# Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 11:01 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 1NT4 |
| Title | : | Crystal structure of Escherichia coli periplasmic glucose-1-phosphatase H18A mutant complexed with glucose-1-phosphate |
| Authors | : | Lee, D.C.; Cottrill, M.A.; Forsberg, C.W.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI) |
| Deposited on | : | 2003-01-28 |
| Resolution | : | 2.40 Å(reported) |

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

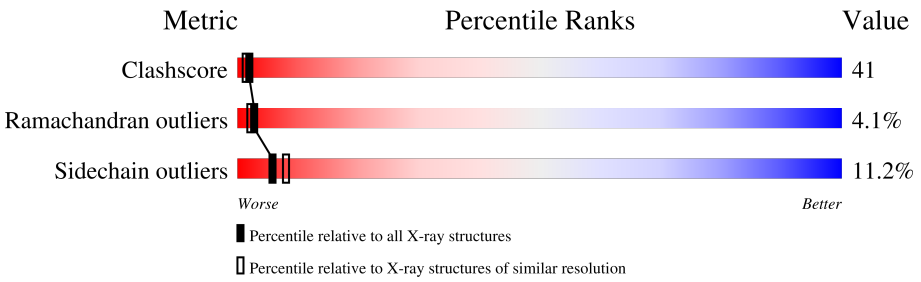
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.23.2 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

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




| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| Clashscore | 141614 | 4398 (2.40-2.40) |
| Ramachandran outliers | 138981 | 4318 (2.40-2.40) |
| Sidechain outliers | 138945 | 4319 (2.40-2.40) |

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

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 391 | 44% 46% 9% • |
| 1 | B | 391 | 46% 43% 10% • |

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 |
|---|---|---|---|---|---|---|---|
| 2 | XGP | A | 2000 | - | - | X | - |
| 2 | XGP | B | 2001 | - | - | X | - |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6499 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.

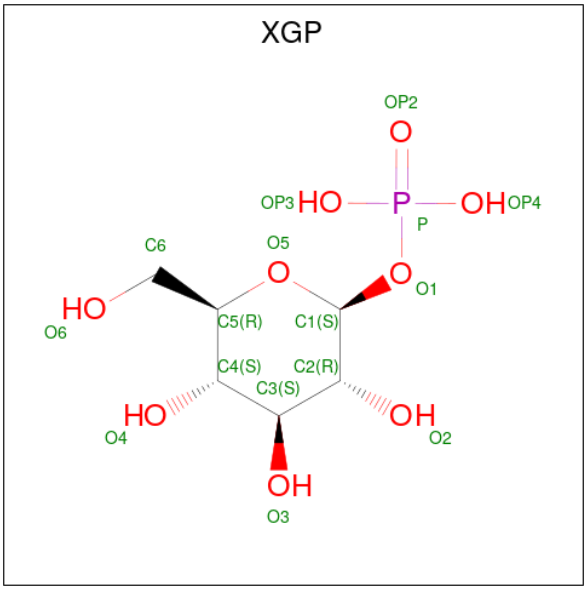
- Molecule 1 is a protein called Glucose-1-phosphatase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 391 | 3058 | 1935 | 513 | 593 | 17 | 0 | 0 | 0 |
| 1 | B | 391 | 3058 | 1935 | 513 | 593 | 17 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 18 | ALA | HIS | engineered mutation | UNP P19926 |
| B | 1018 | ALA | HIS | engineered mutation | UNP P19926 |

- Molecule 2 is 1-O-phosphono-beta-D-glucopyranose (three-letter code: XGP) (formula: $C_6H_{13}O_9P$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | | |
| 2 | A | 1 | 16 | 6 | 9 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | | |
| 2 | B | 1 | 16 | 6 | 9 | 1 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 3 | A | 181 | 181 | 181 | 0 | 0 |
| | | | Total | O | | |
| 3 | B | 170 | 170 | 170 | 0 | 0 |

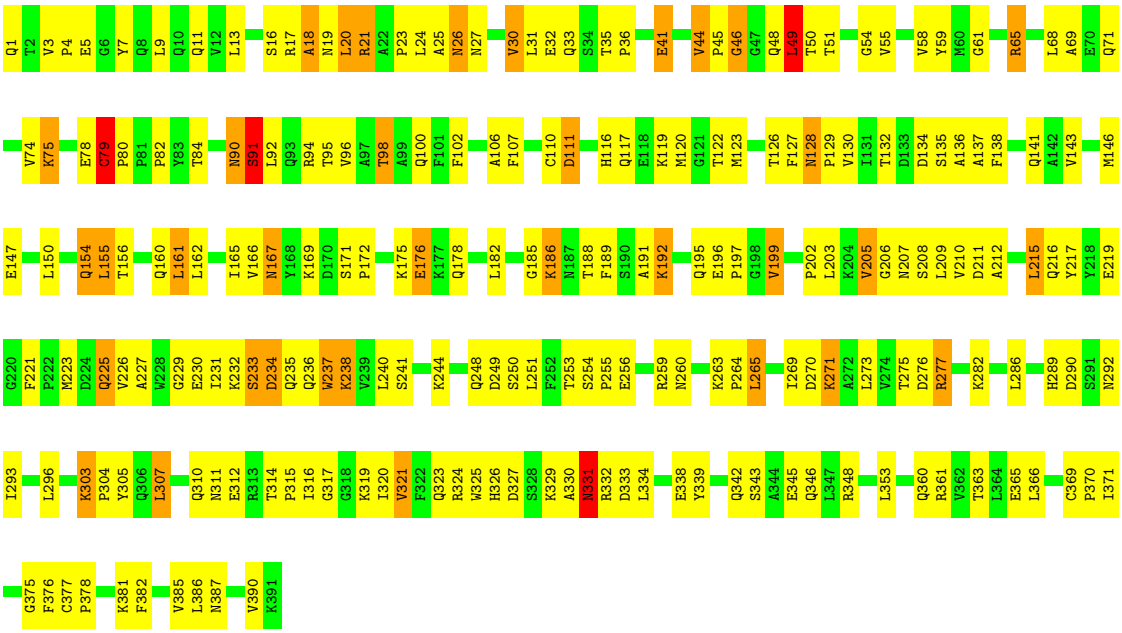
# 3 Residue-property plots (i)

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

Note EDS was not executed.

