T910 |
| K1292 | F1200 | L1043 | A911 |
| E1293 | V1201 | H1044 | F912 |
| P1300 | L1204 | M1047 | R913 |
| A1301 | T1208 | Y1050 | G914 |
| T1302 | L1209 | S1052 | F915 |
| P1303 | S1215 | P1058 | A924 |
| T1315 | P1216 | T1059 | W927 |
| V1319 | E1217 | P1073 | E940 |
| T1320 | T1222 | A1079 | E941 |
| G1321 | A1232 | A1080 | W942 |
| V1322 | P1237 | S1081 | R943 |
| P1323 | I1238 | G1088 | R944 |
| E1324 | E1239 | Q1089 | L947 |
| N1325 | | | W948 |
| G1326 | | | R949 |
| K1327 | | | |
| P1328 | | | |
| V1331 | | | |
| R1332 | | | |
| V1333 | | | |

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 134.57Å 140.94Å 176.48Å 90.00° 91.49° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 2.60 49.47 – 2.58 | Depositor EDS |
| % Data completeness (in resolution range) | 95.0 (50.00-2.60) 94.0 (49.47-2.58) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.09 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.27 (at 2.58Å) | Xtriage |
| Refinement program | CNS 1.0 | Depositor |
| R, R_{free} | 0.192 , 0.246 0.190 , 0.242 | Depositor DCC |
| R_{free} test set | 3840 reflections (2.04%) | DCC |
| Wilson B-factor (Å ²) | 26.4 | Xtriage |
| Anisotropy | 0.154 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 45.2 | EDS |
| Estimated twinning fraction | 0.014 for -k,-h,-l 0.014 for k,h,-l 0.146 for h,-k,-l | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Outliers | 0 of 200786 reflections | Xtriage |
| F_o, F_c correlation | 0.93 | EDS |
| Total number of atoms | 41721 | wwPDB-VP |
| Average B, all atoms (Å ²) | 29.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAL, CA, FES, MOM, BCT, FAD, MTE

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 | 0.35 | 0/10303 | 0.62 | 0/13950 |
| 1 | B | 0.36 | 0/10303 | 0.63 | 1/13950 (0.0%) |
| 1 | C | 0.36 | 0/10303 | 0.62 | 0/13950 |
| 1 | D | 0.36 | 0/10303 | 0.62 | 0/13950 |
| All | All | 0.36 | 0/41212 | 0.63 | 1/55800 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | A | 0 | 1 |
| 1 | C | 0 | 1 |
| All | All | 0 | 2 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 1 | B | 1032 | LEU | CA-CB-CG | 5.62 | 128.22 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|-----------|
| 1 | A | 1105 | TYR | Sidechain |
| 1 | C | 1105 | TYR | Sidechain |

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 | 10088 | 0 | 10112 | 281 | 0 |
| 1 | B | 10088 | 0 | 10111 | 275 | 0 |
| 1 | C | 10088 | 0 | 10110 | 266 | 0 |
| 1 | D | 10088 | 0 | 10112 | 237 | 0 |
| 2 | A | 4 | 0 | 0 | 1 | 0 |
| 2 | B | 4 | 0 | 0 | 1 | 0 |
| 2 | C | 4 | 0 | 0 | 0 | 0 |
| 2 | D | 4 | 0 | 0 | 0 | 0 |
| 3 | A | 2 | 0 | 0 | 0 | 0 |
| 3 | B | 2 | 0 | 0 | 0 | 0 |
| 3 | C | 2 | 0 | 0 | 0 | 0 |
| 3 | D | 2 | 0 | 0 | 0 | 0 |
| 4 | A | 8 | 0 | 0 | 0 | 0 |
| 4 | B | 8 | 0 | 0 | 0 | 0 |
| 4 | C | 8 | 0 | 0 | 0 | 0 |
| 4 | D | 8 | 0 | 0 | 1 | 0 |
| 5 | A | 53 | 0 | 31 | 2 | 0 |
| 5 | B | 53 | 0 | 31 | 3 | 0 |
| 5 | C | 53 | 0 | 31 | 2 | 0 |
| 5 | D | 53 | 0 | 31 | 3 | 0 |
| 6 | A | 24 | 0 | 10 | 4 | 0 |
| 6 | B | 24 | 0 | 8 | 2 | 0 |
| 6 | C | 24 | 0 | 10 | 2 | 0 |
| 6 | D | 24 | 0 | 10 | 2 | 0 |
| 7 | A | 4 | 0 | 0 | 2 | 0 |
| 7 | B | 4 | 0 | 0 | 2 | 0 |
| 7 | C | 4 | 0 | 0 | 2 | 0 |
| 7 | D | 4 | 0 | 0 | 3 | 0 |
| 8 | A | 10 | 0 | 4 | 0 | 0 |
| 8 | B | 10 | 0 | 4 | 0 | 0 |
| 8 | C | 10 | 0 | 4 | 0 | 0 |
| 8 | D | 10 | 0 | 4 | 0 | 0 |
| 9 | A | 234 | 0 | 0 | 7 | 0 |
| 9 | B | 245 | 0 | 0 | 3 | 0 |
| 9 | C | 237 | 0 | 0 | 2 | 0 |
| 9 | D | 233 | 0 | 0 | 6 | 0 |
| All | All | 41721 | 0 | 40623 | 1063 | 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 13.

All (1063) 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) |
|-------------------|-------------------|--------------------------|-------------------|
| 6:A:2004:MTE:N5 | 6:A:2004:MTE:C9 | 1.68 | 1.52 |
| 6:C:4004:MTE:C9 | 6:C:4004:MTE:N5 | 1.68 | 1.51 |
| 1:A:133:GLU:HG2 | 1:A:165:ARG:HB3 | 1.40 | 1.03 |
| 1:D:1320:THR:HG23 | 1:D:1321:GLY:H | 1.26 | 1.00 |
| 1:A:3:ALA:HB1 | 1:A:228:ARG:H | 1.28 | 0.99 |
| 1:C:1287:THR:HG22 | 1:C:1288:GLY:H | 1.31 | 0.95 |
| 1:C:154:ARG:HD3 | 1:C:1197:GLU:OE2 | 1.67 | 0.93 |
| 1:C:956:PHE:HA | 1:C:1146:ASN:HD21 | 1.31 | 0.93 |
| 1:C:131:GLN:HE21 | 1:C:133:GLU:H | 1.15 | 0.92 |
| 1:B:558:VAL:HG22 | 1:B:1241:ARG:HG2 | 1.53 | 0.90 |
| 1:B:1141:TYR:HB2 | 1:B:1150:PRO:HG3 | 1.51 | 0.90 |
| 1:B:538:LYS:H | 1:B:538:LYS:HD2 | 1.36 | 0.89 |
| 1:D:314:ASP:O | 1:D:318:LYS:HD3 | 1.72 | 0.88 |
| 1:B:64:LYS:HD2 | 1:B:65:ILE:H | 1.38 | 0.88 |
| 1:D:264:ILE:HD11 | 5:D:5003:FAD:H3B | 1.56 | 0.87 |
| 1:B:3:ALA:HB1 | 1:B:228:ARG:H | 1.39 | 0.86 |
| 1:B:64:LYS:HD2 | 1:B:65:ILE:N | 1.91 | 0.86 |
| 1:C:558:VAL:HG22 | 1:C:1241:ARG:HG2 | 1.59 | 0.85 |
| 1:B:1313:LYS:O | 1:B:1317:LEU:HD23 | 1.77 | 0.84 |
| 1:B:1323:PRO:HG2 | 1:B:1326:CYS:HB3 | 1.62 | 0.82 |
| 1:D:741:GLU:HG3 | 1:D:834:MET:HG2 | 1.62 | 0.82 |
| 1:D:380:ARG:HH11 | 1:D:380:ARG:HB2 | 1.45 | 0.81 |
| 1:B:461:ASN:OD1 | 1:B:462:ARG:HD3 | 1.81 | 0.81 |
| 1:D:649:ILE:H | 1:D:649:ILE:HD12 | 1.45 | 0.80 |
| 1:D:671:VAL:HG11 | 1:D:682:ALA:HB3 | 1.63 | 0.79 |
| 1:A:558:VAL:HG22 | 1:A:1241:ARG:HG2 | 1.64 | 0.79 |
| 1:A:309:GLU:O | 1:A:313:VAL:HG12 | 1.82 | 0.79 |
| 1:C:133:GLU:HG2 | 1:C:165:ARG:HB2 | 1.64 | 0.79 |
| 1:C:736:TYR:CE2 | 1:C:1332:ARG:HD2 | 2.19 | 0.78 |
| 1:D:154:ARG:HD3 | 1:D:1197:GLU:OE2 | 1.83 | 0.78 |
| 1:C:556:ALA:HB3 | 1:C:1239:GLU:HG2 | 1.65 | 0.78 |
| 1:D:646:ILE:HD11 | 1:D:651:ASN:ND2 | 1.98 | 0.78 |
| 1:B:538:LYS:N | 1:B:538:LYS:HD2 | 1.99 | 0.78 |
| 1:B:480:GLU:CD | 1:B:480:GLU:H | 1.85 | 0.78 |
| 1:C:667:ILE:HD12 | 1:C:808:VAL:HG22 | 1.65 | 0.78 |
| 1:B:193:PRO:HG2 | 1:B:561:PHE:CE2 | 2.20 | 0.77 |
| 1:D:125:TYR:OH | 1:D:209:GLU:HG3 | 1.85 | 0.75 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:215:GLU:HG3 | 1:C:218:ARG:HH22 | 1.51 | 0.75 |
| 1:D:424:ALA:HB1 | 1:D:430:ASP:OD2 | 1.87 | 0.75 |
| 1:D:646:ILE:HD11 | 1:D:651:ASN:CG | 2.06 | 0.74 |
| 1:A:956:PHE:HA | 1:A:1146:ASN:HD21 | 1.51 | 0.74 |
| 1:A:741:GLU:HG3 | 1:A:834:MET:HG2 | 1.68 | 0.74 |
| 1:A:376:SER:HB3 | 1:A:379:THR:OG1 | 1.87 | 0.74 |
| 1:D:649:ILE:N | 1:D:649:ILE:HD12 | 2.03 | 0.74 |
| 1:D:506:ASP:OD1 | 1:D:1320:THR:HG22 | 1.87 | 0.74 |
| 1:C:748:HIS:CD2 | 1:C:837:THR:HG21 | 2.23 | 0.74 |
| 1:C:987:LYS:O | 1:C:991:GLU:HG3 | 1.88 | 0.73 |
| 1:C:374:LEU:HD13 | 1:C:398:LEU:HD13 | 1.71 | 0.73 |
| 1:D:372:LEU:HD11 | 1:D:385:MET:HE2 | 1.71 | 0.73 |
| 1:A:36:LEU:HD22 | 1:A:89:GLU:HG3 | 1.71 | 0.73 |
| 1:C:1115:GLU:O | 1:C:1119:THR:HG23 | 1.88 | 0.72 |
| 1:C:125:TYR:OH | 1:C:209:GLU:HG3 | 1.90 | 0.72 |
| 1:C:374:LEU:HD22 | 1:C:398:LEU:HD11 | 1.72 | 0.72 |
| 1:B:374:LEU:HD22 | 1:B:398:LEU:HD21 | 1.71 | 0.72 |
| 1:D:736:TYR:CE2 | 1:D:1332:ARG:HD2 | 2.24 | 0.72 |
| 1:C:477:LEU:HD23 | 1:C:479:LYS:HE3 | 1.71 | 0.71 |
| 1:B:241:THR:OG1 | 1:B:244:GLU:HG3 | 1.91 | 0.71 |
| 1:A:1204:LEU:HD13 | 1:A:1271:ILE:HD12 | 1.70 | 0.71 |
| 1:C:433:LYS:HE2 | 1:C:504:MET:SD | 2.30 | 0.71 |
| 1:D:1036:GLY:HA3 | 1:D:1043:LEU:HD21 | 1.72 | 0.71 |
| 1:D:867:ASN:ND2 | 1:D:1333:VAL:HG13 | 2.06 | 0.71 |
| 1:D:374:LEU:HD13 | 1:D:398:LEU:HD22 | 1.72 | 0.71 |
| 1:D:310:LYS:HE2 | 1:D:310:LYS:HA | 1.71 | 0.71 |
| 1:B:1115:GLU:O | 1:B:1119:THR:HG23 | 1.90 | 0.70 |
| 1:C:981:ARG:NH1 | 1:C:1176:ARG:HD3 | 2.06 | 0.70 |
| 1:B:215:GLU:HA | 1:B:218:ARG:NH1 | 2.06 | 0.70 |
| 1:A:97:ARG:HB2 | 1:A:97:ARG:NH1 | 2.07 | 0.70 |
| 1:B:953:LEU:HD23 | 1:B:959:LYS:HA | 1.73 | 0.70 |
| 1:C:97:ARG:HB2 | 1:C:97:ARG:NH1 | 2.07 | 0.70 |
| 1:D:164:ALA:C | 1:D:166:ASP:H | 1.95 | 0.70 |
| 1:D:623:THR:HG22 | 1:D:623:THR:O | 1.92 | 0.69 |
| 1:D:312:LEU:O | 1:D:316:VAL:HG23 | 1.92 | 0.69 |
| 1:B:649:ILE:HD11 | 1:B:804:THR:HG21 | 1.75 | 0.69 |
| 1:B:765:VAL:O | 1:B:792:VAL:HG22 | 1.93 | 0.69 |
| 1:B:125:TYR:OH | 1:B:209:GLU:HG3 | 1.93 | 0.69 |
| 6:C:4004:MTE:C6 | 6:C:4004:MTE:C9 | 2.69 | 0.68 |
| 1:D:559:GLN:HB3 | 1:D:1193:ILE:HD13 | 1.76 | 0.68 |
| 1:D:193:PRO:HG2 | 1:D:561:PHE:CE2 | 2.28 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:753:VAL:HG13 | 1:B:762:GLU:HB3 | 1.74 | 0.68 |
| 1:C:765:VAL:O | 1:C:792:VAL:HG22 | 1.93 | 0.68 |
| 1:B:956:PHE:HA | 1:B:1146:ASN:HD21 | 1.58 | 0.68 |
| 1:B:736:TYR:CD2 | 1:B:1332:ARG:HD2 | 2.28 | 0.68 |
| 1:C:1250:ASN:O | 1:C:1256:ALA:HA | 1.94 | 0.68 |
| 1:A:154:ARG:HD3 | 1:A:1197:GLU:OE2 | 1.93 | 0.68 |
| 1:D:1320:THR:HG23 | 1:D:1321:GLY:N | 2.05 | 0.67 |
| 1:A:1135:ARG:HD3 | 1:B:1125:THR:OG1 | 1.94 | 0.67 |
| 1:B:3:ALA:HA | 1:B:227:LEU:HD22 | 1.77 | 0.67 |
| 6:A:2004:MTE:C6 | 6:A:2004:MTE:C9 | 2.73 | 0.67 |
| 1:C:215:GLU:HG3 | 1:C:218:ARG:NH2 | 2.08 | 0.67 |
| 1:C:322:GLN:HA | 1:C:322:GLN:HE21 | 1.60 | 0.67 |
| 1:D:1141:TYR:HB2 | 1:D:1150:PRO:HG3 | 1.76 | 0.67 |
| 1:D:956:PHE:HA | 1:D:1146:ASN:HD21 | 1.59 | 0.67 |
| 1:A:103:GLU:OE2 | 1:A:202:THR:HG23 | 1.95 | 0.67 |
| 1:A:351:ASN:ND2 | 1:A:361:LEU:HB2 | 2.11 | 0.67 |
| 1:B:552:LYS:O | 1:B:553:ASP:HB2 | 1.95 | 0.67 |
| 1:B:623:THR:HG22 | 1:B:623:THR:O | 1.94 | 0.66 |
| 1:C:741:GLU:HG3 | 1:C:834:MET:HG2 | 1.77 | 0.66 |
| 1:A:441:LEU:HB3 | 1:A:451:GLU:HB2 | 1.77 | 0.66 |
| 1:B:656:PHE:HE2 | 1:B:815:LEU:HD23 | 1.60 | 0.66 |
| 1:D:1204:LEU:HD13 | 1:D:1271:ILE:HD12 | 1.78 | 0.66 |
| 1:C:164:ALA:C | 1:C:166:ASP:H | 1.99 | 0.66 |
| 1:C:993:CYS:HA | 1:C:1285:GLN:HE22 | 1.60 | 0.66 |
| 1:B:472:ARG:HD2 | 1:B:485:ASP:OD1 | 1.95 | 0.66 |
| 1:A:604:LEU:HD21 | 1:A:822:ARG:NH2 | 2.10 | 0.66 |
| 1:B:1089:GLN:HG2 | 1:B:1134:TYR:CD1 | 2.31 | 0.65 |
| 1:C:1320:THR:HG23 | 1:C:1321:GLY:H | 1.61 | 0.65 |
| 1:A:748:HIS:CD2 | 1:A:837:THR:HG21 | 2.31 | 0.65 |
| 1:B:309:GLU:O | 1:B:313:VAL:HG13 | 1.96 | 0.65 |
| 1:B:748:HIS:CD2 | 1:B:837:THR:HG21 | 2.31 | 0.65 |
| 1:C:881:ARG:HD2 | 1:C:915:PHE:HB3 | 1.77 | 0.65 |
| 1:D:578:LEU:HD12 | 1:D:579:PRO:HD2 | 1.79 | 0.65 |
| 1:A:473:GLN:HA | 1:A:476:LYS:HD3 | 1.79 | 0.65 |
| 1:D:328:ARG:HH11 | 1:D:328:ARG:HG2 | 1.60 | 0.65 |
| 1:A:400:PRO:HG2 | 1:A:401:GLU:OE2 | 1.97 | 0.65 |
| 1:D:604:LEU:HD21 | 1:D:822:ARG:NH2 | 2.12 | 0.65 |
| 1:B:95:LYS:HG3 | 1:B:590:GLU:OE2 | 1.97 | 0.64 |
| 1:D:944:ARG:O | 1:D:947:LEU:HB2 | 1.97 | 0.64 |
| 1:D:32:ARG:HH11 | 1:D:32:ARG:HG3 | 1.62 | 0.64 |
| 1:D:446:THR:HB | 1:D:535:LYS:NZ | 2.12 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:64:LYS:CD | 1:B:65:ILE:H | 2.08 | 0.64 |
| 1:B:255:ALA:HB2 | 1:B:277:MET:HG2 | 1.79 | 0.64 |
| 1:A:3:ALA:CB | 1:A:228:ARG:H | 2.06 | 0.64 |
| 1:A:1135:ARG:HH12 | 1:A:1137:PRO:HB3 | 1.63 | 0.64 |
| 1:B:531:ASN:O | 1:B:532:LEU:HD12 | 1.97 | 0.64 |
| 1:D:1174:ASN:O | 1:D:1237:PRO:HA | 1.97 | 0.64 |
| 1:A:64:LYS:HE2 | 1:A:65:ILE:H | 1.62 | 0.64 |
| 1:D:649:ILE:H | 1:D:649:ILE:CD1 | 2.11 | 0.64 |
| 1:B:1141:TYR:CB | 1:B:1150:PRO:HG3 | 2.26 | 0.64 |
| 1:B:218:ARG:HH11 | 1:B:218:ARG:CB | 2.11 | 0.64 |
| 1:D:193:PRO:HG2 | 1:D:561:PHE:CZ | 2.33 | 0.64 |
| 1:C:933:VAL:HG11 | 1:C:1280:ARG:HH21 | 1.63 | 0.64 |
| 1:D:241:THR:OG1 | 1:D:244:GLU:HG3 | 1.97 | 0.63 |
| 1:C:1287:THR:HG22 | 1:C:1288:GLY:N | 2.09 | 0.63 |
| 1:D:1115:GLU:O | 1:D:1119:THR:HG22 | 1.98 | 0.63 |
| 1:C:667:ILE:HD12 | 1:C:808:VAL:CG2 | 2.28 | 0.63 |
| 1:B:389:PHE:HA | 1:B:397:LEU:HG | 1.80 | 0.63 |
| 1:C:389:PHE:HA | 1:C:397:LEU:HG | 1.81 | 0.63 |
| 1:A:987:LYS:O | 1:A:991:GLU:HG3 | 1.99 | 0.63 |
| 1:C:1293:GLU:HG2 | 1:C:1294:LEU:N | 2.14 | 0.62 |
| 1:D:748:HIS:CD2 | 1:D:837:THR:HG21 | 2.34 | 0.62 |
| 1:A:1008:ILE:O | 1:A:1009:SER:HB2 | 1.98 | 0.62 |
| 1:A:131:GLN:HE21 | 1:A:133:GLU:H | 1.48 | 0.62 |
| 1:D:607:ARG:NH1 | 1:D:679:THR:OG1 | 2.32 | 0.62 |
| 1:C:1011:THR:O | 1:C:1013:PRO:HD3 | 1.99 | 0.62 |
| 1:A:125:TYR:OH | 1:A:209:GLU:HG3 | 2.00 | 0.62 |