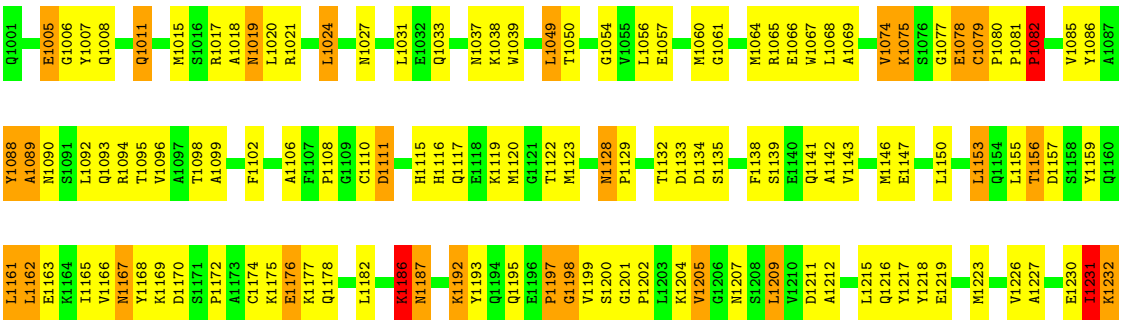
• Molecule 1: Glucose-1-phosphatase

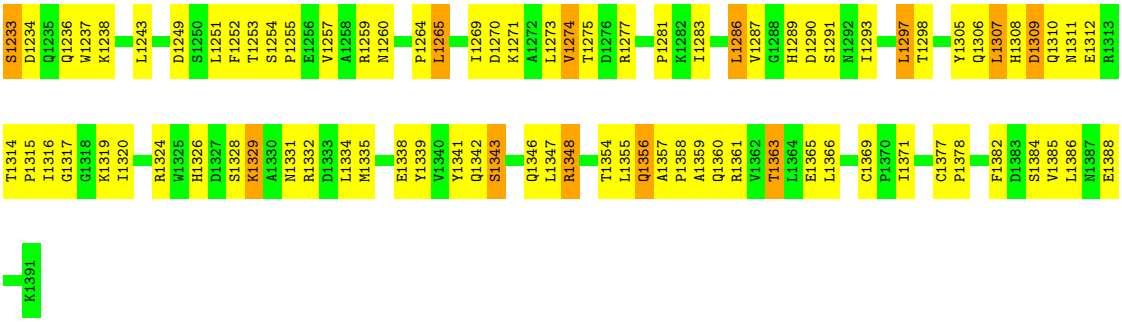
Chain A: 44% 46% 9% •




• Molecule 1: Glucose-1-phosphatase

Chain B: 46% 43% 10% •




S1233
D1234
Q1235
Q1236
W1237
K1238
L1243
D1249
S1250
L1251
F1252
T1253
S1254
P1255
E1256
V1257
A1258
R1259
N1260
P1264
L1265
I1269
D1270
K1271
A1272
L1273
V1274
T1275
D1276
R1277
P1281
K1282
I1283
L1286
V1287
G1288
H1289
D1290
S1291
N1292
I1293
L1297
T1298
Y1305
Q1306
L1307
H1308
D1309
Q1310
N1311
E1312
R1313
T1314
P1315
I1316
G1317
G1318
K1319
I1320
R1324
W1325
H1326
D1327
S1328
K1329
A1330
N1331
R1332
D1333
L1334
M1335
E1338
Y1339
V1340
Y1341
Q1342
S1343
Q1346
L1347
R1348
T1354
L1355
Q1356
A1357
P1358
A1359
Q1360
R1361
V1362
T1363
L1364
E1365
L1366
C1369
P1370
I1371
C1377
P1378
F1382
D1383
S1384
V1385
L1386
N1387
E1388
K1391

# 4 Data and refinement statistics (i)

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

| Property | Value | Source |
|---|---|---|
| Space group | H 3 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 156.26Å 156.26Å 84.58Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 30.00 – 2.40 | Depositor |
| % Data completeness<br>(in resolution range) | 91.9 (30.00-2.40) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | 0.08 | Depositor |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.218 , 0.284 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 6499 | wwPDB-VP |
| Average B, all atoms ($Å^2$) | 30.0 | wwPDB-VP |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| >5$ | RMSZ | $\#\|Z\| >5$ |
| 1 | A | 0.39 | 0/3128 | 0.66 | 1/4248 (0.0%) |
| 1 | B | 0.40 | 0/3128 | 0.68 | 1/4248 (0.0%) |
| All | All | 0.40 | 0/6256 | 0.67 | 2/8496 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 49 | LEU | CA-CB-CG | 6.42 | 130.07 | 115.30 |
| 1 | B | 1356 | GLN | N-CA-C | -5.17 | 97.06 | 111.00 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3058 | 0 | 2996 | 243 | 0 |
| 1 | B | 3058 | 0 | 2993 | 256 | 0 |
| 2 | A | 16 | 0 | 10 | 6 | 0 |
| 2 | B | 16 | 0 | 10 | 6 | 0 |
| 3 | A | 181 | 0 | 0 | 21 | 0 |
| 3 | B | 170 | 0 | 0 | 14 | 0 |
| All | All | 6499 | 0 | 6009 | 501 | 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 41.