| 1:A:1089:GLN:HG2 | 1:A:1134:TYR:CD1 | 2.35 | 0.62 |
| 1:A:722:LYS:O | 1:A:726:GLU:HG3 | 1.99 | 0.62 |
| 7:D:5005:MOM:MO1 | 7:D:5005:MOM:OM2 | 1.71 | 0.62 |
| 1:C:933:VAL:HG11 | 1:C:1280:ARG:NH2 | 2.15 | 0.62 |
| 1:C:103:GLU:OE2 | 1:C:202:THR:HG23 | 2.00 | 0.62 |
| 1:A:981:ARG:HH11 | 1:A:981:ARG:HB3 | 1.64 | 0.62 |
| 1:B:1216:PRO:HG2 | 1:B:1327:LYS:CD | 2.29 | 0.61 |
| 1:B:949:LYS:HG2 | 1:B:952:ASP:OD2 | 2.00 | 0.61 |
| 1:C:958:GLN:OE1 | 1:C:1150:PRO:HD2 | 2.01 | 0.61 |
| 1:D:303:CYS:SG | 1:D:307:ILE:HD11 | 2.40 | 0.61 |
| 1:C:1313:LYS:O | 1:C:1317:LEU:HD23 | 2.01 | 0.61 |
| 7:C:4005:MOM:OM2 | 7:C:4005:MOM:MO1 | 1.72 | 0.61 |
| 7:A:2005:MOM:MO1 | 7:A:2005:MOM:OM2 | 1.72 | 0.61 |
| 1:A:1313:LYS:O | 1:A:1317:LEU:HD23 | 2.01 | 0.61 |
| 1:D:754:PRO:HD3 | 1:D:817:ALA:HB1 | 1.83 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:1280:ARG:HH11 | 1:A:1280:ARG:HG2 | 1.66 | 0.61 |
| 1:A:443:LYS:HG3 | 1:A:448:GLU:HG3 | 1.82 | 0.61 |
| 1:D:131:GLN:HE21 | 1:D:133:GLU:H | 1.49 | 0.61 |
| 1:A:528:GLY:HA2 | 1:A:533:GLU:HB3 | 1.82 | 0.61 |
| 1:D:971:GLU:HG2 | 9:D:7225:HOH:O | 2.00 | 0.61 |
| 1:B:722:LYS:O | 1:B:726:GLU:HG3 | 2.01 | 0.61 |
| 1:C:868:VAL:HB | 1:C:875:SER:OG | 2.01 | 0.60 |
| 7:A:2005:MOM:OM3 | 7:A:2005:MOM:MO1 | 1.72 | 0.60 |
| 1:A:735:ILE:O | 1:A:735:ILE:HD12 | 2.01 | 0.60 |
| 1:A:3:ALA:HA | 1:A:227:LEU:HD22 | 1.82 | 0.60 |
| 7:C:4005:MOM:MO1 | 7:C:4005:MOM:OM3 | 1.72 | 0.60 |
| 1:C:753:VAL:CG2 | 1:C:762:GLU:HB3 | 2.31 | 0.60 |
| 1:D:982:LYS:HG2 | 1:D:999:LEU:HD23 | 1.83 | 0.60 |
| 1:D:1324:GLU:O | 1:D:1325:ASN:HB2 | 2.02 | 0.60 |
| 1:C:623:THR:O | 1:C:627:LYS:HG3 | 2.01 | 0.60 |
| 7:B:3005:MOM:MO1 | 7:B:3005:MOM:OM2 | 1.72 | 0.60 |
| 7:D:5005:MOM:MO1 | 7:D:5005:MOM:OM3 | 1.72 | 0.60 |
| 1:C:638:ALA:O | 1:C:641:VAL:HG22 | 2.02 | 0.60 |
| 1:A:304:PRO:HD2 | 1:A:307:ILE:HD12 | 1.83 | 0.60 |
| 1:A:1332:ARG:HH11 | 1:A:1332:ARG:HG2 | 1.67 | 0.60 |
| 1:D:671:VAL:HG11 | 1:D:682:ALA:CB | 2.30 | 0.60 |
| 1:D:372:LEU:HD11 | 1:D:385:MET:CE | 2.32 | 0.60 |
| 1:C:310:LYS:HE2 | 1:C:310:LYS:HA | 1.84 | 0.59 |
| 7:B:3005:MOM:MO1 | 7:B:3005:MOM:OM3 | 1.73 | 0.59 |
| 1:A:562:GLN:HG3 | 1:A:1246:ARG:CZ | 2.32 | 0.59 |
| 1:A:1100:LYS:O | 1:A:1100:LYS:HE3 | 2.01 | 0.59 |
| 1:A:3:ALA:HB1 | 1:A:228:ARG:N | 2.10 | 0.59 |
| 1:A:322:GLN:O | 1:A:412:SER:HB3 | 2.02 | 0.59 |
| 1:D:566:LYS:HD3 | 1:D:567:GLY:N | 2.17 | 0.59 |
| 1:A:30:LEU:HD23 | 1:A:34:LEU:HD12 | 1.84 | 0.59 |
| 1:B:328:ARG:HG2 | 1:B:328:ARG:HH11 | 1.67 | 0.59 |
| 1:C:131:GLN:HE21 | 1:C:133:GLU:N | 1.95 | 0.59 |
| 1:C:1008:ILE:O | 1:C:1009:SER:HB2 | 2.01 | 0.59 |
| 1:C:1141:TYR:HB2 | 1:C:1150:PRO:HG3 | 1.83 | 0.59 |
| 1:B:649:ILE:HD11 | 1:B:804:THR:CG2 | 2.31 | 0.59 |
| 1:A:720:LEU:HD11 | 1:A:896:ARG:CB | 2.33 | 0.59 |
| 1:B:259:VAL:HG11 | 1:B:347:SER:HB3 | 1.84 | 0.59 |
| 1:A:613:ARG:HH11 | 1:A:692:GLU:HG3 | 1.66 | 0.59 |
| 1:D:242:LEU:HA | 1:D:284:ILE:HD13 | 1.83 | 0.59 |
| 1:A:638:ALA:O | 1:A:641:VAL:HG22 | 2.02 | 0.59 |
| 1:A:389:PHE:HA | 1:A:397:LEU:HG | 1.85 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:613:ARG:NH1 | 1:A:692:GLU:HG3 | 2.18 | 0.59 |
| 1:C:1043:LEU:O | 1:C:1047:MET:HG2 | 2.03 | 0.59 |
| 1:C:1280:ARG:NH2 | 1:C:1293:GLU:O | 2.36 | 0.58 |
| 1:D:471:GLN:NE2 | 1:D:474:LEU:HD11 | 2.18 | 0.58 |
| 1:C:400:PRO:HG2 | 1:C:401:GLU:OE2 | 2.03 | 0.58 |
| 1:B:267:GLU:HA | 1:B:271:LYS:HG2 | 1.83 | 0.58 |
| 1:C:1089:GLN:HG2 | 1:C:1134:TYR:CD1 | 2.38 | 0.58 |
| 1:A:197:LYS:HD2 | 1:A:200:GLU:OE2 | 2.03 | 0.58 |
| 1:A:881:ARG:HD2 | 1:A:915:PHE:HB3 | 1.86 | 0.58 |
| 1:D:656:PHE:HE2 | 1:D:815:LEU:HD23 | 1.66 | 0.58 |
| 1:B:131:GLN:HE21 | 1:B:133:GLU:H | 1.51 | 0.58 |
| 1:D:860:LEU:HD12 | 1:D:861:GLU:H | 1.68 | 0.58 |
| 1:B:558:VAL:CG2 | 1:B:1241:ARG:HG2 | 2.30 | 0.58 |
| 1:D:1324:GLU:CD | 1:D:1325:ASN:H | 2.06 | 0.58 |
| 1:C:407:ILE:HD12 | 1:C:407:ILE:N | 2.19 | 0.58 |
| 1:A:443:LYS:HG3 | 1:A:448:GLU:CG | 2.33 | 0.58 |
| 1:D:215:GLU:O | 1:D:219:LEU:HG | 2.03 | 0.58 |
| 1:D:418:PHE:CD1 | 1:D:439:ARG:HB2 | 2.38 | 0.58 |
| 1:C:965:LEU:HB3 | 1:C:966:PRO:HD3 | 1.85 | 0.58 |
| 1:A:1011:THR:O | 1:A:1013:PRO:HD3 | 2.04 | 0.58 |
| 1:D:1250:ASN:O | 1:D:1256:ALA:HA | 2.04 | 0.58 |
| 1:B:562:GLN:HG3 | 1:B:1246:ARG:HG2 | 1.86 | 0.58 |
| 1:D:351:ASN:ND2 | 1:D:361:LEU:HB2 | 2.19 | 0.58 |
| 1:C:1332:ARG:HH11 | 1:C:1332:ARG:HG2 | 1.69 | 0.58 |
| 1:D:1286:HIS:O | 1:D:1287:THR:HG23 | 2.03 | 0.58 |
| 1:B:304:PRO:HA | 1:B:346:ALA:O | 2.02 | 0.58 |
| 1:A:245:LEU:HD11 | 1:A:257:LEU:HD11 | 1.86 | 0.58 |
| 1:C:1153:TYR:CE1 | 1:C:1258:LYS:HG2 | 2.39 | 0.58 |
| 1:B:1034:HIS:HB2 | 1:B:1087:ASN:HD22 | 1.69 | 0.58 |
| 1:B:880:GLU:HG2 | 1:B:1143:PHE:CZ | 2.39 | 0.58 |
| 1:C:1222:THR:HG22 | 1:C:1228:TYR:HB2 | 1.86 | 0.58 |
| 1:D:641:VAL:HG21 | 1:D:645:ASN:HB2 | 1.85 | 0.57 |
| 1:B:649:ILE:CD1 | 1:B:804:THR:HG21 | 2.34 | 0.57 |
| 1:A:786:ASN:ND2 | 1:B:1029:SER:HB2 | 2.19 | 0.57 |
| 1:D:868:VAL:HG13 | 1:D:902:CYS:O | 2.04 | 0.57 |
| 1:B:559:GLN:HB3 | 1:B:1193:ILE:HD13 | 1.86 | 0.57 |
| 1:B:1287:THR:HG22 | 1:B:1288:GLY:N | 2.19 | 0.57 |
| 1:D:510:THR:HG21 | 1:D:1315:THR:HG22 | 1.86 | 0.57 |
| 1:B:374:LEU:HD22 | 1:B:398:LEU:CD2 | 2.35 | 0.57 |
| 1:C:713:LEU:HD21 | 1:C:876:GLN:HE21 | 1.70 | 0.57 |
| 1:B:372:LEU:HD11 | 1:B:385:MET:CE | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:152:GLY:O | 1:B:1236:ILE:HG21 | 2.05 | 0.57 |
| 1:B:996:LYS:NZ | 1:B:1285:GLN:HE22 | 2.03 | 0.57 |
| 1:A:645:ASN:O | 1:A:654:THR:HA | 2.05 | 0.57 |
| 1:A:1280:ARG:NH2 | 1:A:1293:GLU:O | 2.32 | 0.56 |
| 1:A:215:GLU:HG3 | 1:A:218:ARG:HH22 | 1.70 | 0.56 |
| 1:B:375:VAL:HG12 | 1:B:380:ARG:HG3 | 1.86 | 0.56 |
| 1:A:720:LEU:HD11 | 1:A:896:ARG:HB3 | 1.87 | 0.56 |
| 1:D:553:ASP:HB3 | 1:D:554:PRO:HD2 | 1.85 | 0.56 |
| 1:A:606:LEU:HD23 | 1:A:606:LEU:C | 2.26 | 0.56 |
| 1:C:504:MET:HG2 | 1:C:1304:GLU:OE2 | 2.04 | 0.56 |
| 1:B:743:PHE:HA | 1:B:830:ARG:HH21 | 1.70 | 0.56 |
| 1:A:367:ALA:O | 1:A:439:ARG:HD3 | 2.05 | 0.56 |
| 1:A:479:LYS:HG2 | 1:A:537:GLY:N | 2.21 | 0.56 |
| 1:C:32:ARG:HD2 | 9:C:7058:HOH:O | 2.04 | 0.56 |
| 1:C:735:ILE:O | 1:C:735:ILE:HD12 | 2.06 | 0.56 |
| 1:C:328:ARG:HH11 | 1:C:328:ARG:HG2 | 1.70 | 0.56 |
| 1:C:131:GLN:NE2 | 1:C:133:GLU:H | 1.95 | 0.56 |
| 1:D:881:ARG:HD2 | 1:D:915:PHE:HB3 | 1.86 | 0.56 |
| 1:C:662:THR:O | 1:C:663:CYS:HB3 | 2.05 | 0.56 |
| 1:B:1174:ASN:O | 1:B:1237:PRO:HA | 2.06 | 0.56 |
| 1:B:1216:PRO:HG2 | 1:B:1327:LYS:HD2 | 1.88 | 0.56 |
| 1:B:809:VAL:O | 1:B:813:VAL:HG23 | 2.05 | 0.56 |
| 1:A:650:CYS:HB2 | 1:A:652:ASP:OD2 | 2.05 | 0.56 |
| 1:B:215:GLU:HA | 1:B:218:ARG:HH11 | 1.69 | 0.56 |
| 1:B:1216:PRO:HG2 | 1:B:1327:LYS:HD3 | 1.88 | 0.56 |
| 1:C:193:PRO:HG2 | 1:C:561:PHE:CE2 | 2.41 | 0.56 |
| 1:A:505:VAL:HG21 | 1:A:1320:THR:HG21 | 1.86 | 0.56 |
| 1:A:622:ASP:HB3 | 1:A:687:LYS:HB3 | 1.87 | 0.56 |
| 1:C:1291:VAL:HG13 | 1:C:1292:LYS:HG3 | 1.88 | 0.56 |
| 1:A:510:THR:HG21 | 1:A:1315:THR:HG22 | 1.86 | 0.56 |
| 1:B:218:ARG:HH11 | 1:B:218:ARG:HB3 | 1.70 | 0.55 |
| 1:B:218:ARG:NH1 | 1:B:218:ARG:HB2 | 2.22 | 0.55 |
| 1:C:217:LEU:O | 1:C:220:LYS:HG2 | 2.07 | 0.55 |
| 1:B:720:LEU:HD11 | 1:B:896:ARG:HB3 | 1.89 | 0.55 |
| 1:B:1332:ARG:HH11 | 1:B:1332:ARG:HG2 | 1.71 | 0.55 |
| 1:A:374:LEU:HD13 | 1:A:398:LEU:CD2 | 2.37 | 0.55 |
| 1:A:477:LEU:HD23 | 1:A:479:LYS:HE2 | 1.87 | 0.55 |
| 1:A:667:ILE:HD12 | 1:A:808:VAL:HG13 | 1.89 | 0.55 |
| 1:C:372:LEU:CD2 | 1:C:407:ILE:HG23 | 2.36 | 0.55 |
| 1:A:712:GLU:N | 1:A:900:ARG:HH11 | 2.04 | 0.55 |
| 1:C:1127:SER:HB2 | 1:D:1133:PHE:CG | 2.42 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:623:THR:HG23 | 1:D:626:ALA:HB3 | 1.88 | 0.55 |
| 1:D:498:PRO:HG2 | 1:D:1323:PRO:CD | 2.37 | 0.55 |
| 1:C:1008:ILE:O | 1:C:1009:SER:CB | 2.55 | 0.55 |
| 1:D:880:GLU:HG2 | 1:D:1143:PHE:CZ | 2.41 | 0.55 |
| 1:A:124:MET:HE3 | 1:A:127:LEU:HD23 | 1.89 | 0.55 |
| 1:B:1204:LEU:O | 1:B:1204:LEU:HD12 | 2.06 | 0.55 |
| 1:A:507:PHE:HB2 | 1:A:1304:GLU:HG3 | 1.89 | 0.55 |
| 1:C:744:TYR:O | 1:C:830:ARG:NH2 | 2.31 | 0.55 |
| 1:C:558:VAL:CG2 | 1:C:1241:ARG:HG2 | 2.34 | 0.55 |
| 1:B:799:PHE:HA | 6:B:3004:MTE:S1' | 2.48 | 0.54 |
| 1:C:281:PRO:HB2 | 1:C:287:LEU:CD1 | 2.37 | 0.54 |
| 1:D:196:PHE:CE2 | 1:D:198:PRO:HG3 | 2.42 | 0.54 |
| 1:D:1290:ASN:ND2 | 1:D:1292:LYS:H | 2.05 | 0.54 |
| 1:B:603:GLU:HG3 | 1:B:823:PRO:HB2 | 1.88 | 0.54 |
| 1:A:1199:ALA:HB3 | 1:A:1264:PRO:HB2 | 1.89 | 0.54 |
| 1:A:473:GLN:HA | 1:A:476:LYS:CD | 2.36 | 0.54 |
| 1:A:656:PHE:HE2 | 1:A:815:LEU:HD23 | 1.71 | 0.54 |
| 1:D:535:LYS:O | 1:D:535:LYS:HG2 | 2.07 | 0.54 |
| 1:A:133:GLU:CG | 1:A:165:ARG:HB3 | 2.25 | 0.54 |
| 1:B:224:ARG:HH11 | 1:B:224:ARG:HG2 | 1.72 | 0.54 |
| 1:C:709:TYR:CZ | 1:C:903:LYS:HG3 | 2.43 | 0.54 |
| 1:B:322:GLN:HA | 1:B:322:GLN:OE1 | 2.07 | 0.54 |
| 1:B:538:LYS:H | 1:B:538:LYS:CD | 2.16 | 0.54 |
| 1:C:667:ILE:CD1 | 1:C:808:VAL:HG22 | 2.36 | 0.54 |
| 1:C:3:ALA:HB2 | 1:C:225:LYS:NZ | 2.23 | 0.54 |
| 1:D:95:LYS:HG3 | 1:D:590:GLU:OE2 | 2.07 | 0.54 |
| 1:C:1217:GLU:CD | 1:C:1217:GLU:H | 2.10 | 0.54 |
| 1:A:249:LYS:HD3 | 1:A:257:LEU:HD21 | 1.88 | 0.54 |
| 1:C:940:GLU:HG2 | 1:C:941:GLU:N | 2.22 | 0.54 |
| 1:A:241:THR:OG1 | 1:A:244:GLU:HG3 | 2.08 | 0.54 |
| 1:B:714:LYS:HD2 | 1:B:896:ARG:NH1 | 2.23 | 0.53 |
| 1:D:940:GLU:HG2 | 1:D:941:GLU:N | 2.22 | 0.53 |
| 1:C:891:LYS:HD2 | 1:C:952:ASP:OD2 | 2.09 | 0.53 |
| 1:A:550:PHE:CE2 | 1:A:552:LYS:HD2 | 2.42 | 0.53 |
| 1:C:473:GLN:NE2 | 1:C:482:LEU:HG | 2.23 | 0.53 |
| 1:B:996:LYS:NZ | 1:B:1285:GLN:NE2 | 2.56 | 0.53 |
| 1:B:1109:ASN:ND2 | 1:B:1112:GLY:HA3 | 2.23 | 0.53 |
| 1:A:150:CYS:HB3 | 6:A:2004:MTE:N2 | 2.24 | 0.53 |
| 1:A:87:THR:OG1 | 1:A:89:GLU:HG2 | 2.08 | 0.53 |
| 1:D:1324:GLU:CD | 1:D:1325:ASN:N | 2.62 | 0.53 |
| 1:D:758:ALA:HB1 | 1:D:787:ARG:HE | 1.72 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:616:ALA:HA | 1:A:693:LEU:HG | 1.90 | 0.53 |
| 1:A:958:GLN:OE1 | 1:A:1150:PRO:HD2 | 2.08 | 0.53 |
| 1:D:444:PRO:O | 1:D:446:THR:HG23 | 2.08 | 0.53 |
| 1:B:196:PHE:CE2 | 1:B:198:PRO:HG3 | 2.43 | 0.53 |
| 1:C:322:GLN:HA | 1:C:322:GLN:NE2 | 2.21 | 0.53 |
| 1:D:1263:PRO:HB2 | 1:D:1264:PRO:HD3 | 1.90 | 0.53 |
| 1:A:742:HIS:HA | 1:A:912:PHE:CE2 | 2.44 | 0.53 |
| 1:B:578:LEU:HD12 | 1:B:579:PRO:HD2 | 1.89 | 0.53 |
| 1:B:888:ASN:O | 1:B:1005:LYS:HE2 | 2.07 | 0.53 |
| 1:A:212:PHE:CE2 | 1:A:217:LEU:HD13 | 2.44 | 0.53 |
| 1:C:245:LEU:HD22 | 1:C:281:PRO:HB3 | 1.90 | 0.53 |
| 1:A:910:THR:OG1 | 1:A:911:ALA:N | 2.42 | 0.53 |
| 1:B:910:THR:OG1 | 1:B:911:ALA:N | 2.41 | 0.53 |
| 1:B:753:VAL:CG1 | 1:B:762:GLU:HB3 | 2.37 | 0.53 |
| 1:D:517:PHE:CZ | 1:D:521:LEU:HD11 | 2.43 | 0.53 |
| 1:C:441:LEU:HB3 | 1:C:451:GLU:HB2 | 1.90 | 0.53 |
| 1:D:1008:ILE:O | 1:D:1009:SER:CB | 2.56 | 0.53 |
| 1:B:881:ARG:HD2 | 1:B:915:PHE:O | 2.09 | 0.53 |
| 1:C:805:ARG:O | 1:C:808:VAL:HG12 | 2.07 | 0.53 |
| 1:C:164:ALA:C | 1:C:166:ASP:N | 2.59 | 0.53 |
| 1:A:253:PRO:HB3 | 1:A:400:PRO:HB2 | 1.91 | 0.53 |
| 1:A:124:MET:CE | 1:A:127:LEU:HD23 | 2.38 | 0.53 |
| 1:A:242:LEU:HA | 1:A:284:ILE:HD13 | 1.90 | 0.53 |
| 1:C:1332:ARG:HG2 | 1:C:1332:ARG:NH1 | 2.23 | 0.52 |
| 1:A:787:ARG:HG2 | 1:A:787:ARG:HH11 | 1.75 | 0.52 |
| 1:A:1135:ARG:O | 1:A:1135:ARG:HG3 | 2.09 | 0.52 |
| 1:A:1008:ILE:O | 1:A:1009:SER:CB | 2.57 | 0.52 |
| 1:B:996:LYS:HZ1 | 1:B:1285:GLN:NE2 | 2.07 | 0.52 |
| 1:D:881:ARG:HD2 | 1:D:915:PHE:O | 2.09 | 0.52 |
| 1:C:192:SER:N | 1:C:193:PRO:CD | 2.71 | 0.52 |
| 1:D:65:ILE:HD11 | 1:D:217:LEU:HD11 | 1.92 | 0.52 |
| 1:A:438:MET:HG2 | 1:A:454:LEU:HD22 | 1.90 | 0.52 |
| 1:B:754:PRO:HD3 | 1:B:817:ALA:HB1 | 1.92 | 0.52 |
| 1:A:364:VAL:HG13 | 1:A:418:PHE:CZ | 2.45 | 0.52 |
| 1:C:120:ILE:HD13 | 1:C:146:ASN:HB3 | 1.91 | 0.52 |