All (501) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:332:ARG:HH12 | 1:A:334:LEU:HD11 | 1.17 | 1.08 |
| 1:A:223:MET:HB3 | 1:A:232:LYS:HD2 | 1.37 | 1.07 |
| 1:A:186:LYS:H | 1:A:186:LYS:HD2 | 1.19 | 1.03 |
| 1:B:1231:ILE:CD1 | 1:B:1232:LYS:H | 1.73 | 1.02 |
| 1:B:1277:ARG:HD2 | 1:B:1324:ARG:HH21 | 1.26 | 1.00 |
| 1:B:1231:ILE:HD13 | 1:B:1232:LYS:H | 1.25 | 1.00 |
| 1:B:1031:LEU:HD13 | 1:B:1209:LEU:HD12 | 1.44 | 0.98 |
| 1:B:1186:LYS:HG2 | 1:B:1187:ASN:H | 1.29 | 0.98 |
| 1:A:199:VAL:HG22 | 1:A:251:LEU:HD21 | 1.48 | 0.96 |
| 1:A:92:LEU:O | 1:A:96:VAL:HG12 | 1.67 | 0.95 |
| 1:B:1186:LYS:O | 1:B:1187:ASN:HB2 | 1.67 | 0.94 |
| 1:B:1343:SER:H | 1:B:1346:GLN:HE21 | 1.00 | 0.93 |
| 1:B:1310:GLN:HG2 | 1:B:1315:PRO:HG3 | 1.50 | 0.92 |
| 1:B:1227:ALA:HB3 | 1:B:1231:ILE:HG13 | 1.51 | 0.92 |
| 1:B:1343:SER:H | 1:B:1346:GLN:NE2 | 1.68 | 0.91 |
| 1:B:1293:ILE:HG23 | 1:B:1320:ILE:HD11 | 1.51 | 0.91 |
| 1:B:1289:HIS:CG | 2:B:2001:XGP:O6 | 2.24 | 0.91 |
| 1:A:49:LEU:HD23 | 1:A:98:THR:HG22 | 1.55 | 0.89 |
| 1:A:199:VAL:HG11 | 1:A:203:LEU:HD23 | 1.56 | 0.87 |
| 1:A:169:LYS:O | 1:A:169:LYS:HD3 | 1.75 | 0.86 |
| 2:A:2000:XGP:H6 | 3:A:3181:HOH:O | 1.74 | 0.86 |
| 1:B:1011:GLN:HE21 | 1:B:1277:ARG:HD3 | 1.41 | 0.85 |
| 1:B:1277:ARG:HD2 | 1:B:1324:ARG:NH2 | 1.91 | 0.85 |
| 1:B:1343:SER:N | 1:B:1346:GLN:HE21 | 1.75 | 0.85 |
| 1:B:1019:ASN:HD22 | 1:B:1020:LEU:H | 1.19 | 0.84 |
| 1:B:1146:MET:HE1 | 1:B:1197:PRO:O | 1.76 | 0.84 |
| 1:A:90:ASN:H | 1:A:90:ASN:HD22 | 1.22 | 0.84 |
| 1:B:1234:ASP:OD2 | 1:B:1236:GLN:HG3 | 1.79 | 0.83 |
| 1:B:1005:GLU:CD | 1:B:1006:GLY:H | 1.81 | 0.82 |
| 1:A:332:ARG:NH1 | 1:A:334:LEU:HD11 | 1.95 | 0.81 |
| 1:A:132:THR:H | 1:A:260:ASN:HD21 | 1.27 | 0.80 |
| 1:A:310:GLN:HG2 | 1:A:315:PRO:HG3 | 1.62 | 0.79 |
| 1:A:5:GLU:CD | 1:A:5:GLU:H | 1.85 | 0.79 |
| 1:A:35:THR:HB | 1:A:166:VAL:HG13 | 1.65 | 0.79 |
| 1:B:1226:VAL:O | 1:B:1231:ILE:HD11 | 1.83 | 0.78 |
| 1:B:1289:HIS:ND1 | 2:B:2001:XGP:OP4 | 2.15 | 0.78 |
| 1:A:79:CYS:SG | 1:A:80:PRO:HD2 | 2.25 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:192:LYS:CD | 1:A:195:GLN:HB2 | 2.14 | 0.77 |
| 1:A:289:HIS:CG | 2:A:2000:XGP:O6 | 2.37 | 0.77 |
| 1:B:1238:LYS:HD2 | 1:B:1311:ASN:ND2 | 2.00 | 0.77 |
| 1:A:186:LYS:H | 1:A:186:LYS:CD | 1.89 | 0.77 |
| 1:B:1332:ARG:HE | 1:B:1334:LEU:HD21 | 1.50 | 0.76 |
| 1:B:1132:THR:H | 1:B:1260:ASN:HD21 | 1.33 | 0.76 |
| 1:B:1192:LYS:HD3 | 1:B:1195:GLN:NE2 | 2.01 | 0.76 |
| 1:A:366:LEU:HD23 | 1:A:385:VAL:HG11 | 1.68 | 0.75 |
| 1:B:1031:LEU:HD12 | 1:B:1039:TRP:CZ2 | 2.21 | 0.74 |
| 1:A:303:LYS:HG3 | 1:A:304:PRO:HD2 | 1.69 | 0.74 |
| 1:A:19:ASN:HD22 | 1:A:20:LEU:H | 1.33 | 0.74 |
| 1:A:227:ALA:HB3 | 1:A:231:ILE:HG22 | 1.68 | 0.73 |
| 1:B:1169:LYS:O | 1:B:1170:ASP:HB2 | 1.88 | 0.73 |
| 1:A:90:ASN:HB3 | 1:A:127:PHE:CD2 | 2.24 | 0.73 |
| 1:A:119:LYS:HE2 | 1:A:122:THR:HG21 | 1.69 | 0.73 |
| 1:B:1238:LYS:HD2 | 1:B:1311:ASN:HD21 | 1.50 | 0.72 |
| 1:B:1265:LEU:O | 1:B:1269:ILE:HG12 | 1.89 | 0.72 |
| 1:A:186:LYS:HD2 | 1:A:186:LYS:N | 1.98 | 0.72 |
| 1:B:1186:LYS:HD2 | 1:B:1186:LYS:N | 2.05 | 0.72 |
| 1:B:1231:ILE:CD1 | 1:B:1232:LYS:N | 2.52 | 0.72 |
| 1:B:1270:ASP:O | 1:B:1274:VAL:HG13 | 1.90 | 0.72 |
| 1:A:161:LEU:HD11 | 1:A:236:GLN:HB3 | 1.71 | 0.71 |
| 1:A:265:LEU:O | 1:A:269:ILE:HG12 | 1.90 | 0.71 |
| 1:A:17:ARG:HD2 | 1:A:314:THR:HG22 | 1.73 | 0.71 |
| 1:A:25:ALA:HB2 | 1:A:46:GLY:HA2 | 1.73 | 0.71 |
| 1:A:233:SER:HB3 | 1:A:236:GLN:NE2 | 2.06 | 0.71 |
| 1:B:1186:LYS:HD2 | 1:B:1186:LYS:H | 1.54 | 0.71 |
| 1:A:90:ASN:HB3 | 1:A:127:PHE:HD2 | 1.56 | 0.71 |
| 1:B:1146:MET:CE | 1:B:1197:PRO:HB2 | 2.21 | 0.71 |
| 1:A:51:THR:O | 1:A:55:VAL:HG23 | 1.90 | 0.71 |
| 1:B:1088:TYR:O | 1:B:1089:ALA:HB3 | 1.91 | 0.71 |
| 1:A:377:CYS:SG | 1:A:378:PRO:HD2 | 2.30 | 0.70 |
| 1:B:1186:LYS:CG | 1:B:1187:ASN:H | 2.03 | 0.70 |
| 1:B:1293:ILE:HG23 | 1:B:1320:ILE:CD1 | 2.22 | 0.70 |
| 1:A:44:VAL:HG13 | 1:A:48:GLN:HB2 | 1.74 | 0.70 |
| 1:B:1135:SER:HB3 | 1:B:1138:PHE:HB3 | 1.72 | 0.69 |
| 1:A:249:ASP:O | 1:A:253:THR:HB | 1.92 | 0.69 |
| 1:B:1031:LEU:HD12 | 1:B:1039:TRP:CH2 | 2.27 | 0.69 |
| 1:A:166:VAL:HG21 | 1:A:209:LEU:HD23 | 1.75 | 0.69 |
| 1:B:1231:ILE:O | 1:B:1233:SER:N | 2.26 | 0.69 |
| 1:B:1110:CYS:O | 1:B:1111:ASP:HB2 | 1.93 | 0.68 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:17:ARG:O | 1:A:17:ARG:HG2 | 1.93 | 0.68 |
| 1:A:165:ILE:HG23 | 1:A:230:GLU:CB | 2.24 | 0.68 |
| 1:A:18:ALA:HA | 1:A:98:THR:HG21 | 1.76 | 0.68 |
| 1:B:1249:ASP:O | 1:B:1253:THR:HB | 1.94 | 0.68 |
| 1:B:1289:HIS:CB | 2:B:2001:XGP:O6 | 2.41 | 0.68 |
| 1:A:192:LYS:HD3 | 1:A:195:GLN:HB2 | 1.75 | 0.68 |
| 1:A:123:MET:HE3 | 1:A:128:ASN:HA | 1.76 | 0.67 |
| 1:B:1049:LEU:HD13 | 1:B:1050:THR:O | 1.93 | 0.67 |
| 1:A:143:VAL:O | 1:A:147:GLU:HG3 | 1.95 | 0.67 |
| 1:B:1314:THR:O | 1:B:1314:THR:HG22 | 1.95 | 0.67 |
| 1:B:1018:ALA:O | 1:B:1316:ILE:O | 2.12 | 0.66 |
| 1:A:223:MET:HE2 | 1:A:223:MET:HA | 1.77 | 0.66 |
| 1:B:1227:ALA:CB | 1:B:1231:ILE:HG13 | 2.24 | 0.66 |
| 1:B:1020:LEU:O | 1:B:1049:LEU:O | 2.13 | 0.66 |
| 1:B:1098:THR:HG23 | 1:B:1287:VAL:HG11 | 1.78 | 0.66 |
| 1:A:94:ARG:O | 1:A:98:THR:HG23 | 1.96 | 0.66 |
| 1:B:1290:ASP:HB2 | 1:B:1314:THR:HG21 | 1.78 | 0.66 |
| 1:B:1186:LYS:HG2 | 1:B:1187:ASN:N | 2.08 | 0.65 |
| 1:A:226:VAL:HG23 | 1:A:226:VAL:O | 1.96 | 0.65 |
| 1:B:1186:LYS:H | 1:B:1186:LYS:HZ3 | 1.42 | 0.65 |
| 1:A:18:ALA:O | 1:A:316:ILE:O | 2.15 | 0.65 |
| 1:B:1015:MET:HG3 | 1:B:1293:ILE:CD1 | 2.26 | 0.65 |
| 1:B:1371:ILE:HD11 | 3:B:3175:HOH:O | 1.96 | 0.65 |
| 1:A:270:ASP:HB2 | 1:A:386:LEU:HB3 | 1.79 | 0.65 |
| 1:A:233:SER:HB3 | 1:A:236:GLN:HE21 | 1.61 | 0.65 |
| 1:A:175:LYS:O | 1:A:176:GLU:HB2 | 1.97 | 0.65 |
| 1:A:19:ASN:ND2 | 1:A:20:LEU:H | 1.95 | 0.65 |
| 1:B:1011:GLN:NE2 | 1:B:1277:ARG:NH1 | 2.45 | 0.65 |
| 1:B:1128:ASN:HD22 | 1:B:1129:PRO:HD2 | 1.61 | 0.65 |
| 1:A:96:VAL:O | 1:A:100:GLN:HG3 | 1.95 | 0.64 |
| 1:B:1119:LYS:HD3 | 1:B:1122:THR:HG21 | 1.79 | 0.64 |
| 1:A:20:LEU:HD11 | 1:A:219:GLU:HA | 1.78 | 0.64 |
| 1:A:65:ARG:HH21 | 1:A:74:VAL:HG11 | 1.61 | 0.64 |
| 1:A:192:LYS:HD2 | 1:A:192:LYS:O | 1.98 | 0.64 |
| 1:B:1186:LYS:H | 1:B:1186:LYS:CD | 2.11 | 0.64 |
| 1:B:1172:PRO:O | 1:B:1176:GLU:HB3 | 1.98 | 0.63 |
| 1:A:20:LEU:HD23 | 1:A:215:LEU:HD12 | 1.81 | 0.63 |
| 1:B:1384:SER:O | 1:B:1388:GLU:HB2 | 1.99 | 0.63 |
| 1:B:1175:LYS:HD2 | 1:B:1175:LYS:O | 1.98 | 0.63 |
| 1:A:156:THR:O | 1:A:160:GLN:HG3 | 1.99 | 0.62 |
| 1:A:212:ALA:O | 1:A:216:GLN:HG3 | 1.98 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:175:LYS:O | 1:A:176:GLU:CB | 2.47 | 0.62 |
| 1:A:255:PRO:HG2 | 1:A:256:GLU:OE2 | 1.99 | 0.62 |
| 1:A:254:SER:HB3 | 3:A:3061:HOH:O | 2.00 | 0.62 |
| 1:B:1366:LEU:HD23 | 1:B:1385:VAL:HG11 | 1.81 | 0.62 |
| 1:A:223:MET:HA | 1:A:223:MET:CE | 2.29 | 0.62 |
| 1:A:221:PHE:HB3 | 1:A:225:GLN:HB3 | 1.82 | 0.62 |
| 1:A:343:SER:H | 1:A:346:GLN:NE2 | 1.98 | 0.62 |
| 1:B:1088:TYR:O | 1:B:1115:HIS:O | 2.18 | 0.61 |
| 1:B:1202:PRO:HA | 1:B:1205:VAL:CG1 | 2.30 | 0.61 |
| 1:B:1346:GLN:NE2 | 1:B:1360:GLN:HE21 | 1.98 | 0.61 |
| 1:B:1289:HIS:CD2 | 2:B:2001:XGP:O6 | 2.53 | 0.61 |
| 1:B:1086:TYR:HB2 | 1:B:1281:PRO:HG3 | 1.82 | 0.61 |
| 1:A:231:ILE:HG13 | 1:A:240:LEU:HD12 | 1.83 | 0.61 |
| 1:B:1310:GLN:NE2 | 1:B:1312:GLU:HG2 | 2.15 | 0.61 |
| 1:A:232:LYS:O | 1:A:233:SER:HB3 | 1.99 | 0.61 |
| 1:A:146:MET:HG2 | 1:A:250:SER:O | 2.00 | 0.61 |
| 1:B:1212:ALA:O | 1:B:1216:GLN:HG3 | 2.00 | 0.61 |
| 1:A:21:ARG:HA | 1:A:49:LEU:HA | 1.82 | 0.61 |
| 1:A:165:ILE:HG23 | 1:A:230:GLU:HB2 | 1.83 | 0.61 |
| 1:B:1186:LYS:HB3 | 1:B:1186:LYS:HZ2 | 1.65 | 0.61 |
| 1:B:1015:MET:HG3 | 1:B:1293:ILE:HD13 | 1.83 | 0.60 |
| 1:B:1165:ILE:HG23 | 1:B:1230:GLU:HB2 | 1.83 | 0.60 |
| 1:B:1310:GLN:HE21 | 1:B:1312:GLU:H | 1.50 | 0.60 |
| 1:A:21:ARG:NH2 | 1:A:24:LEU:HD13 | 2.17 | 0.60 |
| 1:B:1090:ASN:N | 1:B:1095:THR:HG21 | 2.16 | 0.60 |
| 1:B:1253:THR:O | 1:B:1298:THR:HG21 | 2.01 | 0.60 |
| 1:B:1219:GLU:HA | 1:B:1219:GLU:OE1 | 2.02 | 0.59 |
| 1:A:277:ARG:HB3 | 1:A:324:ARG:HH12 | 1.66 | 0.59 |
| 1:B:1011:GLN:HB3 | 1:B:1277:ARG:NH1 | 2.17 | 0.59 |
| 1:A:192:LYS:HD3 | 1:A:195:GLN:OE1 | 2.02 | 0.59 |
| 1:B:1098:THR:CG2 | 1:B:1287:VAL:HG11 | 2.33 | 0.59 |
| 1:B:1255:PRO:O | 1:B:1259:ARG:HG2 | 2.01 | 0.59 |
| 1:A:273:LEU:O | 1:A:277:ARG:HG2 | 2.03 | 0.59 |
| 1:B:1019:ASN:ND2 | 1:B:1020:LEU:H | 1.97 | 0.59 |
| 1:A:21:ARG:HD2 | 1:A:94:ARG:HD2 | 1.85 | 0.59 |
| 1:A:71:GLN:OE1 | 1:A:325:TRP:HH2 | 1.86 | 0.59 |
| 1:A:165:ILE:HG23 | 1:A:230:GLU:HB3 | 1.84 | 0.58 |
| 1:A:232:LYS:HG3 | 3:A:3040:HOH:O | 2.02 | 0.58 |
| 1:A:126:THR:O | 1:A:265:LEU:HD13 | 2.03 | 0.58 |
| 1:A:303:LYS:HB2 | 1:A:303:LYS:NZ | 2.19 | 0.58 |
| 1:B:1138:PHE:HA | 1:B:1141:GLN:NE2 | 2.19 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1146:MET:HE3 | 1:B:1197:PRO:HB2 | 1.86 | 0.58 |
| 1:A:227:ALA:HB3 | 1:A:231:ILE:CG2 | 2.33 | 0.58 |
| 1:A:334:LEU:HD23 | 1:A:378:PRO:HA | 1.86 | 0.58 |
| 1:B:1192:LYS:HD2 | 1:B:1192:LYS:O | 2.04 | 0.58 |
| 1:B:1078:GLU:O | 1:B:1079:CYS:HB2 | 2.02 | 0.58 |
| 1:A:5:GLU:CD | 1:A:5:GLU:N | 2.57 | 0.58 |
| 1:B:1316:ILE:CG2 | 1:B:1317:GLY:N | 2.67 | 0.58 |
| 1:B:1192:LYS:CD | 1:B:1195:GLN:HB2 | 2.34 | 0.57 |
| 1:B:1135:SER:HB3 | 1:B:1138:PHE:CB | 2.33 | 0.57 |
| 1:B:1290:ASP:CB | 1:B:1314:THR:HG21 | 2.34 | 0.57 |
| 1:B:1316:ILE:HG23 | 1:B:1317:GLY:N | 2.18 | 0.57 |
| 1:A:231:ILE:HG13 | 1:A:240:LEU:CD1 | 2.35 | 0.57 |