| 1:A:220:LYS:HE2 | 1:A:221:ASP:OD1 | 2.09 | 0.52 |
| 1:B:800:GLY:HA2 | 1:B:803:VAL:HG23 | 1.91 | 0.52 |
| 1:D:1332:ARG:HH11 | 1:D:1332:ARG:HG2 | 1.74 | 0.52 |
| 1:C:389:PHE:O | 1:C:391:PRO:HD3 | 2.09 | 0.52 |
| 1:A:462:ARG:HB3 | 9:A:7121:HOH:O | 2.09 | 0.52 |
| 1:A:3:ALA:HA | 1:A:227:LEU:CD2 | 2.39 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:505:VAL:HG23 | 1:B:506:ASP:N | 2.23 | 0.52 |
| 1:D:1300:PRO:HG2 | 1:D:1302:THR:HG23 | 1.90 | 0.52 |
| 1:D:949:LYS:HG2 | 1:D:952:ASP:OD2 | 2.09 | 0.52 |
| 1:B:422:LYS:HE3 | 1:B:432:ALA:HB2 | 1.92 | 0.52 |
| 1:C:375:VAL:HG12 | 1:C:380:ARG:HG3 | 1.92 | 0.52 |
| 1:B:218:ARG:CB | 1:B:218:ARG:NH1 | 2.72 | 0.52 |
| 1:A:1089:GLN:HG2 | 1:A:1134:TYR:CE1 | 2.45 | 0.52 |
| 1:A:881:ARG:HD2 | 1:A:915:PHE:O | 2.10 | 0.52 |
| 1:B:743:PHE:HA | 1:B:830:ARG:NH2 | 2.24 | 0.52 |
| 1:B:154:ARG:HD3 | 1:B:1197:GLU:OE2 | 2.10 | 0.52 |
| 1:D:467:LEU:O | 1:D:471:GLN:HB2 | 2.10 | 0.52 |
| 1:C:713:LEU:HD21 | 1:C:876:GLN:NE2 | 2.24 | 0.52 |
| 1:C:607:ARG:NH2 | 1:C:829:ASP:OD2 | 2.43 | 0.52 |
| 1:D:1208:THR:O | 1:D:1209:LEU:HD12 | 2.09 | 0.52 |
| 1:D:1038:GLU:HB2 | 1:D:1044:HIS:CD2 | 2.44 | 0.52 |
| 1:B:857:VAL:CG2 | 1:B:892:ILE:HG12 | 2.40 | 0.52 |
| 1:C:322:GLN:HG2 | 1:C:414:GLU:CD | 2.31 | 0.51 |
| 1:C:606:LEU:HD23 | 1:C:606:LEU:C | 2.31 | 0.51 |
| 1:C:736:TYR:CZ | 1:C:1332:ARG:HD2 | 2.45 | 0.51 |
| 1:B:389:PHE:O | 1:B:391:PRO:HD3 | 2.10 | 0.51 |
| 1:C:303:CYS:HB3 | 1:C:307:ILE:HD11 | 1.92 | 0.51 |
| 1:B:135:THR:OG1 | 1:B:138:GLU:HG3 | 2.11 | 0.51 |
| 1:C:517:PHE:CZ | 1:C:521:LEU:HD11 | 2.45 | 0.51 |
| 1:D:633:VAL:HB | 1:D:672:VAL:O | 2.11 | 0.51 |
| 1:D:443:LYS:HD2 | 1:D:450:GLN:NE2 | 2.24 | 0.51 |
| 1:A:1260:VAL:O | 1:A:1260:VAL:HG22 | 2.10 | 0.51 |
| 1:B:720:LEU:HD11 | 1:B:896:ARG:CB | 2.41 | 0.51 |
| 1:D:32:ARG:NH1 | 1:D:32:ARG:HG3 | 2.24 | 0.51 |
| 1:A:117:THR:CG2 | 1:A:587:ALA:HA | 2.40 | 0.51 |
| 1:A:531:ASN:HA | 1:A:533:GLU:OE1 | 2.11 | 0.51 |
| 1:C:224:ARG:HH11 | 1:C:224:ARG:HG2 | 1.75 | 0.51 |
| 1:C:646:ILE:O | 1:C:646:ILE:HG13 | 2.10 | 0.51 |
| 1:B:1179:ILE:HD11 | 1:B:1200:PHE:CD1 | 2.46 | 0.51 |
| 1:A:88:VAL:HG13 | 1:A:89:GLU:N | 2.26 | 0.51 |
| 1:A:981:ARG:HB3 | 1:A:981:ARG:NH1 | 2.26 | 0.51 |
| 1:A:389:PHE:HA | 1:A:397:LEU:CD1 | 2.41 | 0.51 |
| 1:C:490:LEU:HB2 | 1:C:513:LEU:HD22 | 1.93 | 0.51 |
| 1:C:510:THR:HG21 | 1:C:1315:THR:HG22 | 1.92 | 0.51 |
| 1:B:608:LEU:HD13 | 1:B:667:ILE:CD1 | 2.40 | 0.51 |
| 1:A:233:ARG:CZ | 1:A:681:ARG:HD3 | 2.41 | 0.51 |
| 1:C:956:PHE:CA | 1:C:1146:ASN:HD21 | 2.15 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1320:THR:HG23 | 1:C:1321:GLY:N | 2.26 | 0.51 |
| 1:B:1038:GLU:HB2 | 1:B:1044:HIS:CD2 | 2.46 | 0.51 |
| 1:C:787:ARG:HG2 | 1:C:787:ARG:HH11 | 1.76 | 0.51 |
| 1:D:136:MET:HE3 | 1:D:167:GLY:HA2 | 1.92 | 0.51 |
| 1:A:965:LEU:N | 1:A:966:PRO:CD | 2.74 | 0.51 |
| 1:A:953:LEU:HA | 1:A:958:GLN:O | 2.11 | 0.50 |
| 1:A:653:GLU:HB3 | 1:A:871:THR:CG2 | 2.41 | 0.50 |
| 1:B:1022:LEU:HD22 | 1:B:1098:ILE:HG13 | 1.93 | 0.50 |
| 1:A:750:THR:HG21 | 1:A:810:SER:HA | 1.93 | 0.50 |
| 1:A:1038:GLU:HB2 | 1:A:1044:HIS:CD2 | 2.46 | 0.50 |
| 1:D:1332:ARG:HG2 | 1:D:1332:ARG:NH1 | 2.26 | 0.50 |
| 1:D:1081:SER:OG | 1:D:1262:GLU:HG3 | 2.11 | 0.50 |
| 1:D:556:ALA:HB3 | 1:D:1239:GLU:HG2 | 1.93 | 0.50 |
| 1:A:553:ASP:HB3 | 1:A:554:PRO:HD2 | 1.93 | 0.50 |
| 1:B:374:LEU:CD2 | 1:B:398:LEU:HD21 | 2.41 | 0.50 |
| 1:A:1280:ARG:HH11 | 1:A:1280:ARG:CG | 2.24 | 0.50 |
| 1:D:1021:LEU:HD13 | 1:D:1131:THR:HG22 | 1.93 | 0.50 |
| 1:C:753:VAL:O | 1:C:753:VAL:HG23 | 2.12 | 0.50 |
| 1:B:915:PHE:HA | 2:B:6002:BCT:O3 | 2.12 | 0.50 |
| 1:D:400:PRO:HG2 | 1:D:401:GLU:OE2 | 2.11 | 0.50 |
| 1:D:1320:THR:CG2 | 1:D:1321:GLY:H | 2.09 | 0.50 |
| 1:B:607:ARG:HH11 | 1:B:680:GLN:N | 2.09 | 0.50 |
| 1:C:699:ILE:O | 1:C:703:ILE:HG13 | 2.11 | 0.50 |
| 1:C:531:ASN:HA | 1:C:533:GLU:OE1 | 2.11 | 0.50 |
| 1:D:716:GLU:HB2 | 1:D:896:ARG:HG3 | 1.93 | 0.50 |
| 1:A:491:ALA:O | 1:A:495:HIS:HB2 | 2.11 | 0.50 |
| 1:A:696:ILE:HG23 | 1:A:701:ASP:CB | 2.41 | 0.50 |
| 1:A:867:ASN:ND2 | 1:A:1333:VAL:HG13 | 2.26 | 0.50 |
| 1:A:1084:ALA:HB3 | 9:A:7178:HOH:O | 2.11 | 0.50 |
| 1:C:562:GLN:HG3 | 1:C:1246:ARG:CZ | 2.42 | 0.50 |
| 1:C:323:LYS:HA | 1:C:412:SER:O | 2.12 | 0.50 |
| 1:A:736:TYR:CD2 | 1:A:1332:ARG:HD2 | 2.46 | 0.50 |
| 1:B:881:ARG:HD2 | 1:B:915:PHE:HB3 | 1.93 | 0.50 |
| 1:B:104:ARG:HD3 | 1:B:201:PHE:CD2 | 2.47 | 0.50 |
| 1:B:932:ALA:HA | 1:B:942:VAL:HG21 | 1.93 | 0.50 |
| 1:B:3:ALA:O | 1:B:5:LYS:N | 2.41 | 0.50 |
| 1:A:1141:TYR:OH | 1:A:1146:ASN:ND2 | 2.45 | 0.50 |
| 1:A:65:ILE:HD12 | 1:A:212:PHE:CD2 | 2.46 | 0.50 |
| 1:D:58:TYR:OH | 1:D:63:ASN:ND2 | 2.45 | 0.50 |
| 1:B:1271:ILE:O | 1:B:1275:ILE:HG13 | 2.12 | 0.50 |
| 1:A:399:SER:HB2 | 1:A:400:PRO:HD2 | 1.93 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:399:SER:OG | 1:A:402:GLU:HG3 | 2.11 | 0.49 |
| 1:B:958:GLN:OE1 | 1:B:1150:PRO:HD2 | 2.12 | 0.49 |
| 1:D:380:ARG:HH11 | 1:D:380:ARG:CB | 2.22 | 0.49 |
| 1:A:212:PHE:HE2 | 1:A:217:LEU:HD13 | 1.75 | 0.49 |
| 1:B:986:ASP:O | 1:B:990:LYS:HG3 | 2.12 | 0.49 |
| 1:C:264:ILE:HD11 | 5:C:4003:FAD:H3B | 1.92 | 0.49 |
| 1:D:640:ASP:HB3 | 1:D:819:LYS:HE3 | 1.93 | 0.49 |
| 1:A:131:GLN:O | 1:A:134:PRO:HD3 | 2.12 | 0.49 |
| 1:B:374:LEU:HD13 | 1:B:398:LEU:CD2 | 2.41 | 0.49 |
| 1:B:623:THR:HG22 | 1:B:627:LYS:HG3 | 1.95 | 0.49 |
| 1:B:325:GLU:HB2 | 1:B:412:SER:OG | 2.11 | 0.49 |
| 1:A:572:ASP:OD1 | 1:A:1053:ARG:HD3 | 2.12 | 0.49 |
| 1:B:958:GLN:HG3 | 1:B:1149:ASN:OD1 | 2.12 | 0.49 |
| 1:C:322:GLN:HG2 | 1:C:414:GLU:OE1 | 2.12 | 0.49 |
| 1:B:530:GLU:O | 1:B:531:ASN:HB2 | 2.12 | 0.49 |
| 1:D:1324:GLU:OE2 | 1:D:1325:ASN:N | 2.45 | 0.49 |
| 1:D:1008:ILE:O | 1:D:1009:SER:HB2 | 2.11 | 0.49 |
| 1:A:1073:PRO:HD3 | 1:B:1023:HIS:CE1 | 2.47 | 0.49 |
| 1:D:224:ARG:HD3 | 1:D:283:TRP:CE3 | 2.47 | 0.49 |
| 1:B:1184:GLY:HA2 | 1:B:1248:CYS:O | 2.13 | 0.49 |
| 1:D:736:TYR:CZ | 1:D:1332:ARG:HD2 | 2.47 | 0.49 |
| 1:B:1083:SER:HB2 | 6:B:3004:MTE:O3P | 2.13 | 0.49 |
| 1:A:1050:VAL:HG13 | 1:A:1255:TYR:HE2 | 1.78 | 0.49 |
| 1:C:742:HIS:HA | 1:C:912:PHE:CZ | 2.48 | 0.49 |
| 1:B:1152:HIS:CE1 | 1:B:1252:LYS:HD2 | 2.47 | 0.49 |
| 1:C:430:ASP:CG | 1:C:1229:LYS:HE2 | 2.32 | 0.49 |
| 1:A:1033:THR:CG2 | 1:A:1066:GLU:O | 2.60 | 0.49 |
| 1:B:117:THR:HB | 1:B:118:PRO:HD3 | 1.94 | 0.49 |
| 1:B:372:LEU:HD11 | 1:B:385:MET:HE2 | 1.93 | 0.49 |
| 1:A:696:ILE:HG23 | 1:A:701:ASP:HB3 | 1.94 | 0.49 |
| 1:D:1001:ILE:HG23 | 1:D:1001:ILE:O | 2.12 | 0.49 |
| 1:B:374:LEU:HD13 | 1:B:398:LEU:HD23 | 1.93 | 0.49 |
| 1:A:712:GLU:N | 1:A:900:ARG:NH1 | 2.60 | 0.49 |
| 1:B:602:ASN:ND2 | 1:B:823:PRO:HD2 | 2.27 | 0.49 |
| 1:D:910:THR:OG1 | 1:D:911:ALA:N | 2.43 | 0.49 |
| 1:D:376:SER:O | 1:D:377:ARG:C | 2.50 | 0.49 |
| 1:B:5:LYS:HE3 | 1:B:16:VAL:HG13 | 1.93 | 0.49 |
| 1:B:1326:CYS:O | 1:B:1328:PRO:HD3 | 2.13 | 0.49 |
| 1:C:419:SER:HB2 | 1:C:519:PHE:CD1 | 2.47 | 0.49 |
| 1:D:1265:LEU:HD23 | 1:D:1265:LEU:C | 2.33 | 0.49 |
| 1:A:473:GLN:O | 1:A:476:LYS:HB2 | 2.13 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:1089:GLN:HG3 | 9:A:7061:HOH:O | 2.12 | 0.49 |
| 1:C:742:HIS:CE1 | 1:C:839:GLY:HA2 | 2.48 | 0.49 |
| 1:D:1283:ARG:HH21 | 1:D:1293:GLU:CD | 2.16 | 0.49 |
| 1:D:519:PHE:O | 1:D:523:VAL:HG23 | 2.13 | 0.49 |
| 1:A:58:TYR:OH | 1:A:63:ASN:ND2 | 2.45 | 0.49 |
| 1:B:193:PRO:HG2 | 1:B:561:PHE:CZ | 2.48 | 0.48 |
| 1:B:87:THR:OG1 | 1:B:89:GLU:HG2 | 2.13 | 0.48 |
| 1:C:1188:ASN:CG | 1:C:1191:ILE:HG12 | 2.33 | 0.48 |
| 1:D:742:HIS:HA | 1:D:912:PHE:CZ | 2.48 | 0.48 |
| 1:A:393:TYR:N | 1:A:461:ASN:HD21 | 2.11 | 0.48 |
| 1:B:556:ALA:HB3 | 1:B:1239:GLU:HG2 | 1.94 | 0.48 |
| 1:D:748:HIS:CE1 | 1:D:802:LYS:HG2 | 2.48 | 0.48 |
| 1:B:505:VAL:HG23 | 1:B:506:ASP:H | 1.77 | 0.48 |
| 1:A:1321:GLY:O | 1:A:1322:VAL:HB | 2.14 | 0.48 |
| 1:B:58:TYR:HE1 | 1:B:63:ASN:HD22 | 1.59 | 0.48 |
| 1:D:1089:GLN:HG2 | 1:D:1134:TYR:CD1 | 2.47 | 0.48 |
| 1:C:124:MET:HE3 | 1:C:127:LEU:HD23 | 1.96 | 0.48 |
| 1:A:1174:ASN:O | 1:A:1237:PRO:HA | 2.14 | 0.48 |
| 1:D:965:LEU:HB3 | 1:D:966:PRO:HD3 | 1.95 | 0.48 |
| 1:C:351:ASN:ND2 | 1:C:361:LEU:HB2 | 2.28 | 0.48 |
| 1:B:646:ILE:O | 1:B:646:ILE:HG13 | 2.12 | 0.48 |
| 1:C:868:VAL:O | 1:C:868:VAL:HG23 | 2.11 | 0.48 |
| 1:A:1263:PRO:HB2 | 1:A:1264:PRO:HD3 | 1.96 | 0.48 |
| 1:C:419:SER:HB2 | 1:C:519:PHE:HD1 | 1.79 | 0.48 |
| 1:B:1250:ASN:O | 1:B:1256:ALA:HA | 2.12 | 0.48 |
| 1:B:40:LYS:HB3 | 1:B:115:PHE:CZ | 2.48 | 0.48 |
| 1:A:131:GLN:NE2 | 1:A:133:GLU:H | 2.11 | 0.48 |
| 1:D:471:GLN:HE22 | 1:D:474:LEU:HD11 | 1.78 | 0.48 |
| 1:C:62:GLN:HB3 | 1:C:64:LYS:HG2 | 1.95 | 0.48 |
| 1:A:346:ALA:HB1 | 5:A:2003:FAD:H4' | 1.94 | 0.48 |
| 1:D:1331:VAL:HG22 | 1:D:1332:ARG:N | 2.28 | 0.48 |
| 1:A:653:GLU:HB3 | 1:A:871:THR:HG21 | 1.95 | 0.48 |
| 1:D:743:PHE:HA | 1:D:830:ARG:NH2 | 2.27 | 0.48 |
| 1:B:735:ILE:HD12 | 1:B:735:ILE:H | 1.79 | 0.48 |
| 1:C:1320:THR:OG1 | 1:C:1321:GLY:N | 2.45 | 0.48 |
| 1:C:1131:THR:HG23 | 1:D:1131:THR:HG23 | 1.94 | 0.48 |
| 1:A:1033:THR:HG21 | 9:A:7095:HOH:O | 2.13 | 0.48 |
| 1:D:912:PHE:O | 1:D:913:ARG:C | 2.51 | 0.48 |
| 1:C:709:TYR:HB2 | 1:C:901:LEU:HB2 | 1.95 | 0.48 |
| 1:A:623:THR:HG22 | 1:A:627:LYS:HG3 | 1.94 | 0.48 |
| 1:C:338:ALA:HA | 1:C:429:ASP:OD1 | 2.14 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1199:ALA:HB3 | 1:C:1264:PRO:HB2 | 1.96 | 0.48 |
| 1:C:1122:TYR:CD2 | 1:C:1123:MET:HE3 | 2.49 | 0.48 |
| 1:C:389:PHE:HD1 | 1:C:397:LEU:HD12 | 1.77 | 0.48 |
| 1:C:372:LEU:HD11 | 1:C:385:MET:CE | 2.44 | 0.48 |
| 1:D:603:GLU:HA | 1:D:823:PRO:HG2 | 1.95 | 0.48 |
| 1:D:351:ASN:HB2 | 5:D:5003:FAD:O4' | 2.14 | 0.48 |
| 1:B:736:TYR:CE2 | 1:B:1332:ARG:HD2 | 2.48 | 0.48 |
| 1:B:748:HIS:CE1 | 1:B:802:LYS:HG2 | 2.49 | 0.48 |
| 1:C:1009:SER:HA | 1:C:1082:VAL:HG11 | 1.94 | 0.48 |
| 1:C:786:ASN:OD1 | 1:C:787:ARG:NH1 | 2.47 | 0.48 |
| 1:C:97:ARG:HB2 | 1:C:97:ARG:CZ | 2.43 | 0.47 |
| 1:D:623:THR:CG2 | 1:D:623:THR:O | 2.61 | 0.47 |
| 1:C:1089:GLN:HB3 | 1:C:1134:TYR:CG | 2.49 | 0.47 |
| 1:D:228:ARG:HE | 1:D:230:GLU:CD | 2.17 | 0.47 |
| 1:D:646:ILE:HD12 | 1:D:646:ILE:C | 2.34 | 0.47 |
| 1:C:606:LEU:HD23 | 1:C:607:ARG:N | 2.29 | 0.47 |
| 1:C:287:LEU:O | 1:C:302:ALA:HB3 | 2.15 | 0.47 |
| 1:C:346:ALA:HB1 | 5:C:4003:FAD:H4' | 1.96 | 0.47 |
| 1:D:943:ARG:HD2 | 9:D:7129:HOH:O | 2.13 | 0.47 |
| 1:D:117:THR:HB | 1:D:118:PRO:HD3 | 1.95 | 0.47 |
| 1:C:27:LEU:HD21 | 1:C:41:LEU:HB2 | 1.96 | 0.47 |
| 1:D:799:PHE:HA | 6:D:5004:MTE:S1' | 2.54 | 0.47 |
| 1:C:736:TYR:CD2 | 1:C:1332:ARG:HD2 | 2.49 | 0.47 |
| 1:C:96:THR:OG1 | 1:C:97:ARG:N | 2.44 | 0.47 |
| 1:B:592:VAL:HG13 | 1:B:596:ASP:HB2 | 1.96 | 0.47 |
| 1:C:88:VAL:HG13 | 1:C:89:GLU:N | 2.29 | 0.47 |
| 1:B:1162:GLU:HG2 | 1:B:1175:LEU:HD12 | 1.96 | 0.47 |
| 1:A:1192:ASP:O | 1:A:1196:VAL:HG23 | 2.15 | 0.47 |
| 1:D:129:ARG:NE | 1:D:209:GLU:HG2 | 2.30 | 0.47 |
| 1:C:571:GLU:OE2 | 1:C:1058:PRO:HG3 | 2.14 | 0.47 |
| 1:B:786:ASN:OD1 | 1:B:787:ARG:NH1 | 2.46 | 0.47 |
| 1:B:517:PHE:CZ | 1:B:521:LEU:HD11 | 2.49 | 0.47 |
| 1:A:1288:GLY:O | 1:A:1289:ASN:HB3 | 2.13 | 0.47 |
| 1:B:741:GLU:HB3 | 1:B:1228:TYR:CE2 | 2.50 | 0.47 |
| 1:D:346:ALA:HB1 | 5:D:5003:FAD:H4' | 1.96 | 0.47 |
| 1:B:1119:THR:O | 1:B:1123:MET:HG2 | 2.14 | 0.47 |
| 1:D:247:ASP:OD1 | 1:D:377:ARG:HD3 | 2.15 | 0.47 |
| 1:D:115:PHE:HD2 | 1:D:745:LEU:HB3 | 1.80 | 0.47 |
| 1:A:363:PRO:HG2 | 1:A:435:THR:HG23 | 1.96 | 0.47 |
| 1:C:741:GLU:OE1 | 1:C:743:PHE:N | 2.46 | 0.47 |
| 1:A:845:ALA:CB | 1:A:923:ILE:HD13 | 2.44 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:3:ALA:HA | 1:D:227:LEU:CD2 | 2.44 | 0.47 |
| 1:B:510:THR:HG21 | 1:B:1315:THR:HG22 | 1.96 | 0.47 |
| 1:B:709:TYR:CE2 | 1:B:868:VAL:HG22 | 2.49 | 0.47 |
| 1:B:912:PHE:O | 1:B:913:ARG:C | 2.52 | 0.47 |
| 1:B:647:THR:HG23 | 1:B:648:GLY:N | 2.29 | 0.47 |
| 1:D:741:GLU:HG2 | 9:D:7119:HOH:O | 2.14 | 0.47 |
| 1:A:217:LEU:O | 1:A:220:LYS:HG2 | 2.15 | 0.47 |
| 1:C:253:PRO:HB3 | 1:C:400:PRO:HB2 | 1.97 | 0.47 |
| 1:B:1287:THR:HG22 | 1:B:1288:GLY:H | 1.80 | 0.47 |
| 1:A:124:MET:HE2 | 1:A:128:LEU:HG | 1.97 | 0.47 |
| 1:B:607:ARG:NH1 | 1:B:680:GLN:HB2 | 2.30 | 0.47 |
| 1:D:716:GLU:OE2 | 1:D:896:ARG:HD3 | 2.14 | 0.47 |
| 1:A:1033:THR:HG23 | 1:A:1066:GLU:O | 2.14 | 0.47 |
| 1:B:733:GLY:HA3 | 1:B:847:TYR:CZ | 2.50 | 0.47 |
| 1:B:741:GLU:HG2 | 1:B:834:MET:CE | 2.44 | 0.47 |
| 1:B:930:GLU:OE2 | 1:B:1294:LEU:HB3 | 2.15 | 0.47 |
| 1:C:1033:THR:HG23 | 1:C:1066:GLU:O | 2.14 | 0.47 |
| 1:B:535:LYS:HG2 | 1:B:535:LYS:O | 2.15 | 0.47 |
| 1:B:91:ILE:O | 1:B:99:HIS:HB2 | 2.15 | 0.47 |
| 1:A:224:ARG:HG2 | 1:A:224:ARG:HH11 | 1.80 | 0.47 |
| 1:A:1141:TYR:HB2 | 1:A:1150:PRO:HG3 | 1.97 | 0.47 |
| 1:C:322:GLN:O | 1:C:412:SER:HB3 | 2.15 | 0.47 |
| 1:C:352:ILE:CD1 | 1:C:407:ILE:HG12 | 2.44 | 0.47 |
| 1:B:644:SER:OG | 1:B:646:ILE:HG12 | 2.15 | 0.47 |
| 1:D:571:GLU:CD | 1:D:1058:PRO:HG3 | 2.35 | 0.47 |
| 1:A:925:GLU:OE1 | 1:A:943:ARG:NE | 2.47 | 0.47 |
| 1:D:1327:LYS:HD2 | 1:D:1328:PRO:O | 2.14 | 0.47 |
| 1:D:426:ARG:HD2 | 1:D:1232:ALA:HB2 | 1.96 | 0.47 |
| 1:A:1222:THR:HG22 | 1:A:1228:TYR:HB2 | 1.97 | 0.47 |
| 1:A:714:LYS:HD2 | 1:A:896:ARG:NH1 | 2.30 | 0.47 |
| 1:B:1222:THR:HG22 | 1:B:1228:TYR:HB2 | 1.95 | 0.47 |
| 1:C:599:ARG:HH21 | 1:C:825:ARG:HD2 | 1.79 | 0.47 |
| 1:B:668:ILE:HD13 | 1:B:688:ILE:HD13 | 1.96 | 0.47 |
| 1:D:461:ASN:N | 1:D:461:ASN:HD22 | 2.11 | 0.47 |
| 1:A:328:ARG:HH11 | 1:A:328:ARG:HG2 | 1.80 | 0.47 |
| 1:A:351:ASN:HD22 | 1:A:361:LEU:HB2 | 1.79 | 0.46 |
| 1:D:1250:ASN:OD1 | 1:D:1252:LYS:HB2 | 2.15 | 0.46 |
| 1:C:3:ALA:HA | 1:C:227:LEU:HD22 | 1.96 | 0.46 |
| 1:D:740:GLN:HG2 | 1:D:912:PHE:CE2 | 2.50 | 0.46 |
| 1:B:735:ILE:N | 1:B:735:ILE:HD12 | 2.29 | 0.46 |
| 1:C:656:PHE:HE2 | 1:C:815:LEU:HD23 | 1.79 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:1119:THR:O | 1:C:1123:MET:HG2 | 2.15 | 0.46 |
| 1:B:623:THR:O | 1:B:623:THR:CG2 | 2.64 | 0.46 |
| 1:C:124:MET:CE | 1:C:127:LEU:HD23 | 2.44 | 0.46 |
| 1:A:115:PHE:HD2 | 1:A:745:LEU:HB3 | 1.81 | 0.46 |
| 1:C:467:LEU:O | 1:C:471:GLN:HG2 | 2.15 | 0.46 |
| 1:B:257:LEU:O | 5:B:3003:FAD:H2B | 2.15 | 0.46 |
| 1:A:505:VAL:HG23 | 1:A:506:ASP:N | 2.30 | 0.46 |
| 1:D:606:LEU:HD23 | 1:D:606:LEU:C | 2.36 | 0.46 |
| 1:C:881:ARG:HD2 | 1:C:915:PHE:O | 2.16 | 0.46 |
| 1:A:933:VAL:HG11 | 1:A:1280:ARG:NH2 | 2.30 | 0.46 |
| 1:A:374:LEU:HD22 | 1:A:398:LEU:HD21 | 1.98 | 0.46 |
| 1:A:765:VAL:O | 1:A:792:VAL:HG22 | 2.15 | 0.46 |
| 1:B:314:ASP:O | 1:B:318:LYS:HE2 | 2.15 | 0.46 |
| 1:B:1054:ALA:O | 1:B:1099:LEU:HD11 | 2.14 | 0.46 |
| 1:B:987:LYS:O | 1:B:991:GLU:HG3 | 2.16 | 0.46 |
| 1:C:1174:ASN:O | 1:C:1237:PRO:HA | 2.16 | 0.46 |
| 1:D:498:PRO:HG2 | 1:D:1323:PRO:HD3 | 1.97 | 0.46 |
| 1:A:912:PHE:O | 1:A:913:ARG:C | 2.54 | 0.46 |
| 1:C:409:ILE:HA | 1:C:410:PRO:HD3 | 1.74 | 0.46 |
| 1:A:969:TRP:HZ3 | 1:A:1003:PRO:HD3 | 1.79 | 0.46 |
| 1:D:304:PRO:HG2 | 1:D:307:ILE:HG23 | 1.96 | 0.46 |
| 1:C:735:ILE:CD1 | 1:C:845:ALA:HB3 | 2.45 | 0.46 |
| 1:C:304:PRO:O | 1:C:307:ILE:HG13 | 2.16 | 0.46 |
| 1:B:653:GLU:HB3 | 1:B:871:THR:HG21 | 1.97 | 0.46 |
| 1:B:45:GLU:O | 1:B:45:GLU:HG2 | 2.16 | 0.46 |
| 1:C:218:ARG:HH11 | 1:C:218:ARG:CB | 2.29 | 0.46 |
| 1:A:97:ARG:HB2 | 1:A:97:ARG:HH11 | 1.81 | 0.46 |
| 1:B:762:GLU:C | 1:B:763:LEU:HD12 | 2.35 | 0.46 |
| 1:C:709:TYR:CE2 | 1:C:868:VAL:HG22 | 2.51 | 0.46 |
| 1:A:641:VAL:O | 1:A:641:VAL:HG23 | 2.14 | 0.46 |
| 1:A:552:LYS:HD3 | 1:A:552:LYS:N | 2.31 | 0.46 |
| 1:B:506:ASP:OD2 | 1:B:1320:THR:HG22 | 2.16 | 0.46 |
| 1:A:1043:LEU:O | 1:A:1047:MET:HG2 | 2.16 | 0.46 |
| 1:B:1300:PRO:HG2 | 1:B:1302:THR:HG23 | 1.96 | 0.46 |
| 1:C:393:TYR:N | 1:C:461:ASN:ND2 | 2.64 | 0.46 |
| 1:C:117:THR:CG2 | 1:C:587:ALA:HA | 2.45 | 0.46 |
| 1:A:166:ASP:O | 1:A:167:GLY:C | 2.53 | 0.46 |
| 1:B:3:ALA:HB1 | 1:B:228:ARG:N | 2.20 | 0.46 |
| 1:B:1089:GLN:HG2 | 1:B:1134:TYR:CE1 | 2.51 | 0.46 |
| 1:D:924:ALA:HA | 1:D:927:TRP:NE1 | 2.30 | 0.46 |
| 1:A:374:LEU:HD22 | 1:A:398:LEU:CD2 | 2.46 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:1262:GLU:N | 1:D:1263:PRO:CD | 2.79 | 0.46 |
| 1:B:606:LEU:HD23 | 1:B:607:ARG:N | 2.31 | 0.46 |
| 1:C:152:GLY:HA2 | 1:C:1201:VAL:HG21 | 1.98 | 0.46 |
| 1:D:1050:VAL:HG13 | 1:D:1255:TYR:HE2 | 1.80 | 0.46 |
| 1:A:746:GLU:HB3 | 1:A:796:GLY:HA3 | 1.97 | 0.46 |
| 1:D:989:ASN:OD1 | 1:D:996:LYS:HA | 2.15 | 0.46 |
| 1:D:768:GLN:HG3 | 1:D:802:LYS:HB2 | 1.98 | 0.46 |
| 1:B:1005:LYS:HG3 | 1:B:1156:TYR:CE1 | 2.50 | 0.46 |
| 1:C:393:TYR:N | 1:C:461:ASN:HD21 | 2.12 | 0.46 |
| 1:C:890:TYR:OH | 1:C:943:ARG:HD3 | 2.16 | 0.46 |
| 1:A:754:PRO:HD3 | 1:A:817:ALA:HB1 | 1.98 | 0.46 |
| 1:B:829:ASP:HB2 | 1:B:832:GLU:HG3 | 1.97 | 0.46 |
| 1:B:309:GLU:HB2 | 1:B:334:LEU:HD13 | 1.97 | 0.46 |
| 1:A:506:ASP:OD2 | 1:A:1319:VAL:HA | 2.16 | 0.46 |
| 1:B:1320:THR:HG23 | 1:B:1321:GLY:N | 2.31 | 0.46 |
| 1:C:1263:PRO:HB2 | 1:C:1264:PRO:HD3 | 1.98 | 0.46 |
| 1:C:757:GLU:O | 1:C:759:GLY:N | 2.49 | 0.46 |
| 1:D:1109:ASN:ND2 | 1:D:1112:GLY:HA3 | 2.31 | 0.46 |
| 1:B:662:THR:O | 1:B:663:CYS:HB3 | 2.16 | 0.46 |
| 1:C:147:LEU:HD13 | 1:C:1230:ILE:HD11 | 1.98 | 0.46 |
| 1:A:482:LEU:O | 1:A:486:VAL:HG23 | 2.15 | 0.46 |
| 1:A:298:SER:HA | 1:A:408:GLU:HA | 1.97 | 0.46 |
| 1:D:387:HIS:ND1 | 1:D:467:LEU:HD11 | 2.32 | 0.45 |
| 1:C:3:ALA:HA | 1:C:227:LEU:CD2 | 2.46 | 0.45 |
| 1:B:857:VAL:HG21 | 1:B:892:ILE:HG12 | 1.99 | 0.45 |
| 1:C:1319:VAL:HG23 | 1:C:1319:VAL:O | 2.15 | 0.45 |
| 1:B:13:ARG:HH11 | 1:B:13:ARG:CB | 2.29 | 0.45 |
| 1:D:318:LYS:N | 1:D:318:LYS:HD2 | 2.30 | 0.45 |
| 1:A:735:ILE:HD11 | 1:A:923:ILE:HG12 | 1.99 | 0.45 |
| 1:C:840:ARG:HB2 | 1:C:912:PHE:CD2 | 2.51 | 0.45 |
| 1:C:124:MET:HE2 | 1:C:128:LEU:HG | 1.98 | 0.45 |
| 1:A:424:ALA:HB1 | 1:A:430:ASP:OD2 | 2.16 | 0.45 |
| 1:D:612:THR:O | 1:D:613:ARG:HD3 | 2.16 | 0.45 |
| 1:D:649:ILE:HD11 | 1:D:804:THR:HB | 1.99 | 0.45 |
| 1:B:755:LYS:HE2 | 1:B:762:GLU:HB2 | 1.98 | 0.45 |
| 1:A:550:PHE:HE2 | 1:A:552:LYS:HD2 | 1.80 | 0.45 |
| 1:D:217:LEU:HA | 1:D:217:LEU:HD12 | 1.77 | 0.45 |
| 1:C:571:GLU:CD | 1:C:1058:PRO:HG3 | 2.35 | 0.45 |
| 1:B:236:TRP:CZ2 | 1:B:280:CYS:HB2 | 2.51 | 0.45 |
| 1:A:375:VAL:HG12 | 1:A:380:ARG:HG3 | 1.97 | 0.45 |
| 1:C:256:LYS:HG3 | 1:C:275:PHE:CD1 | 2.50 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:62:GLN:HG3 | 1:A:64:LYS:HB2 | 1.99 | 0.45 |
| 1:D:1115:GLU:O | 1:D:1119:THR:CG2 | 2.64 | 0.45 |
| 1:A:372:LEU:HD23 | 1:A:407:ILE:HG13 | 1.97 | 0.45 |
| 1:D:997:ARG:HA | 1:D:1163:VAL:O | 2.16 | 0.45 |
| 1:B:768:GLN:HG3 | 1:B:802:LYS:HB2 | 1.97 | 0.45 |
| 1:A:1332:ARG:NH1 | 1:A:1332:ARG:HG2 | 2.30 | 0.45 |
| 1:C:399:SER:HB2 | 1:C:400:PRO:HD2 | 1.98 | 0.45 |
| 1:A:571:GLU:OE2 | 1:A:1058:PRO:HG3 | 2.17 | 0.45 |
| 1:D:112:GLN:NE2 | 1:D:151:THR:HA | 2.31 | 0.45 |
| 1:A:196:PHE:CE2 | 1:A:198:PRO:HG3 | 2.51 | 0.45 |
| 1:D:630:PRO:HD2 | 1:D:681:ARG:NH2 | 2.32 | 0.45 |
| 1:A:1327:LYS:C | 1:A:1327:LYS:HD2 | 2.37 | 0.45 |
| 1:C:97:ARG:CB | 1:C:97:ARG:HH11 | 2.29 | 0.45 |
| 1:A:154:ARG:NH1 | 1:A:1197:GLU:OE1 | 2.50 | 0.45 |
| 1:C:304:PRO:HG2 | 1:C:307:ILE:HG23 | 1.98 | 0.45 |
| 1:D:1050:VAL:HG13 | 1:D:1255:TYR:CE2 | 2.52 | 0.45 |
| 1:A:95:LYS:HG3 | 1:A:590:GLU:OE2 | 2.16 | 0.45 |
| 1:A:442:PHE:HE1 | 1:A:478:TRP:HB2 | 1.82 | 0.45 |
| 1:B:195:LEU:HD22 | 1:B:1190:ALA:HA | 1.99 | 0.45 |
| 1:D:422:LYS:HE3 | 1:D:432:ALA:HB2 | 1.99 | 0.45 |
| 1:C:851:PHE:N | 1:C:851:PHE:CD1 | 2.84 | 0.45 |
| 1:D:275:PHE:HA | 1:D:276:PRO:HD2 | 1.82 | 0.45 |
| 1:B:257:LEU:HD22 | 1:B:279:VAL:HG13 | 1.98 | 0.45 |
| 1:C:713:LEU:O | 1:C:898:THR:HA | 2.17 | 0.45 |
| 1:C:224:ARG:HD3 | 1:C:283:TRP:CE3 | 2.52 | 0.45 |
| 1:B:709:TYR:HE2 | 1:B:868:VAL:HG22 | 1.81 | 0.45 |
| 1:D:1327:LYS:HD2 | 1:D:1327:LYS:C | 2.37 | 0.45 |
| 1:B:604:LEU:HD21 | 1:B:822:ARG:NH2 | 2.32 | 0.45 |
| 1:C:257:LEU:CD2 | 1:C:279:VAL:HG13 | 2.47 | 0.45 |
| 1:A:98:LEU:HD21 | 1:A:588:SER:HB3 | 1.97 | 0.45 |
| 1:B:656:PHE:CD1 | 1:B:669:GLY:HA2 | 2.51 | 0.45 |
| 1:D:215:GLU:HG3 | 1:D:218:ARG:HH12 | 1.82 | 0.45 |
| 1:D:742:HIS:HA | 1:D:912:PHE:CE2 | 2.52 | 0.45 |
| 1:A:1216:PRO:HD2 | 1:A:1217:GLU:OE2 | 2.17 | 0.45 |
| 1:B:1199:ALA:HB3 | 1:B:1264:PRO:HB2 | 1.99 | 0.45 |
| 1:A:981:ARG:NH1 | 1:A:1162:GLU:OE1 | 2.49 | 0.45 |
| 1:A:530:GLU:O | 1:A:531:ASN:HB2 | 2.16 | 0.45 |
| 1:B:58:TYR:CZ | 1:B:220:LYS:HD2 | 2.52 | 0.45 |
| 1:A:1289:ASN:O | 1:A:1290:ASN:HB2 | 2.17 | 0.45 |
| 1:A:927:TRP:O | 1:A:931:VAL:HG23 | 2.17 | 0.45 |
| 1:A:578:LEU:HD12 | 1:A:579:PRO:HD2 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1184:GLY:HA2 | 1:C:1248:CYS:O | 2.16 | 0.45 |
| 1:D:1119:THR:O | 1:D:1123:MET:HG2 | 2.17 | 0.45 |
| 1:B:96:THR:OG1 | 1:B:97:ARG:N | 2.49 | 0.45 |
| 1:B:906:LEU:HD11 | 1:B:1333:VAL:HG22 | 1.99 | 0.45 |
| 1:C:640:ASP:HB3 | 1:C:819:LYS:HE3 | 1.99 | 0.45 |
| 1:C:533:GLU:HG2 | 1:C:534:ASP:OD1 | 2.17 | 0.44 |
| 1:A:924:ALA:HA | 1:A:927:TRP:NE1 | 2.31 | 0.44 |
| 1:B:97:ARG:HB3 | 1:B:97:ARG:NH1 | 2.31 | 0.44 |
| 1:A:64:LYS:CE | 1:A:65:ILE:H | 2.28 | 0.44 |
| 1:D:1287:THR:OG1 | 1:D:1289:ASN:ND2 | 2.51 | 0.44 |
| 1:B:607:ARG:HB3 | 1:B:679:THR:HB | 1.99 | 0.44 |
| 1:D:224:ARG:HH11 | 1:D:224:ARG:HG2 | 1.83 | 0.44 |
| 1:C:257:LEU:HD23 | 1:C:279:VAL:HG13 | 1.98 | 0.44 |
| 1:D:1052:SER:HB2 | 1:D:1059:THR:HG22 | 1.98 | 0.44 |
| 1:B:439:ARG:NH2 | 1:B:451:GLU:OE1 | 2.50 | 0.44 |
| 1:B:1332:ARG:NH1 | 1:B:1332:ARG:HG2 | 2.31 | 0.44 |
| 1:B:1089:GLN:HG2 | 1:B:1134:TYR:CG | 2.53 | 0.44 |
| 1:C:1320:THR:CG2 | 1:C:1321:GLY:H | 2.22 | 0.44 |
| 1:D:978:TYR:CE2 | 1:D:982:LYS:HD2 | 2.52 | 0.44 |
| 1:A:616:ALA:HB2 | 1:A:692:GLU:HA | 1.99 | 0.44 |
| 1:B:1302:THR:HB | 1:B:1303:PRO:HD2 | 1.99 | 0.44 |
| 1:C:117:THR:HB | 1:C:118:PRO:HD3 | 1.99 | 0.44 |
| 1:D:1022:LEU:HD23 | 1:D:1022:LEU:C | 2.37 | 0.44 |
| 1:C:651:ASN:HD22 | 1:C:651:ASN:HA | 1.59 | 0.44 |
| 1:D:623:THR:CG2 | 1:D:626:ALA:HB3 | 2.47 | 0.44 |
| 1:C:473:GLN:HE21 | 1:C:482:LEU:HG | 1.82 | 0.44 |
| 1:B:667:ILE:HD12 | 1:B:808:VAL:HG13 | 2.00 | 0.44 |
| 1:C:425:SER:HB2 | 1:C:1229:LYS:HG3 | 1.98 | 0.44 |
| 1:D:97:ARG:CZ | 1:D:98:LEU:H | 2.30 | 0.44 |
| 1:B:307:ILE:C | 1:B:307:ILE:HD12 | 2.38 | 0.44 |
| 1:A:65:ILE:HD12 | 1:A:212:PHE:CE2 | 2.52 | 0.44 |
| 1:A:64:LYS:HE2 | 1:A:65:ILE:N | 2.30 | 0.44 |
| 1:A:40:LYS:HB3 | 1:A:115:PHE:CZ | 2.53 | 0.44 |
| 1:C:1287:THR:CG2 | 1:C:1288:GLY:H | 2.14 | 0.44 |
| 1:C:97:ARG:CB | 1:C:97:ARG:NH1 | 2.78 | 0.44 |
| 1:A:448:GLU:O | 1:A:448:GLU:HG3 | 2.18 | 0.44 |
| 1:A:467:LEU:O | 1:A:471:GLN:HG2 | 2.18 | 0.44 |
| 1:A:131:GLN:HE21 | 1:A:133:GLU:N | 2.13 | 0.44 |
| 1:D:164:ALA:C | 1:D:166:ASP:N | 2.65 | 0.44 |
| 1:D:1323:PRO:O | 1:D:1324:GLU:C | 2.56 | 0.44 |
| 1:A:606:LEU:HD13 | 1:A:813:VAL:HA | 1.98 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:1262:GLU:N | 1:C:1263:PRO:CD | 2.80 | 0.44 |
| 1:A:996:LYS:NZ | 1:A:1285:GLN:NE2 | 2.66 | 0.44 |
| 1:D:152:GLY:HA2 | 1:D:1201:VAL:HG21 | 2.00 | 0.44 |
| 1:D:39:THR:HG22 | 1:D:51:CYS:HA | 2.00 | 0.44 |
| 1:B:372:LEU:HD11 | 1:B:385:MET:HE3 | 1.99 | 0.44 |
| 1:B:1204:LEU:C | 1:B:1204:LEU:HD12 | 2.38 | 0.44 |
| 1:A:117:THR:HG21 | 1:A:587:ALA:HA | 1.99 | 0.44 |
| 1:D:1283:ARG:NH2 | 1:D:1293:GLU:OE2 | 2.50 | 0.44 |
| 1:A:1287:THR:O | 1:A:1289:ASN:N | 2.50 | 0.44 |
| 1:B:232:GLU:OE2 | 1:B:681:ARG:NH2 | 2.44 | 0.44 |
| 1:C:443:LYS:HD3 | 1:C:444:PRO:HD2 | 1.99 | 0.44 |
| 1:C:1200:PHE:CE1 | 1:C:1268:ALA:HA | 2.53 | 0.44 |
| 1:C:333:GLN:OE1 | 1:C:333:GLN:HA | 2.18 | 0.44 |