| 1:B:1098:THR:HB | 3:B:3183:HOH:O | 2.04 | 0.57 |
| 1:A:110:CYS:O | 1:A:111:ASP:CB | 2.53 | 0.57 |
| 1:B:1020:LEU:O | 1:B:1049:LEU:HD22 | 2.04 | 0.57 |
| 1:B:1057:GLU:OE2 | 1:B:1102:PHE:HB2 | 2.05 | 0.57 |
| 1:B:1217:TYR:CE2 | 1:B:1348:ARG:HG3 | 2.39 | 0.57 |
| 1:A:65:ARG:HH21 | 1:A:74:VAL:CG1 | 2.18 | 0.57 |
| 1:B:1174:CYS:O | 1:B:1178:GLN:HA | 2.04 | 0.57 |
| 1:B:1343:SER:OG | 1:B:1346:GLN:HG3 | 2.05 | 0.56 |
| 1:A:17:ARG:NH2 | 1:A:316:ILE:HA | 2.21 | 0.56 |
| 1:A:49:LEU:HD13 | 1:A:50:THR:O | 2.04 | 0.56 |
| 1:A:269:ILE:CG2 | 1:A:273:LEU:HD22 | 2.36 | 0.56 |
| 1:B:1021:ARG:NH1 | 1:B:1024:LEU:HD13 | 2.20 | 0.56 |
| 1:A:74:VAL:HG12 | 1:A:75:LYS:N | 2.21 | 0.56 |
| 1:A:84:THR:HG23 | 1:A:282:LYS:HD2 | 1.86 | 0.56 |
| 1:A:21:ARG:CZ | 1:A:24:LEU:HD13 | 2.36 | 0.56 |
| 1:B:1011:GLN:HE21 | 1:B:1277:ARG:CD | 2.16 | 0.56 |
| 1:B:1134:ASP:HB3 | 1:B:1193:TYR:CG | 2.41 | 0.56 |
| 1:B:1015:MET:HE3 | 1:B:1265:LEU:HG | 1.88 | 0.56 |
| 1:B:1142:ALA:O | 1:B:1146:MET:HG3 | 2.07 | 0.56 |
| 1:B:1227:ALA:HB3 | 1:B:1231:ILE:CG1 | 2.32 | 0.55 |
| 1:B:1165:ILE:HG23 | 1:B:1230:GLU:CB | 2.36 | 0.55 |
| 1:A:27:ASN:O | 1:A:31:LEU:HD13 | 2.06 | 0.55 |
| 1:A:165:ILE:HD13 | 1:A:231:ILE:HA | 1.87 | 0.55 |
| 1:A:271:LYS:HA | 1:A:275:THR:OG1 | 2.07 | 0.55 |
| 1:A:4:PRO:HG2 | 1:A:7:TYR:CE1 | 2.41 | 0.55 |
| 1:A:381:LYS:O | 1:A:385:VAL:HG23 | 2.07 | 0.55 |
| 1:A:290:ASP:HA | 1:A:314:THR:HG21 | 1.89 | 0.55 |
| 2:A:2000:XGP:C6 | 3:A:3181:HOH:O | 2.44 | 0.55 |
| 1:B:1202:PRO:HA | 1:B:1205:VAL:HG13 | 1.89 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1075:LYS:HE2 | 1:B:1075:LYS:HA | 1.89 | 0.54 |
| 1:A:90:ASN:HD21 | 1:A:95:THR:HG21 | 1.71 | 0.54 |
| 1:B:1011:GLN:CB | 1:B:1277:ARG:NH1 | 2.70 | 0.54 |
| 1:B:1223:MET:SD | 1:B:1348:ARG:NH2 | 2.80 | 0.54 |
| 1:A:189:PHE:CE1 | 1:A:199:VAL:HG13 | 2.42 | 0.54 |
| 1:A:202:PRO:HA | 1:A:205:VAL:CG1 | 2.38 | 0.54 |
| 1:A:303:LYS:HG3 | 1:A:304:PRO:CD | 2.37 | 0.54 |
| 1:B:1006:GLY:O | 1:B:1007:TYR:HB2 | 2.08 | 0.54 |
| 1:B:1186:LYS:N | 1:B:1186:LYS:HZ3 | 2.06 | 0.53 |
| 1:B:1297:LEU:CD1 | 1:B:1320:ILE:HD13 | 2.38 | 0.53 |
| 1:B:1086:TYR:CB | 1:B:1281:PRO:HG3 | 2.39 | 0.53 |
| 1:B:1232:LYS:O | 1:B:1233:SER:C | 2.46 | 0.53 |
| 1:B:1065:ARG:HG2 | 1:B:1065:ARG:HH11 | 1.73 | 0.53 |
| 1:A:321:VAL:O | 1:A:321:VAL:CG2 | 2.56 | 0.53 |
| 1:A:365:GLU:OE1 | 1:A:370:PRO:HA | 2.09 | 0.53 |
| 1:A:17:ARG:O | 1:A:17:ARG:CG | 2.56 | 0.53 |
| 1:A:248:GLN:HE22 | 1:A:290:ASP:HB2 | 1.73 | 0.53 |
| 1:A:21:ARG:HH21 | 1:A:23:PRO:HA | 1.73 | 0.53 |
| 1:A:91:SER:HB2 | 1:A:120:MET:HA | 1.91 | 0.53 |
| 1:B:1271:LYS:HA | 1:B:1275:THR:OG1 | 2.08 | 0.53 |
| 1:B:1085:VAL:HG13 | 1:B:1283:ILE:HG22 | 1.91 | 0.52 |
| 1:A:263:LYS:HE2 | 1:A:264:PRO:HD3 | 1.90 | 0.52 |
| 1:B:1186:LYS:HB3 | 1:B:1186:LYS:NZ | 2.24 | 0.52 |
| 1:A:175:LYS:NZ | 1:A:175:LYS:HB3 | 2.24 | 0.52 |
| 1:A:310:GLN:HE21 | 1:A:312:GLU:HG2 | 1.74 | 0.52 |
| 1:B:1123:MET:HE2 | 1:B:1128:ASN:HA | 1.91 | 0.52 |
| 1:B:1153:LEU:HB3 | 1:B:1155:LEU:HD13 | 1.91 | 0.52 |
| 1:A:75:LYS:N | 1:A:75:LYS:HD3 | 2.25 | 0.52 |
| 1:B:1146:MET:HE1 | 1:B:1197:PRO:HB2 | 1.91 | 0.52 |
| 1:A:41:GLU:HG2 | 3:A:3057:HOH:O | 2.10 | 0.52 |
| 1:A:44:VAL:CG1 | 1:A:48:GLN:HB2 | 2.39 | 0.52 |
| 1:B:1199:VAL:HG22 | 1:B:1200:SER:N | 2.25 | 0.52 |
| 1:B:1162:LEU:O | 1:B:1166:VAL:HB | 2.09 | 0.52 |
| 1:A:74:VAL:CG1 | 1:A:75:LYS:N | 2.73 | 0.52 |
| 1:A:74:VAL:HG13 | 3:A:3030:HOH:O | 2.10 | 0.52 |
| 1:B:1011:GLN:HB3 | 1:B:1277:ARG:HH12 | 1.73 | 0.52 |
| 1:B:1015:MET:CE | 1:B:1265:LEU:HG | 2.40 | 0.52 |
| 1:B:1116:HIS:HD2 | 1:B:1117:GLN:O | 1.91 | 0.52 |
| 1:A:90:ASN:HD22 | 1:A:90:ASN:N | 1.94 | 0.52 |
| 1:A:24:LEU:HG | 1:A:26:ASN:ND2 | 2.25 | 0.52 |
| 1:A:75:LYS:HG2 | 3:A:3030:HOH:O | 2.08 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:223:MET:HE3 | 1:A:348:ARG:NH2 | 2.25 | 0.51 |
| 1:A:235:GLN:OE1 | 1:A:235:GLN:HA | 2.10 | 0.51 |
| 1:A:320:ILE:N | 1:A:320:ILE:HD12 | 2.25 | 0.51 |
| 1:B:1186:LYS:N | 1:B:1186:LYS:CD | 2.73 | 0.51 |
| 1:A:17:ARG:CZ | 1:A:316:ILE:HD12 | 2.40 | 0.51 |
| 1:A:165:ILE:HD12 | 1:A:240:LEU:HD11 | 1.92 | 0.51 |
| 1:A:69:ALA:HA | 1:A:74:VAL:O | 2.09 | 0.51 |
| 1:B:1088:TYR:O | 1:B:1089:ALA:CB | 2.56 | 0.51 |
| 1:A:137:ALA:O | 1:A:141:GLN:HG3 | 2.11 | 0.51 |
| 1:A:205:VAL:O | 1:A:209:LEU:HD13 | 2.11 | 0.51 |
| 1:B:1167:ASN:O | 1:B:1169:LYS:O | 2.28 | 0.51 |
| 1:A:110:CYS:O | 1:A:111:ASP:HB2 | 2.10 | 0.51 |
| 1:A:128:ASN:HD22 | 1:A:129:PRO:HD2 | 1.74 | 0.51 |
| 1:B:1065:ARG:HE | 1:B:1074:VAL:CG1 | 2.23 | 0.51 |
| 1:A:49:LEU:CD2 | 1:A:98:THR:HG22 | 2.35 | 0.51 |
| 1:B:1005:GLU:CD | 1:B:1006:GLY:N | 2.60 | 0.51 |
| 1:A:263:LYS:HE2 | 3:A:3038:HOH:O | 2.10 | 0.51 |