| 1:A:117:THR:HB | 1:A:118:PRO:HD3 | 1.99 | 0.44 |
| 1:A:256:LYS:HG3 | 1:A:275:PHE:CG | 2.53 | 0.44 |
| 1:D:46:GLY:HA2 | 4:D:2002:FES:S1 | 2.58 | 0.44 |
| 1:A:443:LYS:HG2 | 1:A:450:GLN:HB2 | 2.00 | 0.43 |
| 1:C:58:TYR:OH | 1:C:63:ASN:ND2 | 2.46 | 0.43 |
| 1:B:507:PHE:HB2 | 1:B:1304:GLU:HG3 | 1.99 | 0.43 |
| 1:C:65:ILE:HD12 | 1:C:212:PHE:CD2 | 2.53 | 0.43 |
| 1:C:1038:GLU:HB2 | 1:C:1044:HIS:CD2 | 2.53 | 0.43 |
| 1:C:720:LEU:HD11 | 1:C:896:ARG:CB | 2.48 | 0.43 |
| 1:A:1188:ASN:CG | 1:A:1191:ILE:HG12 | 2.38 | 0.43 |
| 1:A:97:ARG:CB | 1:A:97:ARG:HH11 | 2.31 | 0.43 |
| 1:C:310:LYS:CA | 1:C:310:LYS:HE2 | 2.47 | 0.43 |
| 1:D:196:PHE:O | 1:D:198:PRO:HD3 | 2.19 | 0.43 |
| 1:B:58:TYR:OH | 1:B:63:ASN:ND2 | 2.52 | 0.43 |
| 1:C:932:ALA:HA | 1:C:942:VAL:HG21 | 2.00 | 0.43 |
| 1:B:3:ALA:HA | 1:B:227:LEU:CD2 | 2.46 | 0.43 |
| 1:A:602:ASN:O | 1:A:822:ARG:HD2 | 2.17 | 0.43 |
| 1:D:1302:THR:HB | 1:D:1303:PRO:HD2 | 2.00 | 0.43 |
| 1:B:667:ILE:HD12 | 1:B:808:VAL:CG1 | 2.48 | 0.43 |
| 1:A:298:SER:HA | 1:A:407:ILE:O | 2.18 | 0.43 |
| 1:C:257:LEU:HD23 | 1:C:279:VAL:CG1 | 2.48 | 0.43 |
| 1:C:550:PHE:CE2 | 1:C:552:LYS:HG3 | 2.53 | 0.43 |
| 1:B:606:LEU:C | 1:B:606:LEU:HD23 | 2.38 | 0.43 |
| 1:B:58:TYR:CE1 | 1:B:63:ASN:ND2 | 2.86 | 0.43 |
| 1:C:117:THR:O | 1:C:121:VAL:HG23 | 2.19 | 0.43 |
| 1:D:733:GLY:HA3 | 1:D:847:TYR:CZ | 2.54 | 0.43 |
| 1:D:1047:MET:SD | 1:D:1088:GLY:HA2 | 2.59 | 0.43 |
| 1:B:1183:VAL:HG22 | 9:B:7068:HOH:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:267:GLU:HB3 | 1:C:273:MET:HG3 | 2.00 | 0.43 |
| 1:C:154:ARG:N | 1:C:155:PRO:HD2 | 2.33 | 0.43 |
| 1:A:616:ALA:CB | 1:A:692:GLU:HA | 2.48 | 0.43 |
| 1:B:1320:THR:OG1 | 1:B:1321:GLY:N | 2.49 | 0.43 |
| 1:B:58:TYR:HE1 | 1:B:63:ASN:ND2 | 2.16 | 0.43 |
| 1:A:1220:LEU:HD21 | 1:A:1222:THR:O | 2.18 | 0.43 |
| 1:D:298:SER:HA | 1:D:408:GLU:HA | 1.99 | 0.43 |
| 1:A:1083:SER:HB2 | 6:A:2004:MTE:O3P | 2.19 | 0.43 |
| 1:A:1009:SER:HA | 1:A:1082:VAL:HG11 | 2.01 | 0.43 |
| 1:B:888:ASN:ND2 | 1:B:925:GLU:OE2 | 2.51 | 0.43 |
| 1:B:1008:ILE:O | 1:B:1009:SER:CB | 2.66 | 0.43 |
| 1:A:1133:PHE:CG | 1:B:1127:SER:HB2 | 2.53 | 0.43 |
| 1:C:131:GLN:O | 1:C:134:PRO:HD3 | 2.19 | 0.43 |
| 1:D:1323:PRO:O | 1:D:1325:ASN:N | 2.51 | 0.43 |
| 1:A:197:LYS:HB2 | 1:A:200:GLU:HG3 | 2.01 | 0.43 |
| 1:C:490:LEU:HB2 | 1:C:513:LEU:CD2 | 2.49 | 0.43 |
| 1:D:87:THR:OG1 | 1:D:89:GLU:HG2 | 2.18 | 0.43 |
| 1:C:506:ASP:OD1 | 1:C:1320:THR:N | 2.52 | 0.43 |
| 1:A:967:ARG:O | 1:A:971:GLU:HB2 | 2.19 | 0.43 |
| 1:D:1215:SER:HG | 1:D:1217:GLU:HG2 | 1.83 | 0.43 |
| 1:C:1133:PHE:CG | 1:D:1127:SER:HB2 | 2.54 | 0.43 |
| 1:B:362:ASN:N | 1:B:363:PRO:CD | 2.82 | 0.43 |
| 1:B:1291:VAL:HG13 | 1:B:1292:LYS:HG3 | 2.00 | 0.43 |
| 1:D:374:LEU:HD13 | 1:D:398:LEU:CD2 | 2.45 | 0.43 |
| 1:A:443:LYS:HA | 1:A:450:GLN:NE2 | 2.33 | 0.43 |
| 1:D:1089:GLN:HG2 | 1:D:1134:TYR:CE1 | 2.53 | 0.43 |
| 1:A:1222:THR:CG2 | 1:A:1228:TYR:HB2 | 2.49 | 0.43 |
| 1:C:656:PHE:CD1 | 1:C:669:GLY:HA2 | 2.54 | 0.43 |
| 1:C:1208:THR:C | 1:C:1209:LEU:HD12 | 2.39 | 0.43 |
| 1:C:1141:TYR:OH | 1:C:1146:ASN:ND2 | 2.52 | 0.43 |
| 1:B:623:THR:HG23 | 1:B:626:ALA:HB3 | 2.01 | 0.43 |
| 1:A:389:PHE:HA | 1:A:397:LEU:CG | 2.47 | 0.43 |
| 1:C:28:ALA:CB | 1:C:32:ARG:HH12 | 2.32 | 0.43 |
| 1:C:912:PHE:O | 1:C:913:ARG:C | 2.57 | 0.43 |
| 1:A:256:LYS:HG3 | 1:A:275:PHE:CD1 | 2.54 | 0.43 |
| 1:C:204:LEU:HG | 1:C:206:PRO:HD3 | 2.01 | 0.43 |
| 1:A:1034:HIS:HB2 | 1:A:1087:ASN:HD22 | 1.83 | 0.43 |
| 1:D:646:ILE:O | 1:D:646:ILE:HG13 | 2.19 | 0.42 |
| 1:A:734:GLU:O | 1:A:735:ILE:HG23 | 2.19 | 0.42 |
| 1:B:758:ALA:O | 1:B:787:ARG:HD2 | 2.19 | 0.42 |
| 1:A:32:ARG:HD2 | 9:A:7112:HOH:O | 2.18 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:582:ALA:O | 1:A:586:GLN:HG3 | 2.19 | 0.42 |
| 1:A:96:THR:OG1 | 1:A:97:ARG:N | 2.51 | 0.42 |
| 1:B:552:LYS:O | 1:B:553:ASP:CB | 2.65 | 0.42 |
| 1:A:428:GLU:O | 1:A:429:ASP:C | 2.57 | 0.42 |
| 1:C:572:ASP:OD1 | 1:C:1053:ARG:HD3 | 2.19 | 0.42 |
| 1:A:632:PHE:HE1 | 1:A:671:VAL:HG22 | 1.83 | 0.42 |
| 1:A:1279:ILE:HG21 | 1:A:1309:ALA:HB1 | 2.01 | 0.42 |
| 1:C:869:GLY:HA3 | 1:C:908:SER:HA | 2.01 | 0.42 |
| 1:B:859:ALA:HA | 1:B:894:ASN:O | 2.19 | 0.42 |
| 1:B:558:VAL:HG21 | 1:B:1241:ARG:NH1 | 2.34 | 0.42 |
| 1:B:652:ASP:HB3 | 1:B:871:THR:HB | 2.01 | 0.42 |
| 1:C:357:PRO:HG3 | 1:C:461:ASN:O | 2.18 | 0.42 |
| 1:C:550:PHE:HE2 | 1:C:552:LYS:HG3 | 1.83 | 0.42 |
| 1:A:428:GLU:OE2 | 1:A:1234:GLY:HA3 | 2.20 | 0.42 |
| 1:C:108:SER:O | 1:C:109:HIS:HB2 | 2.20 | 0.42 |
| 1:C:74:LEU:O | 1:C:76:PRO:HD3 | 2.19 | 0.42 |
| 1:B:550:PHE:CE1 | 1:B:1173:LYS:HD3 | 2.53 | 0.42 |
| 1:A:97:ARG:HB2 | 1:A:97:ARG:CZ | 2.49 | 0.42 |
| 1:D:446:THR:HB | 1:D:535:LYS:HZ2 | 1.83 | 0.42 |
| 1:A:419:SER:HB2 | 1:A:519:PHE:CD1 | 2.54 | 0.42 |
| 1:D:661:VAL:HA | 1:D:666:HIS:ND1 | 2.34 | 0.42 |
| 1:A:977:GLN:O | 1:A:981:ARG:HG3 | 2.18 | 0.42 |
| 1:A:562:GLN:HG3 | 1:A:1246:ARG:NH2 | 2.35 | 0.42 |
| 1:B:346:ALA:HB1 | 5:B:3003:FAD:H4' | 2.00 | 0.42 |
| 1:D:641:VAL:O | 1:D:641:VAL:HG23 | 2.19 | 0.42 |
| 1:C:735:ILE:HG21 | 1:C:926:CYS:SG | 2.59 | 0.42 |
| 1:D:117:THR:CG2 | 1:D:587:ALA:HA | 2.50 | 0.42 |
| 1:D:1034:HIS:NE2 | 1:D:1047:MET:HG3 | 2.35 | 0.42 |
| 1:B:835:LEU:HD22 | 1:B:1223:ARG:NH1 | 2.35 | 0.42 |
| 1:C:363:PRO:HG3 | 1:C:463:THR:HG23 | 2.01 | 0.42 |
| 1:D:592:VAL:HG13 | 1:D:596:ASP:HB2 | 2.02 | 0.42 |
| 1:B:55:LEU:CD2 | 1:B:85:VAL:HG22 | 2.50 | 0.42 |
| 1:A:425:SER:HB2 | 1:A:1229:LYS:HG3 | 2.02 | 0.42 |
| 1:D:1079:ALA:HB1 | 7:D:5005:MOM:OM1 | 2.19 | 0.42 |
| 1:A:498:PRO:HG3 | 1:A:1320:THR:OG1 | 2.20 | 0.42 |
| 1:B:1109:ASN:N | 1:B:1110:PRO:HD3 | 2.35 | 0.42 |
| 1:D:136:MET:CE | 1:D:167:GLY:HA2 | 2.49 | 0.42 |
| 1:B:642:PRO:HG2 | 1:B:781:LEU:HA | 2.00 | 0.42 |
| 1:A:532:LEU:C | 1:A:534:ASP:H | 2.23 | 0.42 |
| 1:B:1141:TYR:HE1 | 1:B:1146:ASN:HD22 | 1.68 | 0.42 |
| 1:D:649:ILE:HD13 | 1:D:873:ASP:OD1 | 2.19 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:217:LEU:HD12 | 1:C:217:LEU:HA | 1.92 | 0.42 |
| 1:A:742:HIS:HA | 1:A:912:PHE:CZ | 2.55 | 0.42 |
| 1:D:613:ARG:NH1 | 1:D:692:GLU:HG3 | 2.34 | 0.42 |
| 1:A:112:GLN:NE2 | 1:A:151:THR:HA | 2.34 | 0.42 |
| 1:B:886:MET:SD | 1:B:897:GLY:HA3 | 2.59 | 0.42 |
| 1:C:1019:GLY:HA2 | 1:C:1132:GLY:O | 2.20 | 0.42 |
| 1:C:950:GLU:OE2 | 1:C:961:GLU:HA | 2.19 | 0.42 |
| 1:B:29:TYR:CE1 | 1:B:33:LYS:HG2 | 2.54 | 0.42 |
| 1:D:307:ILE:HG13 | 1:D:308:VAL:N | 2.35 | 0.42 |
| 1:C:399:SER:OG | 1:C:402:GLU:HG3 | 2.19 | 0.42 |
| 1:B:735:ILE:HD11 | 1:B:847:TYR:HD1 | 1.85 | 0.42 |
| 1:B:787:ARG:HG2 | 1:B:787:ARG:HH11 | 1.85 | 0.42 |
| 1:D:841:HIS:CE1 | 1:D:878:ILE:HD12 | 2.55 | 0.42 |
| 1:A:68:PHE:HD2 | 1:A:344:SER:HB3 | 1.84 | 0.42 |
| 1:A:1149:ASN:HA | 1:A:1150:PRO:HD3 | 1.85 | 0.42 |
| 1:D:860:LEU:HD22 | 1:D:927:TRP:CZ2 | 2.54 | 0.42 |
| 1:D:650:CYS:HB2 | 1:D:652:ASP:HB2 | 2.01 | 0.42 |
| 1:B:500:ALA:HA | 1:B:501:PRO:HD3 | 1.93 | 0.42 |
| 1:D:124:MET:HE2 | 1:D:128:LEU:HD11 | 2.02 | 0.42 |
| 1:A:749:CYS:HA | 1:A:826:CYS:O | 2.20 | 0.42 |
| 1:D:558:VAL:HG13 | 1:D:1241:ARG:HG2 | 2.01 | 0.42 |
| 1:A:1113:SER:O | 1:A:1116:ASP:HB2 | 2.20 | 0.42 |
| 1:C:1105:TYR:N | 1:C:1105:TYR:CD1 | 2.88 | 0.42 |
| 1:C:786:ASN:ND2 | 1:D:1029:SER:HB2 | 2.35 | 0.42 |
| 1:B:572:ASP:OD2 | 1:B:1053:ARG:HD2 | 2.20 | 0.42 |
| 1:A:640:ASP:OD1 | 1:A:819:LYS:HE3 | 2.20 | 0.42 |
| 1:C:1260:VAL:O | 1:C:1260:VAL:HG22 | 2.19 | 0.42 |
| 1:A:1105:TYR:CD1 | 1:A:1105:TYR:N | 2.88 | 0.42 |
| 1:A:443:LYS:HA | 1:A:450:GLN:HE21 | 1.85 | 0.41 |
| 1:C:1089:GLN:HG2 | 1:C:1134:TYR:CE1 | 2.55 | 0.41 |
| 1:A:257:LEU:HD13 | 1:A:279:VAL:HG13 | 2.02 | 0.41 |
| 1:B:233:ARG:HD3 | 1:B:681:ARG:CZ | 2.50 | 0.41 |
| 1:A:1210:GLU:O | 1:A:1300:PRO:HG3 | 2.19 | 0.41 |
| 1:D:561:PHE:HB2 | 9:D:7144:HOH:O | 2.20 | 0.41 |
| 1:C:933:VAL:CG1 | 1:C:1280:ARG:HH21 | 2.29 | 0.41 |
| 1:D:566:LYS:HD3 | 1:D:566:LYS:C | 2.41 | 0.41 |
| 1:A:10:VAL:HG21 | 1:A:34:LEU:HD11 | 2.01 | 0.41 |
| 1:B:233:ARG:HD3 | 1:B:681:ARG:NH1 | 2.35 | 0.41 |
| 1:B:212:PHE:CD1 | 1:B:213:PRO:HD2 | 2.54 | 0.41 |
| 1:C:953:LEU:HD23 | 1:C:959:LYS:HA | 2.03 | 0.41 |
| 1:C:242:LEU:O | 1:C:246:LEU:HG | 2.20 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:C:924:ALA:HA | 1:C:927:TRP:NE1 | 2.35 | 0.41 |
| 1:D:741:GLU:CG | 1:D:834:MET:HG2 | 2.40 | 0.41 |
| 1:B:552:LYS:HG2 | 1:B:552:LYS:H | 1.44 | 0.41 |
| 1:B:752:ALA:HB3 | 1:B:813:VAL:HG12 | 2.03 | 0.41 |
| 1:C:87:THR:OG1 | 1:C:89:GLU:HG2 | 2.21 | 0.41 |
| 1:C:152:GLY:O | 1:C:1236:ILE:HG21 | 2.20 | 0.41 |
| 1:B:927:TRP:O | 1:B:931:VAL:HG23 | 2.20 | 0.41 |
| 1:C:1135:ARG:O | 1:C:1135:ARG:HD2 | 2.21 | 0.41 |
| 1:A:225:LYS:HE2 | 1:A:226:GLN:O | 2.19 | 0.41 |
| 1:A:1176:ARG:HH21 | 1:A:1241:ARG:CD | 2.33 | 0.41 |
| 1:A:650:CYS:O | 1:A:651:ASN:C | 2.57 | 0.41 |
| 1:D:3:ALA:HA | 1:D:227:LEU:HD22 | 2.02 | 0.41 |
| 1:C:573:MET:HA | 1:C:576:ARG:HD2 | 2.02 | 0.41 |
| 1:A:143:PHE:HB3 | 1:A:1233:PHE:CE1 | 2.55 | 0.41 |
| 1:D:441:LEU:HB3 | 1:D:451:GLU:HB2 | 2.02 | 0.41 |
| 1:D:1107:LYS:HB3 | 1:D:1107:LYS:HE2 | 1.85 | 0.41 |
| 1:B:671:VAL:HG11 | 1:B:682:ALA:HB3 | 2.03 | 0.41 |
| 1:C:218:ARG:NH1 | 1:C:218:ARG:HB2 | 2.35 | 0.41 |
| 1:D:860:LEU:HD12 | 1:D:861:GLU:N | 2.34 | 0.41 |
| 1:C:607:ARG:HB3 | 1:C:671:VAL:HG12 | 2.03 | 0.41 |
| 1:C:632:PHE:HE1 | 1:C:671:VAL:HG22 | 1.86 | 0.41 |
| 1:C:303:CYS:SG | 1:C:307:ILE:HD11 | 2.60 | 0.41 |
| 1:B:1103:GLU:O | 1:B:1107:LYS:HG3 | 2.20 | 0.41 |
| 1:D:750:THR:HG23 | 1:D:765:VAL:HG22 | 2.01 | 0.41 |
| 1:D:584:ASP:HB2 | 9:D:7063:HOH:O | 2.21 | 0.41 |
| 1:B:549:LEU:O | 1:B:551:GLN:HG2 | 2.20 | 0.41 |
| 1:C:722:LYS:HD3 | 1:C:726:GLU:OE2 | 2.19 | 0.41 |
| 1:A:154:ARG:CD | 1:A:1197:GLU:OE2 | 2.67 | 0.41 |
| 1:C:650:CYS:O | 1:C:651:ASN:C | 2.58 | 0.41 |
| 1:A:619:LYS:HD2 | 1:A:691:GLU:HB2 | 2.01 | 0.41 |
| 1:D:1106:LYS:HE3 | 1:D:1117:TRP:CH2 | 2.56 | 0.41 |
| 1:D:560:LEU:O | 1:D:1243:SER:HA | 2.20 | 0.41 |
| 1:D:614:ALA:O | 1:D:905:ASN:HB3 | 2.21 | 0.41 |
| 1:C:1084:ALA:HB3 | 9:C:7132:HOH:O | 2.21 | 0.41 |
| 1:A:1317:LEU:N | 1:A:1317:LEU:HD22 | 2.35 | 0.41 |
| 1:B:303:CYS:HA | 1:B:304:PRO:HD2 | 1.96 | 0.41 |
| 1:C:829:ASP:O | 1:C:830:ARG:C | 2.59 | 0.41 |
| 1:B:224:ARG:HG2 | 1:B:224:ARG:NH1 | 2.36 | 0.41 |
| 1:C:1236:ILE:HB | 1:C:1237:PRO:HD2 | 2.02 | 0.41 |
| 1:B:236:TRP:C | 1:B:236:TRP:CD1 | 2.94 | 0.41 |
| 1:D:562:GLN:HG3 | 1:D:1246:ARG:NH1 | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:D:56:SER:HA | 1:D:66:VAL:O | 2.20 | 0.41 |
| 1:A:254:ASP:O | 1:A:255:ALA:C | 2.59 | 0.41 |
| 1:D:1253:ALA:HB3 | 1:D:1257:SER:O | 2.21 | 0.41 |
| 1:B:747:THR:HG23 | 9:B:7032:HOH:O | 2.20 | 0.41 |
| 1:C:1092:TYR:O | 1:C:1096:GLN:HG2 | 2.21 | 0.41 |
| 1:A:59:ASP:OD1 | 1:A:62:GLN:HB3 | 2.21 | 0.41 |
| 1:D:303:CYS:HB3 | 1:D:307:ILE:HD11 | 2.03 | 0.41 |
| 1:B:351:ASN:HB2 | 5:B:3003:FAD:O4' | 2.21 | 0.41 |
| 1:C:3:ALA:HB2 | 1:C:225:LYS:HE3 | 2.01 | 0.41 |
| 1:D:1039:MET:HG3 | 6:D:5004:MTE:C4 | 2.50 | 0.41 |
| 1:C:357:PRO:HA | 1:C:462:ARG:HA | 2.02 | 0.41 |
| 1:B:504:MET:HG2 | 1:B:1304:GLU:OE2 | 2.20 | 0.41 |
| 1:A:68:PHE:CD2 | 1:A:344:SER:HB3 | 2.56 | 0.41 |
| 1:B:568:GLN:HG2 | 1:B:572:ASP:HB3 | 2.03 | 0.41 |
| 1:C:1210:GLU:O | 1:C:1300:PRO:HG3 | 2.21 | 0.41 |
| 1:A:1253:ALA:HB3 | 1:A:1257:SER:O | 2.21 | 0.41 |
| 1:C:732:SER:HA | 1:C:847:TYR:O | 2.20 | 0.41 |
| 1:A:315:ALA:O | 1:A:319:LEU:HG | 2.20 | 0.41 |
| 1:C:1193:ILE:O | 1:C:1197:GLU:HG3 | 2.20 | 0.41 |
| 1:B:215:GLU:O | 1:B:218:ARG:HB3 | 2.20 | 0.41 |
| 1:D:165:ARG:O | 1:D:166:ASP:O | 2.39 | 0.41 |
| 1:A:606:LEU:HD23 | 1:A:607:ARG:N | 2.35 | 0.41 |
| 1:C:192:SER:N | 1:C:193:PRO:HD3 | 2.35 | 0.41 |
| 1:A:1174:ASN:HB3 | 9:A:7076:HOH:O | 2.19 | 0.41 |
| 1:B:758:ALA:HB1 | 1:B:787:ARG:HE | 1.86 | 0.41 |
| 1:D:97:ARG:NH1 | 1:D:97:ARG:HA | 2.36 | 0.41 |
| 1:A:334:LEU:HA | 1:A:337:PHE:HB2 | 2.02 | 0.41 |
| 1:B:430:ASP:CG | 1:B:1229:LYS:HE2 | 2.41 | 0.41 |
| 1:C:1140:GLY:O | 1:C:1148:GLY:HA3 | 2.21 | 0.41 |
| 1:C:298:SER:HA | 1:C:407:ILE:O | 2.21 | 0.41 |
| 1:A:418:PHE:HD1 | 1:A:439:ARG:HB2 | 1.86 | 0.41 |
| 1:A:742:HIS:CE1 | 1:A:839:GLY:HA2 | 2.56 | 0.41 |
| 1:B:154:ARG:HD2 | 9:B:7076:HOH:O | 2.21 | 0.41 |
| 1:B:117:THR:CG2 | 1:B:587:ALA:HA | 2.51 | 0.41 |
| 1:B:646:ILE:HG13 | 1:B:779:LYS:NZ | 2.36 | 0.41 |
| 1:B:740:GLN:HG2 | 1:B:912:PHE:CE2 | 2.56 | 0.41 |
| 1:B:1036:GLY:HA3 | 1:B:1043:LEU:HD21 | 2.03 | 0.41 |
| 1:B:981:ARG:O | 1:B:985:VAL:HG23 | 2.20 | 0.41 |
| 1:B:9:PHE:CE2 | 1:B:14:LYS:HB2 | 2.55 | 0.41 |
| 1:B:645:ASN:O | 1:B:654:THR:HA | 2.21 | 0.41 |
| 1:A:1022:LEU:HD23 | 1:A:1032:LEU:HD13 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:B:477:LEU:HB3 | 1:B:479:LYS:HG2 | 2.03 | 0.41 |
| 1:A:384:GLN:O | 1:A:384:GLN:HG3 | 2.21 | 0.41 |
| 1:B:205:ASP:HA | 1:B:206:PRO:HD2 | 1.91 | 0.41 |
| 1:B:301:ALA:O | 1:B:347:SER:HB2 | 2.21 | 0.40 |
| 1:C:443:LYS:HD3 | 1:C:450:GLN:NE2 | 2.37 | 0.40 |
| 1:D:56:SER:HB2 | 1:D:84:ALA:HB3 | 2.03 | 0.40 |
| 1:B:981:ARG:CZ | 1:B:1176:ARG:HD3 | 2.52 | 0.40 |
| 1:A:886:MET:SD | 1:A:897:GLY:HA3 | 2.61 | 0.40 |
| 1:A:1159:ALA:HA | 1:A:1178:ASP:O | 2.21 | 0.40 |
| 1:C:234:VAL:HG12 | 1:C:235:THR:N | 2.37 | 0.40 |
| 1:A:647:THR:HG21 | 9:A:7205:HOH:O | 2.20 | 0.40 |
| 1:C:780:MET:C | 1:C:780:MET:SD | 3.00 | 0.40 |
| 1:C:1327:LYS:HD2 | 1:C:1327:LYS:C | 2.42 | 0.40 |
| 1:C:735:ILE:CD1 | 1:C:923:ILE:HG12 | 2.52 | 0.40 |
| 1:A:6:LEU:HB3 | 1:A:17:GLU:HB3 | 2.03 | 0.40 |
| 1:B:157:LEU:HA | 1:B:157:LEU:HD23 | 1.92 | 0.40 |
| 1:D:418:PHE:HD1 | 1:D:439:ARG:HB2 | 1.85 | 0.40 |
| 1:C:328:ARG:CG | 1:C:328:ARG:HH11 | 2.35 | 0.40 |
| 1:D:1199:ALA:HB3 | 1:D:1264:PRO:HB2 | 2.03 | 0.40 |
| 1:B:154:ARG:CD | 1:B:1197:GLU:OE2 | 2.69 | 0.40 |
| 1:B:709:TYR:CE2 | 1:B:868:VAL:CG2 | 3.04 | 0.40 |
| 1:A:74:LEU:O | 1:A:76:PRO:HD3 | 2.21 | 0.40 |
| 1:D:29:TYR:O | 1:D:33:LYS:HB3 | 2.21 | 0.40 |
| 1:D:362:ASN:N | 1:D:363:PRO:CD | 2.85 | 0.40 |
| 1:B:480:GLU:O | 1:B:483:LEU:HB3 | 2.21 | 0.40 |
| 1:C:750:THR:HG23 | 1:C:765:VAL:HG22 | 2.04 | 0.40 |
| 1:A:400:PRO:HG2 | 1:A:401:GLU:CD | 2.42 | 0.40 |
| 1:A:218:ARG:NH1 | 1:A:218:ARG:HB2 | 2.37 | 0.40 |
| 1:B:1200:PHE:CE1 | 1:B:1268:ALA:HA | 2.56 | 0.40 |
| 1:A:263:GLU:HB3 | 5:A:2003:FAD:H52A | 2.03 | 0.40 |
| 1:A:840:ARG:HG3 | 2:A:6001:BCT:O1 | 2.21 | 0.40 |
| 1:B:1032:LEU:O | 1:B:1064:ILE:HG12 | 2.22 | 0.40 |
| 1:C:860:LEU:HD22 | 1:C:892:ILE:HD13 | 2.03 | 0.40 |
| 1:B:442:PHE:CE2 | 1:B:527:LEU:HD21 | 2.56 | 0.40 |
| 1:A:1107:LYS:HB3 | 1:A:1107:LYS:HE2 | 1.90 | 0.40 |
| 1:D:505:VAL:HG23 | 1:D:506:ASP:N | 2.37 | 0.40 |
| 1:C:1122:TYR:HD1 | 9:D:7164:HOH:O | 2.04 | 0.40 |
| 1:A:242:LEU:O | 1:A:246:LEU:HG | 2.21 | 0.40 |
| 1:B:965:LEU:N | 1:B:966:PRO:CD | 2.84 | 0.40 |
| 1:D:500:ALA:HA | 1:D:501:PRO:HD3 | 1.96 | 0.40 |
| 1:D:332:GLU:O | 1:D:335:ARG:HB3 | 2.22 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|------------------|--------------------------|-------------------|
| 1:B:217:LEU:HA | 1:B:217:LEU:HD12 | 1.79 | 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 | 1303/1333 (98%) | 1225 (94%) | 64 (5%) | 14 (1%) | 17 | 36 |
| 1 | B | 1303/1333 (98%) | 1228 (94%) | 65 (5%) | 10 (1%) | 24 | 46 |
| 1 | C | 1303/1333 (98%) | 1228 (94%) | 69 (5%) | 6 (0%) | 34 | 60 |
| 1 | D | 1303/1333 (98%) | 1223 (94%) | 64 (5%) | 16 (1%) | 16 | 33 |
| All | All | 5212/5332 (98%) | 4904 (94%) | 262 (5%) | 46 (1%) | 21 | 42 |

All (46) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1009 | SER |
| 1 | A | 1290 | ASN |
| 1 | B | 553 | ASP |
| 1 | B | 1009 | SER |
| 1 | C | 758 | ALA |
| 1 | C | 1009 | SER |
| 1 | C | 1320 | THR |
| 1 | D | 166 | ASP |
| 1 | D | 1009 | SER |
| 1 | D | 1324 | GLU |
| 1 | D | 1325 | ASN |
| 1 | D | 377 | ARG |
| 1 | D | 391 | PRO |
| 1 | D | 758 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 798 | GLY |
| 1 | D | 1319 | VAL |
| 1 | D | 1320 | THR |
| 1 | A | 429 | ASP |
| 1 | A | 1288 | GLY |
| 1 | B | 552 | LYS |
| 1 | B | 798 | GLY |
| 1 | D | 1290 | ASN |
| 1 | A | 4 | ASP |
| 1 | A | 533 | GLU |
| 1 | A | 624 | SER |
| 1 | A | 798 | GLY |
| 1 | A | 913 | ARG |
| 1 | B | 4 | ASP |
| 1 | B | 913 | ARG |
| 1 | D | 429 | ASP |
| 1 | D | 1323 | PRO |
| 1 | B | 1323 | PRO |
| 1 | C | 798 | GLY |
| 1 | C | 1289 | ASN |
| 1 | D | 978 | TYR |
| 1 | A | 1247 | ASP |
| 1 | A | 1319 | VAL |
| 1 | B | 213 | PRO |
| 1 | B | 1081 | SER |
| 1 | A | 1260 | VAL |
| 1 | A | 1322 | VAL |
| 1 | A | 1323 | PRO |
| 1 | B | 1321 | GLY |
| 1 | C | 1003 | PRO |
| 1 | D | 1003 | PRO |
| 1 | D | 213 | PRO |

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 | 1104/1126 (98%) | 1066 (97%) | 38 (3%) | 44 | 72 |
| 1 | B | 1104/1126 (98%) | 1063 (96%) | 41 (4%) | 41 | 69 |
| 1 | C | 1104/1126 (98%) | 1070 (97%) | 34 (3%) | 47 | 76 |
| 1 | D | 1104/1126 (98%) | 1060 (96%) | 44 (4%) | 38 | 67 |
| All | All | 4416/4504 (98%) | 4259 (96%) | 157 (4%) | 42 | 71 |

All (157) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 4 | ASP |
| 1 | A | 60 | ARG |
| 1 | A | 62 | GLN |
| 1 | A | 64 | LYS |
| 1 | A | 89 | GLU |
| 1 | A | 129 | ARG |
| 1 | A | 154 | ARG |
| 1 | A | 202 | THR |
| 1 | A | 209 | GLU |
| 1 | A | 220 | LYS |
| 1 | A | 254 | ASP |
| 1 | A | 257 | LEU |
| 1 | A | 313 | VAL |
| 1 | A | 328 | ARG |
| 1 | A | 462 | ARG |
| 1 | A | 529 | GLN |
| 1 | A | 552 | LYS |
| 1 | A | 619 | LYS |
| 1 | A | 649 | ILE |
| 1 | A | 652 | ASP |
| 1 | A | 671 | VAL |
| 1 | A | 741 | GLU |
| 1 | A | 744 | TYR |
| 1 | A | 753 | VAL |
| 1 | A | 857 | VAL |
| 1 | A | 868 | VAL |
| 1 | A | 912 | PHE |
| 1 | A | 947 | LEU |
| 1 | A | 970 | GLU |
| 1 | A | 1033 | THR |
| 1 | A | 1053 | ARG |
| 1 | A | 1100 | LYS |
| 1 | A | 1146 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 1240 | PHE |
| 1 | A | 1280 | ARG |
| 1 | A | 1291 | VAL |
| 1 | A | 1319 | VAL |
| 1 | A | 1327 | LYS |
| 1 | B | 13 | ARG |
| 1 | B | 62 | GLN |
| 1 | B | 64 | LYS |
| 1 | B | 89 | GLU |
| 1 | B | 100 | PRO |
| 1 | B | 129 | ARG |
| 1 | B | 144 | GLN |
| 1 | B | 154 | ARG |
| 1 | B | 209 | GLU |
| 1 | B | 254 | ASP |
| 1 | B | 277 | MET |
| 1 | B | 328 | ARG |
| 1 | B | 462 | ARG |
| 1 | B | 468 | LYS |
| 1 | B | 477 | LEU |
| 1 | B | 534 | ASP |
| 1 | B | 552 | LYS |
| 1 | B | 553 | ASP |
| 1 | B | 619 | LYS |
| 1 | B | 641 | VAL |
| 1 | B | 652 | ASP |
| 1 | B | 671 | VAL |
| 1 | B | 735 | ILE |
| 1 | B | 744 | TYR |
| 1 | B | 789 | VAL |
| 1 | B | 857 | VAL |
| 1 | B | 912 | PHE |
| 1 | B | 940 | GLU |
| 1 | B | 965 | LEU |
| 1 | B | 970 | GLU |
| 1 | B | 1032 | LEU |
| 1 | B | 1033 | THR |
| 1 | B | 1053 | ARG |
| 1 | B | 1073 | PRO |
| 1 | B | 1119 | THR |
| 1 | B | 1135 | ARG |
| 1 | B | 1146 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | B | 1204 | LEU |
| 1 | B | 1240 | PHE |
| 1 | B | 1327 | LYS |
| 1 | B | 1333 | VAL |
| 1 | C | 62 | GLN |
| 1 | C | 89 | GLU |
| 1 | C | 100 | PRO |
| 1 | C | 129 | ARG |
| 1 | C | 154 | ARG |
| 1 | C | 199 | GLU |
| 1 | C | 202 | THR |
| 1 | C | 209 | GLU |
| 1 | C | 310 | LYS |
| 1 | C | 322 | GLN |
| 1 | C | 328 | ARG |
| 1 | C | 433 | LYS |
| 1 | C | 462 | ARG |
| 1 | C | 529 | GLN |
| 1 | C | 553 | ASP |
| 1 | C | 599 | ARG |
| 1 | C | 607 | ARG |
| 1 | C | 652 | ASP |
| 1 | C | 671 | VAL |
| 1 | C | 722 | LYS |
| 1 | C | 744 | TYR |
| 1 | C | 789 | VAL |
| 1 | C | 853 | LYS |
| 1 | C | 1003 | PRO |
| 1 | C | 1032 | LEU |
| 1 | C | 1033 | THR |
| 1 | C | 1053 | ARG |
| 1 | C | 1073 | PRO |
| 1 | C | 1119 | THR |
| 1 | C | 1146 | ASN |
| 1 | C | 1217 | GLU |
| 1 | C | 1240 | PHE |
| 1 | C | 1317 | LEU |
| 1 | C | 1327 | LYS |
| 1 | D | 32 | ARG |
| 1 | D | 89 | GLU |
| 1 | D | 97 | ARG |
| 1 | D | 100 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | D | 133 | GLU |
| 1 | D | 154 | ARG |
| 1 | D | 166 | ASP |
| 1 | D | 209 | GLU |
| 1 | D | 254 | ASP |
| 1 | D | 310 | LYS |
| 1 | D | 312 | LEU |
| 1 | D | 328 | ARG |
| 1 | D | 380 | ARG |
| 1 | D | 461 | ASN |
| 1 | D | 462 | ARG |
| 1 | D | 468 | LYS |
| 1 | D | 513 | LEU |
| 1 | D | 532 | LEU |
| 1 | D | 533 | GLU |
| 1 | D | 558 | VAL |
| 1 | D | 566 | LYS |
| 1 | D | 620 | SER |
| 1 | D | 646 | ILE |
| 1 | D | 741 | GLU |
| 1 | D | 744 | TYR |
| 1 | D | 753 | VAL |
| 1 | D | 789 | VAL |
| 1 | D | 808 | VAL |
| 1 | D | 857 | VAL |
| 1 | D | 868 | VAL |
| 1 | D | 912 | PHE |
| 1 | D | 970 | GLU |
| 1 | D | 971 | GLU |
| 1 | D | 1003 | PRO |
| 1 | D | 1073 | PRO |
| 1 | D | 1119 | THR |
| 1 | D | 1135 | ARG |
| 1 | D | 1146 | ASN |
| 1 | D | 1217 | GLU |
| 1 | D | 1222 | THR |
| 1 | D | 1240 | PHE |
| 1 | D | 1277 | ASP |
| 1 | D | 1325 | ASN |
| 1 | D | 1327 | LYS |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | A | 63 | ASN |
| 1 | A | 71 | ASN |
| 1 | A | 131 | GLN |
| 1 | A | 351 | ASN |
| 1 | A | 450 | GLN |
| 1 | A | 473 | GLN |
| 1 | A | 531 | ASN |
| 1 | A | 551 | GLN |
| 1 | A | 586 | GLN |
| 1 | A | 651 | ASN |
| 1 | A | 1087 | ASN |
| 1 | A | 1146 | ASN |
| 1 | A | 1285 | GLN |
| 1 | A | 1290 | ASN |
| 1 | B | 63 | ASN |
| 1 | B | 131 | GLN |
| 1 | B | 351 | ASN |
| 1 | B | 450 | GLN |
| 1 | B | 473 | GLN |
| 1 | B | 531 | ASN |
| 1 | B | 651 | ASN |
| 1 | B | 748 | HIS |
| 1 | B | 1087 | ASN |
| 1 | B | 1109 | ASN |
| 1 | B | 1146 | ASN |
| 1 | B | 1285 | GLN |
| 1 | B | 1289 | ASN |
| 1 | B | 1325 | ASN |
| 1 | C | 63 | ASN |
| 1 | C | 131 | GLN |
| 1 | C | 322 | GLN |
| 1 | C | 351 | ASN |
| 1 | C | 450 | GLN |
| 1 | C | 461 | ASN |
| 1 | C | 473 | GLN |
| 1 | C | 484 | GLN |
| 1 | C | 529 | GLN |
| 1 | C | 586 | GLN |
| 1 | C | 651 | ASN |
| 1 | C | 684 | GLN |
| 1 | C | 876 | GLN |
| 1 | C | 1087 | ASN |
| 1 | C | 1109 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|------|------|
| 1 | C | 1146 | ASN |
| 1 | C | 1285 | GLN |
| 1 | D | 62 | GLN |
| 1 | D | 63 | ASN |
| 1 | D | 131 | GLN |
| 1 | D | 450 | GLN |
| 1 | D | 461 | ASN |
| 1 | D | 471 | GLN |
| 1 | D | 473 | GLN |
| 1 | D | 529 | GLN |
| 1 | D | 586 | GLN |
| 1 | D | 841 | HIS |
| 1 | D | 1087 | ASN |
| 1 | D | 1146 | ASN |
| 1 | D | 1285 | GLN |
| 1 | D | 1289 | ASN |
| 1 | D | 1290 | ASN |
| 1 | D | 1325 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 8 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 4 | FES | A | 2001 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 4 | FES | A | 2002 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 5 | FAD | A | 2003 | - | 48,58,58 | 2.70 | 20 (41%) | 54,89,89 | 3.28 | 20 (37%) |
| 6 | MTE | A | 2004 | 7 | 19,26,26 | 7.11 | 10 (52%) | 19,40,40 | 2.89 | 8 (42%) |
| 7 | MOM | A | 2005 | 6 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 8 | SAL | A | 2006 | - | 7,10,10 | 1.89 | 3 (42%) | 10,13,13 | 1.26 | 1 (10%) |
| 2 | BCT | A | 6001 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | FES | B | 2001 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 4 | FES | B | 2002 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 5 | FAD | B | 3003 | - | 48,58,58 | 2.73 | 22 (45%) | 54,89,89 | 3.26 | 20 (37%) |
| 6 | MTE | B | 3004 | 7 | 19,26,26 | 6.00 | 11 (57%) | 19,40,40 | 3.04 | 9 (47%) |
| 7 | MOM | B | 3005 | 6 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 8 | SAL | B | 3006 | - | 7,10,10 | 1.76 | 3 (42%) | 10,13,13 | 1.20 | 0 |