| 1:A:217:TYR:CE2 | 1:A:348:ARG:HD2 | 2.46 | 0.51 |
| 1:B:1074:VAL:HG22 | 1:B:1080:PRO:HB3 | 1.93 | 0.51 |
| 1:A:134:ASP:HA | 3:A:3154:HOH:O | 2.10 | 0.50 |
| 1:A:192:LYS:HD3 | 1:A:195:GLN:CB | 2.41 | 0.50 |
| 1:A:4:PRO:HG2 | 1:A:7:TYR:CD1 | 2.46 | 0.50 |
| 1:B:1365:GLU:HB2 | 1:B:1371:ILE:HD12 | 1.93 | 0.50 |
| 1:A:155:LEU:N | 1:A:155:LEU:HD22 | 2.27 | 0.50 |
| 1:B:1066:GLU:HB3 | 1:B:1355:LEU:HG | 1.93 | 0.50 |
| 1:B:1277:ARG:CZ | 1:B:1324:ARG:HE | 2.25 | 0.50 |
| 1:A:11:GLN:NE2 | 1:A:324:ARG:NH1 | 2.60 | 0.50 |
| 1:B:1326:HIS:HE1 | 1:B:1328:SER:HA | 1.76 | 0.50 |
| 1:A:333:ASP:O | 1:A:334:LEU:HD23 | 2.11 | 0.50 |
| 1:A:17:ARG:O | 1:A:18:ALA:O | 2.29 | 0.50 |
| 1:A:18:ALA:CA | 1:A:98:THR:HG21 | 2.40 | 0.50 |
| 1:A:146:MET:HE3 | 1:A:197:PRO:HB2 | 1.93 | 0.50 |
| 1:B:1231:ILE:HD12 | 1:B:1232:LYS:H | 1.72 | 0.50 |
| 1:A:256:GLU:HA | 1:A:259:ARG:NH2 | 2.27 | 0.49 |
| 1:B:1011:GLN:NE2 | 1:B:1277:ARG:HD3 | 2.20 | 0.49 |
| 1:B:1155:LEU:HG | 1:B:1243:LEU:HD23 | 1.93 | 0.49 |
| 1:B:1088:TYR:HB3 | 1:B:1286:LEU:HD12 | 1.93 | 0.49 |
| 1:B:1186:LYS:H | 1:B:1186:LYS:NZ | 2.10 | 0.49 |
| 1:B:1377:CYS:SG | 1:B:1378:PRO:HD2 | 2.52 | 0.49 |
| 1:B:1139:SER:O | 1:B:1143:VAL:HG23 | 2.12 | 0.49 |
| 1:B:1143:VAL:O | 1:B:1147:GLU:HG3 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1155:LEU:O | 1:B:1157:ASP:N | 2.46 | 0.49 |
| 1:B:1192:LYS:HD3 | 1:B:1195:GLN:CD | 2.32 | 0.49 |
| 1:B:1335:MET:HG2 | 1:B:1382:PHE:CD1 | 2.48 | 0.49 |
| 1:B:1231:ILE:O | 1:B:1232:LYS:C | 2.50 | 0.49 |
| 1:A:3:VAL:HG21 | 1:A:325:TRP:CZ3 | 2.48 | 0.49 |
| 1:A:167:ASN:C | 1:A:167:ASN:HD22 | 2.16 | 0.49 |
| 1:A:226:VAL:O | 1:A:226:VAL:CG2 | 2.60 | 0.49 |
| 1:A:343:SER:H | 1:A:346:GLN:HE21 | 1.59 | 0.49 |
| 1:B:1291:SER:OG | 2:B:2001:XGP:H5 | 2.13 | 0.49 |
| 1:A:232:LYS:O | 1:A:236:GLN:NE2 | 2.46 | 0.49 |
| 1:B:1207:ASN:O | 1:B:1211:ASP:HB2 | 2.13 | 0.49 |
| 1:B:1231:ILE:HD12 | 1:B:1232:LYS:N | 2.28 | 0.48 |
| 1:A:221:PHE:O | 1:A:348:ARG:NH2 | 2.46 | 0.48 |
| 1:B:1146:MET:HE2 | 1:B:1251:LEU:HA | 1.94 | 0.48 |
| 1:B:1226:VAL:O | 1:B:1226:VAL:HG13 | 2.13 | 0.48 |
| 1:B:1310:GLN:HE21 | 1:B:1312:GLU:HG2 | 1.77 | 0.48 |
| 1:A:206:GLY:O | 1:A:210:VAL:HG23 | 2.13 | 0.48 |
| 1:A:59:TYR:HB3 | 1:A:353:LEU:HB2 | 1.96 | 0.48 |
| 1:B:1169:LYS:HG2 | 3:B:3186:HOH:O | 2.14 | 0.48 |
| 1:A:20:LEU:HD11 | 1:A:219:GLU:CA | 2.43 | 0.48 |
| 1:A:79:CYS:SG | 1:A:107:PHE:HB3 | 2.53 | 0.48 |
| 1:B:1049:LEU:O | 1:B:1050:THR:HG23 | 2.14 | 0.48 |
| 1:B:1031:LEU:HD21 | 3:B:3012:HOH:O | 2.14 | 0.48 |
| 1:B:1186:LYS:O | 1:B:1187:ASN:CB | 2.49 | 0.48 |
| 1:A:248:GLN:NE2 | 1:A:290:ASP:HB2 | 2.29 | 0.48 |
| 1:B:1020:LEU:HA | 1:B:1316:ILE:HG12 | 1.96 | 0.48 |
| 1:B:1159:TYR:O | 1:B:1163:GLU:HG3 | 2.14 | 0.48 |
| 1:A:21:ARG:O | 1:A:215:LEU:HG | 2.14 | 0.47 |
| 1:A:305:TYR:CD1 | 1:A:307:LEU:HD13 | 2.49 | 0.47 |
| 1:B:1192:LYS:HD2 | 1:B:1195:GLN:HB2 | 1.96 | 0.47 |
| 1:A:30:VAL:HG12 | 3:A:3091:HOH:O | 2.14 | 0.47 |
| 1:A:45:PRO:O | 1:A:46:GLY:C | 2.52 | 0.47 |
| 1:B:1049:LEU:HD23 | 3:B:3183:HOH:O | 2.13 | 0.47 |
| 1:A:13:LEU:HD23 | 1:A:13:LEU:C | 2.34 | 0.47 |
| 1:A:33:GLN:O | 1:A:171:SER:HB2 | 2.14 | 0.47 |
| 1:A:35:THR:HA | 1:A:171:SER:HB3 | 1.96 | 0.47 |
| 1:A:303:LYS:CG | 1:A:304:PRO:HD2 | 2.42 | 0.47 |
| 1:A:155:LEU:HD22 | 1:A:155:LEU:H | 1.79 | 0.47 |
| 1:A:326:HIS:NE2 | 1:A:331:ASN:ND2 | 2.63 | 0.47 |
| 1:A:332:ARG:NH1 | 1:A:334:LEU:HD21 | 2.30 | 0.47 |
| 1:B:1094:ARG:O | 1:B:1098:THR:HG22 | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1146:MET:CE | 1:B:1251:LEU:HA | 2.45 | 0.47 |
| 1:B:1270:ASP:OD1 | 1:B:1386:LEU:HB3 | 2.14 | 0.47 |
| 1:B:1310:GLN:HG2 | 1:B:1315:PRO:CG | 2.34 | 0.47 |
| 1:A:130:VAL:HB | 1:A:195:GLN:N | 2.30 | 0.47 |
| 1:A:289:HIS:CB | 2:A:2000:XGP:O6 | 2.62 | 0.47 |
| 1:A:321:VAL:CG2 | 1:A:323:GLN:HE21 | 2.28 | 0.47 |
| 1:B:1033:GLN:HA | 1:B:1172:PRO:HG2 | 1.97 | 0.47 |
| 1:B:1357:ALA:N | 1:B:1358:PRO:HD3 | 2.29 | 0.47 |
| 1:A:271:LYS:O | 1:A:276:ASP:HB2 | 2.15 | 0.47 |
| 1:A:342:GLN:HA | 1:A:346:GLN:NE2 | 2.30 | 0.47 |
| 1:B:1161:LEU:O | 1:B:1165:ILE:HG12 | 2.15 | 0.47 |
| 1:A:21:ARG:HD2 | 1:A:94:ARG:CD | 2.44 | 0.47 |
| 1:A:314:THR:HG22 | 1:A:314:THR:O | 2.15 | 0.47 |
| 1:B:1060:MET:HE1 | 1:B:1341:TYR:HA | 1.96 | 0.47 |
| 1:A:231:ILE:HG12 | 1:A:231:ILE:O | 2.15 | 0.46 |
| 1:A:386:LEU:O | 1:A:390:VAL:HG23 | 2.15 | 0.46 |
| 1:B:1289:HIS:HB2 | 2:B:2001:XGP:O6 | 2.14 | 0.46 |
| 1:B:1326:HIS:CE1 | 1:B:1328:SER:HA | 2.49 | 0.46 |
| 1:B:1096:VAL:HG21 | 1:B:1120:MET:HE1 | 1.97 | 0.46 |
| 1:B:1264:PRO:HG2 | 3:B:3065:HOH:O | 2.14 | 0.46 |
| 1:B:1297:LEU:HD11 | 1:B:1320:ILE:HD13 | 1.97 | 0.46 |
| 1:A:74:VAL:HG12 | 1:A:75:LYS:O | 2.14 | 0.46 |