| 2 | BCT | B | 6002 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | FES | C | 2001 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 4 | FES | C | 2002 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 5 | FAD | C | 4003 | - | 48,58,58 | 2.73 | 20 (41%) | 54,89,89 | 3.27 | 20 (37%) |
| 6 | MTE | C | 4004 | 7 | 19,26,26 | 6.73 | 11 (57%) | 19,40,40 | 3.18 | 8 (42%) |
| 7 | MOM | C | 4005 | 6 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 8 | SAL | C | 4006 | - | 7,10,10 | 1.82 | 3 (42%) | 10,13,13 | 1.21 | 0 |
| 2 | BCT | C | 6003 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 4 | FES | D | 2001 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 4 | FES | D | 2002 | 1 | 0,4,4 | 0.00 | - | 0,4,4 | 0.00 | - |
| 5 | FAD | D | 5003 | - | 48,58,58 | 2.63 | 20 (41%) | 54,89,89 | 3.24 | 22 (40%) |
| 6 | MTE | D | 5004 | 7 | 19,26,26 | 6.61 | 12 (63%) | 19,40,40 | 2.79 | 9 (47%) |
| 7 | MOM | D | 5005 | 6 | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |
| 8 | SAL | D | 5006 | - | 7,10,10 | 1.89 | 3 (42%) | 10,13,13 | 1.24 | 0 |
| 2 | BCT | D | 6004 | - | 0,3,3 | 0.00 | - | 0,3,3 | 0.00 | - |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|----------|---------|
| 4 | FES | A | 2001 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 4 | FES | A | 2002 | 1 | - | 0/0/4/4 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|------------|---------|
| 5 | FAD | A | 2003 | - | - | 0/30/50/50 | 0/6/6/6 |
| 6 | MTE | A | 2004 | 7 | - | 0/6/34/34 | 0/3/3/3 |
| 7 | MOM | A | 2005 | 6 | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SAL | A | 2006 | - | - | 0/0/4/4 | 0/1/1/1 |
| 2 | BCT | A | 6001 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | FES | B | 2001 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 4 | FES | B | 2002 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 5 | FAD | B | 3003 | - | - | 0/30/50/50 | 0/6/6/6 |
| 6 | MTE | B | 3004 | 7 | - | 0/6/34/34 | 0/3/3/3 |
| 7 | MOM | B | 3005 | 6 | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SAL | B | 3006 | - | - | 0/0/4/4 | 0/1/1/1 |
| 2 | BCT | B | 6002 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | FES | C | 2001 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 4 | FES | C | 2002 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 5 | FAD | C | 4003 | - | - | 0/30/50/50 | 0/6/6/6 |
| 6 | MTE | C | 4004 | 7 | - | 0/6/34/34 | 0/3/3/3 |
| 7 | MOM | C | 4005 | 6 | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SAL | C | 4006 | - | - | 0/0/4/4 | 0/1/1/1 |
| 2 | BCT | C | 6003 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | FES | D | 2001 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 4 | FES | D | 2002 | 1 | - | 0/0/4/4 | 0/1/1/1 |
| 5 | FAD | D | 5003 | - | - | 0/30/50/50 | 0/6/6/6 |
| 6 | MTE | D | 5004 | 7 | - | 0/6/34/34 | 0/3/3/3 |
| 7 | MOM | D | 5005 | 6 | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SAL | D | 5006 | - | - | 0/0/4/4 | 0/1/1/1 |
| 2 | BCT | D | 6004 | - | - | 0/0/0/0 | 0/0/0/0 |

All (138) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | C | 4004 | MTE | O4'-C4' | -8.04 | 1.11 | 1.44 |
| 6 | D | 5004 | MTE | O4'-C4' | -7.83 | 1.12 | 1.44 |
| 6 | B | 3004 | MTE | P-O4' | -6.53 | 1.38 | 1.60 |
| 6 | C | 4004 | MTE | P-O4' | -6.40 | 1.38 | 1.60 |
| 6 | D | 5004 | MTE | P-O4' | -6.26 | 1.39 | 1.60 |
| 6 | A | 2004 | MTE | P-O4' | -6.20 | 1.39 | 1.60 |
| 6 | C | 4004 | MTE | C6-N5 | -5.14 | 1.38 | 1.45 |
| 6 | C | 4004 | MTE | P-O3P | -5.03 | 1.36 | 1.54 |
| 6 | D | 5004 | MTE | P-O3P | -4.93 | 1.37 | 1.54 |
| 6 | A | 2004 | MTE | P-O3P | -4.93 | 1.37 | 1.54 |
| 6 | B | 3004 | MTE | P-O3P | -4.69 | 1.37 | 1.54 |
| 5 | B | 3003 | FAD | C5A-N7A | -2.09 | 1.32 | 1.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 5 | C | 4003 | FAD | PA-O1A | 2.09 | 1.58 | 1.51 |
| 5 | B | 3003 | FAD | C6-C5X | 2.10 | 1.44 | 1.41 |
| 5 | B | 3003 | FAD | PA-O1A | 2.13 | 1.59 | 1.51 |
| 5 | D | 5003 | FAD | P-O1P | 2.14 | 1.59 | 1.51 |
| 5 | B | 3003 | FAD | P-O1P | 2.18 | 1.59 | 1.51 |
| 5 | C | 4003 | FAD | P-O1P | 2.18 | 1.59 | 1.51 |
| 5 | A | 2003 | FAD | PA-O1A | 2.18 | 1.59 | 1.51 |
| 6 | D | 5004 | MTE | P-O1P | 2.20 | 1.58 | 1.51 |
| 6 | B | 3004 | MTE | O3'-C3' | 2.21 | 1.46 | 1.43 |
| 6 | D | 5004 | MTE | C10-N8 | 2.21 | 1.39 | 1.35 |
| 5 | B | 3003 | FAD | C4'-C3' | 2.22 | 1.58 | 1.53 |
| 5 | D | 5003 | FAD | PA-O1A | 2.22 | 1.59 | 1.51 |
| 5 | B | 3003 | FAD | C5'-C4' | 2.23 | 1.55 | 1.51 |
| 8 | C | 4006 | SAL | C3-C2 | 2.26 | 1.43 | 1.39 |
| 5 | C | 4003 | FAD | C6-C7 | 2.26 | 1.44 | 1.37 |
| 5 | D | 5003 | FAD | C5'-C4' | 2.27 | 1.55 | 1.51 |
| 8 | B | 3006 | SAL | C6-C1 | 2.28 | 1.43 | 1.39 |
| 8 | D | 5006 | SAL | C3-C2 | 2.28 | 1.43 | 1.39 |
| 5 | C | 4003 | FAD | C4'-C3' | 2.28 | 1.58 | 1.53 |
| 8 | B | 3006 | SAL | C3-C2 | 2.30 | 1.43 | 1.39 |
| 5 | D | 5003 | FAD | C5X-N5 | 2.30 | 1.39 | 1.35 |
| 5 | A | 2003 | FAD | P-O1P | 2.31 | 1.59 | 1.51 |
| 5 | D | 5003 | FAD | C4'-C3' | 2.33 | 1.58 | 1.53 |
| 5 | A | 2003 | FAD | C6-C5X | 2.33 | 1.45 | 1.41 |
| 8 | A | 2006 | SAL | C3-C2 | 2.38 | 1.43 | 1.39 |
| 5 | B | 3003 | FAD | C5X-N5 | 2.41 | 1.39 | 1.35 |
| 5 | A | 2003 | FAD | C2A-N1A | 2.42 | 1.38 | 1.33 |
| 5 | C | 4003 | FAD | C2A-N1A | 2.44 | 1.38 | 1.33 |
| 8 | C | 4006 | SAL | C6-C1 | 2.45 | 1.44 | 1.39 |
| 5 | C | 4003 | FAD | C5X-N5 | 2.50 | 1.39 | 1.35 |
| 5 | B | 3003 | FAD | C8-C7 | 2.51 | 1.47 | 1.41 |
| 5 | D | 5003 | FAD | C8-C7 | 2.55 | 1.47 | 1.41 |
| 6 | D | 5004 | MTE | C2-N1 | 2.56 | 1.39 | 1.35 |
| 5 | A | 2003 | FAD | C6-C7 | 2.57 | 1.44 | 1.37 |
| 6 | A | 2004 | MTE | C10-N8 | 2.57 | 1.39 | 1.35 |
| 5 | D | 5003 | FAD | C6-C7 | 2.58 | 1.44 | 1.37 |
| 5 | A | 2003 | FAD | C8-C7 | 2.58 | 1.47 | 1.41 |
| 8 | D | 5006 | SAL | C6-C1 | 2.59 | 1.44 | 1.39 |
| 6 | C | 4004 | MTE | O4-C4 | 2.59 | 1.30 | 1.24 |
| 5 | D | 5003 | FAD | C2A-N1A | 2.59 | 1.38 | 1.33 |
| 8 | A | 2006 | SAL | C6-C1 | 2.61 | 1.44 | 1.39 |
| 5 | B | 3003 | FAD | C6-C7 | 2.62 | 1.45 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|------|-------------|----------|
| 6 | A | 2004 | MTE | O4-C4 | 2.63 | 1.31 | 1.24 |
| 5 | C | 4003 | FAD | C8-C7 | 2.64 | 1.48 | 1.41 |
| 5 | D | 5003 | FAD | C9-C9A | 2.67 | 1.46 | 1.40 |
| 5 | B | 3003 | FAD | C2A-N1A | 2.68 | 1.39 | 1.33 |
| 6 | B | 3004 | MTE | C10-N8 | 2.70 | 1.40 | 1.35 |
| 5 | A | 2003 | FAD | C5'-C4' | 2.73 | 1.55 | 1.51 |
| 6 | C | 4004 | MTE | C2-N1 | 2.76 | 1.40 | 1.35 |
| 5 | C | 4003 | FAD | C5'-C4' | 2.77 | 1.55 | 1.51 |
| 5 | B | 3003 | FAD | C9A-C5X | 2.78 | 1.48 | 1.42 |
| 8 | C | 4006 | SAL | C5-C6 | 2.78 | 1.44 | 1.38 |
| 5 | A | 2003 | FAD | C5X-N5 | 2.79 | 1.39 | 1.35 |
| 5 | B | 3003 | FAD | C4X-C10 | 2.79 | 1.46 | 1.41 |
| 5 | C | 4003 | FAD | C9-C9A | 2.80 | 1.46 | 1.40 |
| 5 | D | 5003 | FAD | C9A-C5X | 2.82 | 1.48 | 1.42 |
| 5 | D | 5003 | FAD | C4X-C10 | 2.82 | 1.46 | 1.41 |
| 8 | B | 3006 | SAL | C5-C6 | 2.83 | 1.44 | 1.38 |
| 5 | A | 2003 | FAD | C2A-N3A | 2.84 | 1.37 | 1.32 |
| 5 | C | 4003 | FAD | C4X-C10 | 2.86 | 1.46 | 1.41 |
| 5 | A | 2003 | FAD | C9-C9A | 2.88 | 1.47 | 1.40 |
| 5 | C | 4003 | FAD | C2A-N3A | 2.91 | 1.37 | 1.32 |
| 8 | D | 5006 | SAL | C5-C6 | 2.94 | 1.45 | 1.38 |
| 5 | A | 2003 | FAD | C4X-C10 | 2.95 | 1.46 | 1.41 |
| 6 | C | 4004 | MTE | C10-N8 | 2.97 | 1.40 | 1.35 |
| 6 | D | 5004 | MTE | O4-C4 | 2.98 | 1.31 | 1.24 |
| 5 | C | 4003 | FAD | C9A-C5X | 2.99 | 1.48 | 1.42 |
| 8 | A | 2006 | SAL | C5-C6 | 3.00 | 1.45 | 1.38 |
| 6 | B | 3004 | MTE | O4-C4 | 3.01 | 1.31 | 1.24 |
| 5 | B | 3003 | FAD | C9-C9A | 3.01 | 1.47 | 1.40 |
| 5 | D | 5003 | FAD | C2A-N3A | 3.01 | 1.37 | 1.32 |
| 5 | B | 3003 | FAD | O4B-C1B | 3.02 | 1.45 | 1.41 |
| 5 | A | 2003 | FAD | C9A-C5X | 3.09 | 1.48 | 1.42 |
| 5 | B | 3003 | FAD | C2A-N3A | 3.18 | 1.37 | 1.32 |
| 6 | B | 3004 | MTE | C2-N1 | 3.21 | 1.41 | 1.35 |
| 5 | B | 3003 | FAD | C4A-N3A | 3.35 | 1.40 | 1.35 |
| 5 | A | 2003 | FAD | C4A-N3A | 3.36 | 1.40 | 1.35 |
| 6 | A | 2004 | MTE | C2-N1 | 3.38 | 1.41 | 1.35 |
| 5 | D | 5003 | FAD | C4A-N3A | 3.39 | 1.40 | 1.35 |
| 5 | D | 5003 | FAD | O4B-C1B | 3.46 | 1.45 | 1.41 |
| 6 | B | 3004 | MTE | C9-N5 | 3.47 | 1.46 | 1.38 |
| 5 | C | 4003 | FAD | C4A-N3A | 3.48 | 1.40 | 1.35 |
| 5 | C | 4003 | FAD | O4B-C1B | 3.70 | 1.45 | 1.41 |
| 5 | C | 4003 | FAD | C4X-N5 | 3.74 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 6 | A | 2004 | MTE | C4-N3 | 3.76 | 1.40 | 1.33 |
| 5 | A | 2003 | FAD | O4B-C1B | 3.79 | 1.46 | 1.41 |
| 5 | B | 3003 | FAD | C4X-N5 | 3.83 | 1.39 | 1.33 |
| 6 | C | 4004 | MTE | C4-N3 | 3.88 | 1.40 | 1.33 |
| 5 | D | 5003 | FAD | C4X-N5 | 3.97 | 1.39 | 1.33 |
| 5 | A | 2003 | FAD | C4X-N5 | 4.04 | 1.39 | 1.33 |
| 6 | D | 5004 | MTE | C4-N3 | 4.32 | 1.41 | 1.33 |
| 6 | B | 3004 | MTE | C4-N3 | 4.49 | 1.41 | 1.33 |
| 5 | A | 2003 | FAD | C1'-N10 | 4.56 | 1.53 | 1.48 |
| 5 | B | 3003 | FAD | C1'-N10 | 4.77 | 1.53 | 1.48 |
| 5 | D | 5003 | FAD | C1'-N10 | 4.90 | 1.53 | 1.48 |
| 5 | C | 4003 | FAD | C1'-N10 | 5.12 | 1.53 | 1.48 |
| 5 | D | 5003 | FAD | C10-N1 | 5.28 | 1.44 | 1.35 |
| 5 | C | 4003 | FAD | C10-N1 | 5.46 | 1.44 | 1.35 |
| 5 | D | 5003 | FAD | C4-N3 | 5.71 | 1.43 | 1.33 |
| 5 | A | 2003 | FAD | C10-N1 | 5.76 | 1.45 | 1.35 |
| 5 | A | 2003 | FAD | C4-N3 | 6.01 | 1.44 | 1.33 |
| 5 | C | 4003 | FAD | C4-N3 | 6.11 | 1.44 | 1.33 |
| 5 | B | 3003 | FAD | C4-N3 | 6.16 | 1.44 | 1.33 |
| 5 | B | 3003 | FAD | C10-N1 | 6.18 | 1.45 | 1.35 |
| 6 | D | 5004 | MTE | C6-N5 | 6.36 | 1.54 | 1.45 |
| 5 | D | 5003 | FAD | C10-N10 | 6.95 | 1.47 | 1.39 |
| 5 | A | 2003 | FAD | C10-N10 | 7.10 | 1.47 | 1.39 |
| 5 | B | 3003 | FAD | C9A-N10 | 7.16 | 1.48 | 1.38 |
| 5 | D | 5003 | FAD | C9A-N10 | 7.16 | 1.48 | 1.38 |
| 6 | B | 3004 | MTE | C6-N5 | 7.31 | 1.55 | 1.45 |
| 5 | A | 2003 | FAD | C9A-N10 | 7.41 | 1.49 | 1.38 |
| 5 | C | 4003 | FAD | C10-N10 | 7.47 | 1.47 | 1.39 |
| 5 | C | 4003 | FAD | C9A-N10 | 7.60 | 1.49 | 1.38 |
| 5 | B | 3003 | FAD | C10-N10 | 7.70 | 1.48 | 1.39 |
| 6 | D | 5004 | MTE | C9-N5 | 10.07 | 1.61 | 1.38 |
| 6 | D | 5004 | MTE | C9-C10 | 10.39 | 1.62 | 1.41 |
| 6 | B | 3004 | MTE | C9-C10 | 10.43 | 1.62 | 1.41 |
| 6 | C | 4004 | MTE | C9-C10 | 10.44 | 1.62 | 1.41 |
| 6 | A | 2004 | MTE | C9-C10 | 10.63 | 1.63 | 1.41 |
| 6 | A | 2004 | MTE | C6-N5 | 12.86 | 1.63 | 1.45 |
| 6 | A | 2004 | MTE | C9-N5 | 13.15 | 1.68 | 1.38 |
| 6 | C | 4004 | MTE | C9-N5 | 13.28 | 1.68 | 1.38 |
| 6 | C | 4004 | MTE | C7-C6 | 19.21 | 1.67 | 1.53 |
| 6 | B | 3004 | MTE | C7-C6 | 19.49 | 1.68 | 1.53 |
| 6 | A | 2004 | MTE | C7-C6 | 19.95 | 1.68 | 1.53 |
| 6 | D | 5004 | MTE | C7-C6 | 20.07 | 1.68 | 1.53 |

All (117) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|--------|-------------|----------|
| 5 | C | 4003 | FAD | N3A-C2A-N1A | -14.56 | 117.75 | 128.89 |
| 5 | A | 2003 | FAD | N3A-C2A-N1A | -14.54 | 117.77 | 128.89 |
| 5 | B | 3003 | FAD | N3A-C2A-N1A | -14.37 | 117.89 | 128.89 |
| 5 | D | 5003 | FAD | N3A-C2A-N1A | -14.33 | 117.92 | 128.89 |
| 6 | C | 4004 | MTE | C10-C9-N5 | -6.10 | 111.16 | 118.85 |
| 6 | B | 3004 | MTE | C10-C9-N5 | -4.00 | 113.81 | 118.85 |
| 6 | B | 3004 | MTE | N3-C2-N1 | -3.82 | 119.27 | 125.53 |
| 6 | C | 4004 | MTE | N3-C2-N1 | -3.69 | 119.49 | 125.53 |
| 6 | D | 5004 | MTE | N3-C2-N1 | -3.68 | 119.50 | 125.53 |
| 6 | A | 2004 | MTE | N3-C2-N1 | -3.66 | 119.54 | 125.53 |
| 6 | C | 4004 | MTE | O3'-C7-C6 | -3.59 | 106.51 | 108.96 |
| 6 | B | 3004 | MTE | O3'-C7-C6 | -3.48 | 106.58 | 108.96 |
| 6 | A | 2004 | MTE | O3'-C7-C6 | -3.33 | 106.69 | 108.96 |
| 5 | C | 4003 | FAD | O3P-PA-O5B | -3.22 | 94.39 | 102.94 |
| 5 | A | 2003 | FAD | O3P-PA-O5B | -3.11 | 94.69 | 102.94 |
| 5 | B | 3003 | FAD | O3P-PA-O5B | -3.11 | 94.70 | 102.94 |
| 5 | D | 5003 | FAD | O3P-PA-O5B | -2.93 | 95.16 | 102.94 |
| 6 | A | 2004 | MTE | C9-N5-C6 | -2.78 | 111.16 | 118.65 |
| 5 | B | 3003 | FAD | C4X-C10-N10 | -2.75 | 118.90 | 120.52 |
| 5 | C | 4003 | FAD | C4X-C4-N3 | -2.59 | 120.04 | 123.59 |
| 5 | C | 4003 | FAD | O3B-C3B-C4B | -2.58 | 103.31 | 111.05 |
| 5 | A | 2003 | FAD | O3B-C3B-C4B | -2.57 | 103.34 | 111.05 |
| 5 | B | 3003 | FAD | O4B-C1B-N9A | -2.56 | 102.73 | 108.10 |
| 5 | B | 3003 | FAD | O3B-C3B-C4B | -2.54 | 103.43 | 111.05 |
| 5 | A | 2003 | FAD | C1B-N9A-C4A | -2.52 | 123.13 | 126.94 |
| 5 | C | 4003 | FAD | C1B-N9A-C4A | -2.50 | 123.17 | 126.94 |
| 5 | A | 2003 | FAD | C4-C4X-C10 | -2.49 | 118.35 | 119.94 |
| 6 | A | 2004 | MTE | C9-C10-N1 | -2.47 | 113.64 | 118.76 |
| 5 | B | 3003 | FAD | C4X-C4-N3 | -2.46 | 120.22 | 123.59 |
| 5 | D | 5003 | FAD | C4X-C4-N3 | -2.46 | 120.22 | 123.59 |
| 5 | A | 2003 | FAD | C4X-C4-N3 | -2.45 | 120.24 | 123.59 |
| 5 | C | 4003 | FAD | C4-C4X-C10 | -2.42 | 118.39 | 119.94 |
| 5 | D | 5003 | FAD | O3B-C3B-C4B | -2.39 | 103.87 | 111.05 |
| 6 | B | 3004 | MTE | C9-C10-N1 | -2.39 | 113.81 | 118.76 |
| 5 | D | 5003 | FAD | C1B-N9A-C4A | -2.39 | 123.34 | 126.94 |
| 5 | C | 4003 | FAD | C4X-C10-N10 | -2.38 | 119.12 | 120.52 |
| 6 | C | 4004 | MTE | C9-C10-N1 | -2.37 | 113.85 | 118.76 |
| 5 | D | 5003 | FAD | C4-C4X-C10 | -2.36 | 118.43 | 119.94 |
| 5 | D | 5003 | FAD | C4X-C10-N10 | -2.35 | 119.14 | 120.52 |
| 5 | B | 3003 | FAD | C9A-C5X-N5 | -2.27 | 118.99 | 122.36 |
| 5 | D | 5003 | FAD | C9A-C5X-N5 | -2.26 | 119.02 | 122.36 |
| 6 | D | 5004 | MTE | C9-C10-N1 | -2.23 | 114.14 | 118.76 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 5 | A | 2003 | FAD | C9A-C5X-N5 | -2.22 | 119.07 | 122.36 |
| 5 | C | 4003 | FAD | C9A-C5X-N5 | -2.21 | 119.09 | 122.36 |
| 5 | B | 3003 | FAD | C1B-N9A-C4A | -2.20 | 123.62 | 126.94 |
| 5 | D | 5003 | FAD | O4B-C1B-N9A | -2.20 | 103.50 | 108.10 |
| 5 | A | 2003 | FAD | C4X-C10-N10 | -2.11 | 119.28 | 120.52 |
| 5 | D | 5003 | FAD | C8M-C8-C9 | -2.03 | 114.75 | 120.28 |
| 5 | C | 4003 | FAD | C4A-C5A-N7A | -2.00 | 107.64 | 109.48 |
| 6 | D | 5004 | MTE | C10-C9-N5 | -2.00 | 116.33 | 118.85 |
| 8 | A | 2006 | SAL | C2-C1-C1' | 2.00 | 123.65 | 121.60 |
| 6 | D | 5004 | MTE | C9-C10-N8 | 2.03 | 120.47 | 118.34 |
| 6 | D | 5004 | MTE | O2P-P-O4' | 2.08 | 112.54 | 106.56 |
| 5 | A | 2003 | FAD | O5'-P-O1P | 2.09 | 117.72 | 109.62 |
| 5 | B | 3003 | FAD | C8M-C8-C7 | 2.12 | 125.39 | 120.73 |
| 5 | C | 4003 | FAD | C8M-C8-C7 | 2.14 | 125.43 | 120.73 |
| 6 | B | 3004 | MTE | C9-N5-C6 | 2.14 | 124.41 | 118.65 |
| 5 | A | 2003 | FAD | C8M-C8-C7 | 2.15 | 125.44 | 120.73 |
| 5 | B | 3003 | FAD | C2A-N1A-C6A | 2.19 | 122.68 | 118.77 |
| 5 | B | 3003 | FAD | O2'-C2'-C1' | 2.19 | 115.33 | 109.94 |
| 5 | D | 5003 | FAD | C8M-C8-C7 | 2.22 | 125.61 | 120.73 |
| 5 | B | 3003 | FAD | O5B-PA-O1A | 2.23 | 118.28 | 109.62 |
| 5 | D | 5003 | FAD | O2'-C2'-C1' | 2.26 | 115.49 | 109.94 |
| 5 | C | 4003 | FAD | O5B-PA-O1A | 2.30 | 118.54 | 109.62 |
| 5 | D | 5003 | FAD | C2A-N1A-C6A | 2.31 | 122.89 | 118.77 |
| 5 | D | 5003 | FAD | O5B-PA-O1A | 2.34 | 118.72 | 109.62 |
| 5 | C | 4003 | FAD | C2A-N1A-C6A | 2.35 | 122.96 | 118.77 |
| 5 | A | 2003 | FAD | O5B-PA-O1A | 2.38 | 118.86 | 109.62 |
| 5 | A | 2003 | FAD | C2A-N1A-C6A | 2.42 | 123.10 | 118.77 |
| 5 | C | 4003 | FAD | O2B-C2B-C3B | 2.54 | 120.07 | 111.83 |
| 5 | A | 2003 | FAD | O2B-C2B-C3B | 2.54 | 120.09 | 111.83 |
| 5 | A | 2003 | FAD | O3'-C3'-C4' | 2.66 | 115.45 | 108.75 |
| 5 | C | 4003 | FAD | O3'-C3'-C4' | 2.71 | 115.59 | 108.75 |
| 5 | B | 3003 | FAD | C4-C4X-N5 | 2.71 | 122.01 | 118.72 |
| 5 | D | 5003 | FAD | O2B-C2B-C3B | 2.75 | 120.77 | 111.83 |
| 5 | B | 3003 | FAD | O2B-C2B-C3B | 2.75 | 120.78 | 111.83 |
| 5 | D | 5003 | FAD | C4-C4X-N5 | 2.83 | 122.15 | 118.72 |
| 5 | C | 4003 | FAD | C4-C4X-N5 | 2.84 | 122.16 | 118.72 |
| 5 | D | 5003 | FAD | O3'-C3'-C4' | 2.87 | 115.97 | 108.75 |
| 5 | A | 2003 | FAD | C4-C4X-N5 | 2.90 | 122.23 | 118.72 |
| 5 | B | 3003 | FAD | O3'-C3'-C4' | 3.07 | 116.50 | 108.75 |
| 5 | A | 2003 | FAD | O4'-C4'-C3' | 3.96 | 118.97 | 109.02 |
| 5 | D | 5003 | FAD | O4'-C4'-C3' | 4.11 | 119.36 | 109.02 |
| 6 | A | 2004 | MTE | N2-C2-N3 | 4.12 | 124.02 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|------|-------------|----------|
| 6 | B | 3004 | MTE | N2-C2-N3 | 4.13 | 124.04 | 117.20 |
| 5 | C | 4003 | FAD | O4'-C4'-C3' | 4.14 | 119.43 | 109.02 |
| 6 | C | 4004 | MTE | N2-C2-N3 | 4.15 | 124.08 | 117.20 |
| 5 | B | 3003 | FAD | O4'-C4'-C3' | 4.24 | 119.68 | 109.02 |
| 6 | D | 5004 | MTE | N2-C2-N3 | 4.29 | 124.31 | 117.20 |
| 6 | D | 5004 | MTE | C4-N3-C2 | 4.98 | 122.85 | 115.94 |
| 6 | A | 2004 | MTE | C4-N3-C2 | 5.00 | 122.87 | 115.94 |
| 6 | C | 4004 | MTE | C4-N3-C2 | 5.02 | 122.91 | 115.94 |
| 6 | B | 3004 | MTE | C4-N3-C2 | 5.09 | 123.00 | 115.94 |
| 6 | D | 5004 | MTE | N8-C10-N1 | 5.52 | 125.40 | 116.62 |
| 6 | C | 4004 | MTE | C2-N1-C10 | 5.79 | 127.56 | 114.54 |
| 6 | A | 2004 | MTE | C2-N1-C10 | 5.81 | 127.60 | 114.54 |
| 6 | B | 3004 | MTE | N8-C10-N1 | 5.93 | 126.05 | 116.62 |
| 6 | A | 2004 | MTE | N8-C10-N1 | 5.93 | 126.06 | 116.62 |
| 6 | B | 3004 | MTE | C2-N1-C10 | 5.96 | 127.95 | 114.54 |
| 6 | C | 4004 | MTE | N8-C10-N1 | 5.97 | 126.13 | 116.62 |
| 6 | D | 5004 | MTE | C2-N1-C10 | 5.97 | 127.97 | 114.54 |
| 5 | A | 2003 | FAD | C4X-N5-C5X | 6.93 | 124.73 | 116.76 |
| 5 | D | 5003 | FAD | C4-N3-C2 | 6.95 | 121.25 | 115.25 |
| 5 | D | 5003 | FAD | C4X-N5-C5X | 7.01 | 124.83 | 116.76 |
| 5 | C | 4003 | FAD | C4-N3-C2 | 7.04 | 121.33 | 115.25 |
| 5 | C | 4003 | FAD | C4X-N5-C5X | 7.21 | 125.05 | 116.76 |
| 5 | B | 3003 | FAD | C2B-C1B-N9A | 7.23 | 125.33 | 114.29 |
| 5 | B | 3003 | FAD | C4-N3-C2 | 7.25 | 121.51 | 115.25 |
| 5 | B | 3003 | FAD | C1'-N10-C9A | 7.33 | 127.10 | 118.86 |
| 5 | B | 3003 | FAD | C4X-N5-C5X | 7.34 | 125.21 | 116.76 |
| 5 | A | 2003 | FAD | C4-N3-C2 | 7.38 | 121.62 | 115.25 |
| 5 | C | 4003 | FAD | C1'-N10-C9A | 7.55 | 127.33 | 118.86 |
| 5 | C | 4003 | FAD | C2B-C1B-N9A | 7.55 | 125.83 | 114.29 |
| 5 | D | 5003 | FAD | C2B-C1B-N9A | 7.57 | 125.86 | 114.29 |
| 5 | D | 5003 | FAD | C1'-N10-C9A | 7.60 | 127.39 | 118.86 |
| 5 | A | 2003 | FAD | C1'-N10-C9A | 7.71 | 127.52 | 118.86 |
| 5 | A | 2003 | FAD | C2B-C1B-N9A | 7.90 | 126.36 | 114.29 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 32 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 5 | A | 2003 | FAD | 2 | 0 |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6 | A | 2004 | MTE | 4 | 0 |
| 7 | A | 2005 | MOM | 2 | 0 |
| 2 | A | 6001 | BCT | 1 | 0 |
| 5 | B | 3003 | FAD | 3 | 0 |
| 6 | B | 3004 | MTE | 2 | 0 |
| 7 | B | 3005 | MOM | 2 | 0 |
| 2 | B | 6002 | BCT | 1 | 0 |
| 5 | C | 4003 | FAD | 2 | 0 |
| 6 | C | 4004 | MTE | 2 | 0 |
| 7 | C | 4005 | MOM | 2 | 0 |
| 4 | D | 2002 | FES | 1 | 0 |
| 5 | D | 5003 | FAD | 3 | 0 |
| 6 | D | 5004 | MTE | 2 | 0 |
| 7 | D | 5005 | MOM | 3 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1 | A | 1307/1333 (98%) | -0.36 | 11 (0%) 87 85 | 10, 27, 56, 169 | 0 |
| 1 | B | 1307/1333 (98%) | -0.44 | 5 (0%) 93 91 | 10, 25, 52, 166 | 0 |
| 1 | C | 1307/1333 (98%) | -0.40 | 8 (0%) 90 88 | 9, 26, 54, 156 | 0 |
| 1 | D | 1307/1333 (98%) | -0.43 | 9 (0%) 89 87 | 8, 25, 55, 150 | 0 |
| All | All | 5228/5332 (98%) | -0.41 | 33 (0%) 90 88 | 8, 26, 55, 169 | 0 |

All (33) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | B | 1321 | GLY | 5.0 |
| 1 | B | 1325 | ASN | 4.8 |
| 1 | C | 1289 | ASN | 4.8 |
| 1 | D | 1325 | ASN | 4.5 |
| 1 | B | 566 | LYS | 4.2 |
| 1 | A | 538 | LYS | 3.9 |
| 1 | B | 1324 | GLU | 3.9 |
| 1 | A | 1288 | GLY | 3.4 |
| 1 | D | 566 | LYS | 3.3 |
| 1 | D | 167 | GLY | 3.2 |
| 1 | C | 1112 | GLY | 3.1 |
| 1 | D | 1324 | GLU | 2.9 |
| 1 | C | 1111 | SER | 2.8 |
| 1 | C | 60 | ARG | 2.8 |
| 1 | A | 1289 | ASN | 2.8 |
| 1 | D | 3 | ALA | 2.7 |
| 1 | A | 566 | LYS | 2.7 |
| 1 | C | 566 | LYS | 2.6 |
| 1 | A | 219 | LEU | 2.5 |
| 1 | D | 1323 | PRO | 2.5 |
| 1 | A | 3 | ALA | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|------|------|------|
| 1 | A | 223 | PRO | 2.4 |
| 1 | B | 1323 | PRO | 2.3 |
| 1 | A | 1325 | ASN | 2.3 |
| 1 | C | 167 | GLY | 2.3 |
| 1 | C | 472 | ARG | 2.2 |
| 1 | A | 1111 | SER | 2.1 |
| 1 | D | 1332 | ARG | 2.1 |
| 1 | A | 192 | SER | 2.1 |
| 1 | D | 377 | ARG | 2.1 |
| 1 | A | 1110 | PRO | 2.0 |
| 1 | D | 1322 | VAL | 2.0 |
| 1 | C | 687 | LYS | 2.0 |

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|----------------------------|-------|
| 3 | CA | B | 7004 | 1/1 | 0.97 | 0.38 | 11.52 | 18,18,18,18 | 0 |
| 3 | CA | A | 7002 | 1/1 | 0.97 | 0.38 | 10.86 | 18,18,18,18 | 0 |
| 3 | CA | C | 7006 | 1/1 | 0.98 | 0.36 | 7.63 | 18,18,18,18 | 0 |
| 3 | CA | D | 7008 | 1/1 | 0.98 | 0.26 | 6.98 | 23,23,23,23 | 0 |
| 8 | SAL | D | 5006 | 10/10 | 0.92 | 0.20 | 3.43 | 41,42,42,43 | 0 |
| 8 | SAL | B | 3006 | 10/10 | 0.91 | 0.20 | 2.32 | 41,42,42,43 | 0 |
| 8 | SAL | A | 2006 | 10/10 | 0.93 | 0.18 | 2.17 | 36,37,37,38 | 0 |
| 8 | SAL | C | 4006 | 10/10 | 0.91 | 0.19 | 2.01 | 36,37,37,38 | 0 |
| 5 | FAD | C | 4003 | 53/53 | 0.96 | 0.17 | 1.87 | 26,36,47,49 | 0 |

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| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-------|-----------------------------|-------|
| 5 | FAD | D | 5003 | 53/53 | 0.96 | 0.16 | 1.41 | 26,35,45,47 | 0 |
| 2 | BCT | C | 6003 | 4/4 | 0.94 | 0.19 | 1.33 | 17,18,19,19 | 0 |
| 3 | CA | B | 7003 | 1/1 | 0.91 | 0.20 | 1.31 | 20,20,20,20 | 0 |
| 5 | FAD | B | 3003 | 53/53 | 0.96 | 0.16 | 1.30 | 26,34,47,49 | 0 |
| 5 | FAD | A | 2003 | 53/53 | 0.97 | 0.15 | 0.92 | 26,36,46,48 | 0 |
| 3 | CA | D | 7007 | 1/1 | 0.96 | 0.18 | 0.61 | 20,20,20,20 | 0 |
| 3 | CA | A | 7001 | 1/1 | 0.95 | 0.18 | 0.59 | 20,20,20,20 | 0 |
| 2 | BCT | A | 6001 | 4/4 | 0.95 | 0.17 | 0.53 | 17,18,19,19 | 0 |
| 2 | BCT | D | 6004 | 4/4 | 0.94 | 0.17 | -0.31 | 17,18,19,19 | 0 |
| 3 | CA | C | 7005 | 1/1 | 0.97 | 0.14 | -0.80 | 20,20,20,20 | 0 |
| 7 | MOM | A | 2005 | 4/4 | 0.99 | 0.14 | -0.91 | 28,29,30,31 | 0 |
| 7 | MOM | C | 4005 | 4/4 | 0.99 | 0.14 | -1.21 | 28,29,30,31 | 0 |
| 4 | FES | A | 2001 | 4/4 | 0.96 | 0.12 | -1.39 | 14,14,14,33 | 0 |
| 7 | MOM | D | 5005 | 4/4 | 0.99 | 0.14 | -1.45 | 27,28,28,29 | 0 |
| 6 | MTE | D | 5004 | 24/24 | 0.94 | 0.13 | -1.53 | 19,23,28,30 | 0 |
| 4 | FES | C | 2002 | 4/4 | 0.99 | 0.09 | -1.73 | 14,14,14,14 | 0 |
| 4 | FES | B | 2002 | 4/4 | 0.99 | 0.09 | -1.84 | 14,14,14,14 | 0 |
| 2 | BCT | B | 6002 | 4/4 | 0.97 | 0.12 | -1.88 | 17,18,19,19 | 0 |
| 4 | FES | D | 2002 | 4/4 | 0.99 | 0.08 | -1.94 | 14,14,14,14 | 0 |
| 7 | MOM | B | 3005 | 4/4 | 0.99 | 0.13 | -1.96 | 27,28,28,29 | 0 |
| 6 | MTE | C | 4004 | 24/24 | 0.95 | 0.12 | -2.09 | 20,24,28,30 | 0 |
| 6 | MTE | B | 3004 | 24/24 | 0.95 | 0.12 | -2.15 | 19,23,28,30 | 0 |
| 6 | MTE | A | 2004 | 24/24 | 0.96 | 0.12 | -2.19 | 20,24,28,30 | 0 |
| 4 | FES | D | 2001 | 4/4 | 0.99 | 0.09 | -2.55 | 14,14,14,14 | 0 |
| 4 | FES | A | 2002 | 4/4 | 0.99 | 0.08 | -2.65 | 14,14,14,14 | 0 |
| 4 | FES | B | 2001 | 4/4 | 0.99 | 0.10 | -3.00 | 14,14,14,14 | 0 |
| 4 | FES | C | 2001 | 4/4 | 0.99 | 0.09 | -3.15 | 14,14,14,14 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.