| 1:B:1049:LEU:HD11 | 1:B:1054:GLY:N | 2.30 | 0.46 |
| 1:B:1331:ASN:OD1 | 1:B:1331:ASN:O | 2.33 | 0.46 |
| 1:B:1017:ARG:HG2 | 1:B:1018:ALA:N | 2.30 | 0.46 |
| 1:B:1293:ILE:CG2 | 1:B:1320:ILE:HD11 | 2.35 | 0.46 |
| 1:B:1309:ASP:HB3 | 1:B:1343:SER:HB2 | 1.96 | 0.46 |
| 1:B:1357:ALA:N | 1:B:1358:PRO:CD | 2.78 | 0.46 |
| 1:B:1011:GLN:CB | 1:B:1277:ARG:HH11 | 2.27 | 0.46 |
| 1:A:207:ASN:O | 1:A:211:ASP:HB2 | 2.16 | 0.46 |
| 1:A:371:ILE:HG13 | 1:A:375:GLY:C | 2.35 | 0.46 |
| 1:B:1354:THR:OG1 | 1:B:1356:GLN:O | 2.30 | 0.46 |
| 1:B:1064:MET:O | 1:B:1068:LEU:HB2 | 2.16 | 0.46 |
| 1:B:1138:PHE:C | 1:B:1138:PHE:CD1 | 2.89 | 0.46 |
| 1:B:1254:SER:HB3 | 1:B:1257:VAL:HG13 | 1.98 | 0.46 |
| 1:A:327:ASP:OD2 | 1:A:327:ASP:C | 2.53 | 0.46 |
| 1:A:154:GLN:C | 1:A:155:LEU:HD13 | 2.36 | 0.45 |
| 1:B:1274:VAL:HG22 | 1:B:1275:THR:N | 2.31 | 0.45 |
| 1:B:1359:ALA:HA | 3:B:3191:HOH:O | 2.16 | 0.45 |
| 1:A:192:LYS:HD2 | 1:A:195:GLN:HB2 | 1.93 | 0.45 |
| 1:A:256:GLU:CD | 1:A:256:GLU:H | 2.19 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1356:GLN:O | 1:B:1357:ALA:HB3 | 2.16 | 0.45 |
| 1:A:35:THR:OG1 | 1:A:36:PRO:HD2 | 2.16 | 0.45 |
| 1:A:196:GLU:OE2 | 2:A:2000:XGP:O4 | 2.35 | 0.45 |
| 1:A:316:ILE:CG2 | 1:A:317:GLY:N | 2.79 | 0.45 |
| 1:A:238:LYS:O | 1:A:238:LYS:NZ | 2.38 | 0.45 |
| 1:A:292:ASN:O | 1:A:296:LEU:HB2 | 2.17 | 0.45 |
| 1:B:1310:GLN:NE2 | 1:B:1312:GLU:CG | 2.78 | 0.45 |
| 1:A:31:LEU:HD11 | 1:A:208:SER:HB3 | 1.98 | 0.45 |
| 1:A:32:GLU:HA | 3:A:3218:HOH:O | 2.17 | 0.45 |
| 1:B:1233:SER:HB2 | 1:B:1236:GLN:OE1 | 2.17 | 0.45 |
| 1:B:1067:TRP:CE3 | 1:B:1068:LEU:HD12 | 2.52 | 0.45 |
| 1:A:227:ALA:O | 1:A:230:GLU:HB2 | 2.17 | 0.45 |
| 1:A:310:GLN:NE2 | 1:A:312:GLU:CG | 2.80 | 0.45 |
| 1:A:310:GLN:NE2 | 1:A:312:GLU:HG2 | 2.32 | 0.45 |
| 1:B:1197:PRO:O | 1:B:1198:GLY:O | 2.35 | 0.45 |
| 1:A:54:GLY:O | 1:A:58:VAL:HG23 | 2.17 | 0.45 |
| 1:A:65:ARG:HD2 | 1:A:106:ALA:O | 2.17 | 0.45 |
| 1:A:269:ILE:O | 1:A:273:LEU:HB2 | 2.17 | 0.45 |
| 1:A:293:ILE:HG21 | 1:A:320:ILE:HD11 | 1.98 | 0.45 |
| 1:A:310:GLN:HE21 | 1:A:312:GLU:CG | 2.29 | 0.45 |
| 1:A:61:GLY:HA2 | 1:A:102:PHE:CE1 | 2.52 | 0.44 |
| 1:A:136:ALA:N | 3:A:3203:HOH:O | 2.49 | 0.44 |
| 1:A:189:PHE:CD1 | 1:A:199:VAL:HG13 | 2.52 | 0.44 |
| 1:A:229:GLY:O | 1:A:232:LYS:HB2 | 2.17 | 0.44 |
| 1:A:321:VAL:O | 1:A:321:VAL:HG23 | 2.17 | 0.44 |
| 1:B:1057:GLU:HG2 | 1:B:1098:THR:O | 2.16 | 0.44 |
| 1:B:1177:LYS:HD2 | 3:B:3287:HOH:O | 2.17 | 0.44 |
| 1:A:377:CYS:SG | 1:A:378:PRO:CD | 3.05 | 0.44 |
| 1:B:1133:ASP:C | 1:B:1135:SER:H | 2.20 | 0.44 |
| 1:A:13:LEU:HD13 | 1:A:273:LEU:HD13 | 1.98 | 0.44 |
| 1:B:1011:GLN:CD | 1:B:1277:ARG:NH1 | 2.70 | 0.44 |
| 1:B:1305:TYR:CD2 | 1:B:1307:LEU:HD13 | 2.53 | 0.44 |
| 1:B:1363:THR:HG22 | 3:B:3151:HOH:O | 2.17 | 0.44 |
| 1:A:223:MET:O | 1:A:226:VAL:HG22 | 2.17 | 0.44 |
| 1:B:1085:VAL:HG13 | 1:B:1283:ILE:CG2 | 2.48 | 0.44 |
| 1:B:1027:ASN:O | 1:B:1031:LEU:HD23 | 2.17 | 0.44 |
| 1:B:1201:GLY:O | 1:B:1205:VAL:HG12 | 2.17 | 0.44 |
| 1:A:9:LEU:HD13 | 1:A:325:TRP:CE2 | 2.52 | 0.44 |
| 1:B:1074:VAL:HG22 | 3:B:3070:HOH:O | 2.17 | 0.44 |
| 1:B:1090:ASN:ND2 | 1:B:1092:LEU:HG | 2.33 | 0.44 |
| 1:B:1090:ASN:H | 1:B:1095:THR:HG21 | 1.82 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1249:ASP:HA | 1:B:1253:THR:OG1 | 2.17 | 0.44 |
| 1:A:20:LEU:HD13 | 1:A:219:GLU:OE2 | 2.17 | 0.44 |
| 1:A:33:GLN:HA | 1:A:172:PRO:HG2 | 1.99 | 0.44 |
| 1:A:175:LYS:HE2 | 3:A:3307:HOH:O | 2.17 | 0.44 |
| 1:B:1146:MET:HE2 | 1:B:1251:LEU:HD23 | 1.99 | 0.44 |
| 1:A:35:THR:HB | 1:A:166:VAL:CG1 | 2.43 | 0.43 |
| 1:B:1270:ASP:HA | 1:B:1386:LEU:HD23 | 2.00 | 0.43 |
| 1:A:79:CYS:N | 3:A:3277:HOH:O | 2.49 | 0.43 |
| 1:A:234:ASP:OD1 | 1:A:236:GLN:HG3 | 2.18 | 0.43 |
| 1:B:1037:ASN:C | 1:B:1038:LYS:HE2 | 2.39 | 0.43 |
| 1:B:1106:ALA:C | 1:B:1108:PRO:HD3 | 2.38 | 0.43 |
| 1:B:1329:LYS:HG2 | 3:B:3214:HOH:O | 2.17 | 0.43 |
| 1:A:290:ASP:OD2 | 2:A:2000:XGP:C1 | 2.66 | 0.43 |
| 1:B:1011:GLN:NE2 | 1:B:1277:ARG:HH11 | 2.15 | 0.43 |
| 1:B:1017:ARG:NH2 | 1:B:1314:THR:O | 2.51 | 0.43 |
| 1:A:327:ASP:O | 1:A:330:ALA:O | 2.37 | 0.43 |
| 1:B:1169:LYS:O | 1:B:1170:ASP:CB | 2.60 | 0.43 |
| 1:B:1231:ILE:HD12 | 1:B:1231:ILE:N | 2.33 | 0.43 |
| 1:B:1252:PHE:CE2 | 1:B:1291:SER:HB3 | 2.53 | 0.43 |
| 1:A:325:TRP:CG | 1:A:376:PHE:HE2 | 2.37 | 0.43 |
| 1:A:90:ASN:N | 1:A:90:ASN:ND2 | 2.65 | 0.43 |
| 1:A:235:GLN:C | 1:A:237:TRP:N | 2.70 | 0.43 |
| 1:B:1049:LEU:C | 1:B:1050:THR:HG23 | 2.39 | 0.43 |
| 1:A:316:ILE:HG23 | 1:A:317:GLY:N | 2.32 | 0.43 |
| 1:B:1065:ARG:HG2 | 1:B:1065:ARG:NH1 | 2.33 | 0.43 |
| 1:B:1265:LEU:HD12 | 1:B:1265:LEU:HA | 1.73 | 0.43 |
| 1:B:1277:ARG:HD2 | 1:B:1324:ARG:CZ | 2.49 | 0.43 |
| 1:B:1061:GLY:HA2 | 1:B:1102:PHE:CE1 | 2.54 | 0.43 |
| 1:B:1273:LEU:CB | 1:B:1277:ARG:NH2 | 2.82 | 0.43 |
| 1:A:361:ARG:CZ | 3:A:3059:HOH:O | 2.67 | 0.42 |
| 1:B:1168:TYR:CE1 | 1:B:1182:LEU:HD13 | 2.54 | 0.42 |
| 1:B:1216:GLN:OE1 | 1:B:1226:VAL:HA | 2.19 | 0.42 |
| 1:A:65:ARG:NH2 | 1:A:74:VAL:HG11 | 2.32 | 0.42 |
| 1:A:273:LEU:HD23 | 1:A:382:PHE:CZ | 2.54 | 0.42 |
| 1:B:1075:LYS:HG3 | 1:B:1077:GLY:H | 1.85 | 0.42 |
| 1:A:16:SER:CB | 1:A:319:LYS:HG2 | 2.50 | 0.42 |
| 1:B:1099:ALA:HB2 | 1:B:1287:VAL:HG21 | 2.01 | 0.42 |
| 1:B:1226:VAL:HG13 | 1:B:1231:ILE:HD11 | 2.01 | 0.42 |
| 1:A:217:TYR:CZ | 1:A:348:ARG:HD2 | 2.54 | 0.42 |
| 1:A:310:GLN:CG | 1:A:315:PRO:HG3 | 2.42 | 0.42 |
| 1:B:1168:TYR:C | 1:B:1169:LYS:O | 2.53 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1277:ARG:NH1 | 1:B:1324:ARG:HE | 2.17 | 0.42 |
| 1:B:1338:GLU:OE2 | 1:B:1361:ARG:NH1 | 2.53 | 0.42 |
| 1:A:135:SER:C | 1:A:137:ALA:H | 2.23 | 0.42 |
| 1:B:1232:LYS:HE3 | 3:B:3098:HOH:O | 2.18 | 0.42 |
| 1:A:330:ALA:O | 1:A:332:ARG:N | 2.45 | 0.42 |
| 1:B:1308:HIS:O | 1:B:1309:ASP:HB2 | 2.20 | 0.42 |
| 1:B:1326:HIS:ND1 | 1:B:1326:HIS:C | 2.73 | 0.42 |
| 1:A:138:PHE:HB3 | 3:A:3203:HOH:O | 2.20 | 0.42 |
| 1:A:211:ASP:OD2 | 1:A:244:LYS:HE2 | 2.20 | 0.42 |
| 1:B:1132:THR:N | 1:B:1260:ASN:HD21 | 2.11 | 0.42 |
| 1:A:265:LEU:HD12 | 1:A:265:LEU:HA | 1.91 | 0.42 |
| 1:A:241:SER:HB3 | 3:A:3265:HOH:O | 2.20 | 0.41 |
| 1:B:1081:PRO:HA | 1:B:1082:PRO:HD3 | 1.93 | 0.41 |
| 1:B:1168:TYR:O | 1:B:1169:LYS:C | 2.59 | 0.41 |
| 1:A:1:GLN:HG2 | 3:A:3171:HOH:O | 2.20 | 0.41 |
| 1:A:185:GLY:HA3 | 1:A:202:PRO:HG3 | 2.02 | 0.41 |
| 1:A:270:ASP:OD1 | 1:A:387:ASN:OD1 | 2.38 | 0.41 |
| 1:A:346:GLN:NE2 | 1:A:360:GLN:HE21 | 2.18 | 0.41 |
| 1:B:1168:TYR:CZ | 1:B:1182:LEU:HD13 | 2.56 | 0.41 |
| 1:B:1290:ASP:HB2 | 1:B:1314:THR:CG2 | 2.48 | 0.41 |
| 1:B:1218:TYR:CE1 | 1:B:1347:LEU:HD12 | 2.56 | 0.41 |
| 1:A:244:LYS:NZ | 1:A:312:GLU:HB3 | 2.36 | 0.41 |
| 1:B:1069:ALA:HA | 1:B:1074:VAL:O | 2.20 | 0.41 |
| 1:A:25:ALA:HB2 | 1:A:46:GLY:CA | 2.47 | 0.41 |
| 1:A:138:PHE:CD1 | 1:A:138:PHE:C | 2.94 | 0.41 |
| 1:A:21:ARG:NH2 | 1:A:23:PRO:HA | 2.35 | 0.41 |
| 1:A:116:HIS:HD2 | 1:A:117:GLN:O | 2.03 | 0.41 |
| 1:B:1319:LYS:HE2 | 1:B:1319:LYS:HB3 | 1.94 | 0.41 |
| 1:A:91:SER:HA | 1:A:120:MET:SD | 2.61 | 0.41 |
| 1:A:175:LYS:HD2 | 3:A:3253:HOH:O | 2.19 | 0.41 |
| 1:A:269:ILE:HG22 | 1:A:273:LEU:HD22 | 2.02 | 0.41 |
| 1:A:338:GLU:HG2 | 1:A:363:THR:HG22 | 2.02 | 0.41 |
| 1:B:1201:GLY:O | 1:B:1204:LYS:HB3 | 2.20 | 0.41 |
| 1:B:1233:SER:O | 1:B:1234:ASP:OD2 | 2.37 | 0.41 |
| 1:A:269:ILE:HG23 | 1:A:273:LEU:HD22 | 2.03 | 0.41 |
| 1:B:1056:LEU:HB3 | 1:B:1342:GLN:HE22 | 1.86 | 0.41 |
| 1:B:1128:ASN:HD22 | 1:B:1129:PRO:CD | 2.31 | 0.41 |
| 1:B:1259:ARG:HD2 | 3:B:3254:HOH:O | 2.21 | 0.41 |
| 1:A:311:ASN:HB2 | 3:A:3205:HOH:O | 2.20 | 0.40 |
| 1:B:1093:GLN:HA | 3:B:3258:HOH:O | 2.21 | 0.40 |
| 1:B:1095:THR:O | 1:B:1098:THR:CG2 | 2.69 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:1049:LEU:O | 1:B:1050:THR:CB | 2.69 | 0.40 |
| 1:B:1297:LEU:HD12 | 1:B:1297:LEU:HA | 1.85 | 0.40 |
| 1:B:1049:LEU:CD1 | 1:B:1050:THR:O | 2.67 | 0.40 |
| 1:B:1134:ASP:HB3 | 1:B:1193:TYR:CD2 | 2.57 | 0.40 |
| 1:A:26:ASN:ND2 | 3:A:3105:HOH:O | 2.54 | 0.40 |
| 1:A:175:LYS:O | 1:A:176:GLU:CG | 2.69 | 0.40 |
| 1:B:1065:ARG:NE | 1:B:1074:VAL:HG11 | 2.36 | 0.40 |
| 1:B:1132:THR:HG22 | 1:B:1260:ASN:OD1 | 2.21 | 0.40 |
| 1:B:1307:LEU:HD23 | 1:B:1315:PRO:HD3 | 2.02 | 0.40 |
| 1:B:1310:GLN:NE2 | 1:B:1311:ASN:H | 2.19 | 0.40 |
| 1:B:1020:LEU:HD11 | 1:B:1219:GLU:HA | 2.03 | 0.40 |
| 1:B:1297:LEU:HD13 | 1:B:1320:ILE:HD13 | 2.03 | 0.40 |
| 1:B:1307:LEU:HD23 | 1:B:1315:PRO:CD | 2.51 | 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 | 389/391 (100%) | 352 (90%) | 22 (6%) | 15 (4%) | 3 2 |
| 1 | B | 389/391 (100%) | 347 (89%) | 25 (6%) | 17 (4%) | 2 2 |
| All | All | 778/782 (100%) | 699 (90%) | 47 (6%) | 32 (4%) | 3 2 |

All (32) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 79 | CYS |
| 1 | A | 91 | SER |
| 1 | A | 111 | ASP |
| 1 | A | 176 | GLU |
| 1 | A | 234 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1186 | LYS |
| 1 | B | 1187 | ASN |
| 1 | B | 1198 | GLY |
| 1 | B | 1232 | LYS |
| 1 | A | 18 | ALA |
| 1 | A | 46 | GLY |
| 1 | A | 78 | GLU |
| 1 | A | 271 | LYS |
| 1 | A | 329 | LYS |
| 1 | A | 331 | ASN |
| 1 | B | 1156 | THR |
| 1 | B | 1231 | ILE |
| 1 | A | 82 | PRO |
| 1 | A | 178 | GLN |
| 1 | B | 1078 | GLU |
| 1 | B | 1176 | GLU |
| 1 | B | 1008 | GLN |
| 1 | B | 1079 | CYS |
| 1 | B | 1233 | SER |
| 1 | B | 1329 | LYS |
| 1 | A | 191 | ALA |
| 1 | B | 1082 | PRO |
| 1 | B | 1089 | ALA |
| 1 | B | 1111 | ASP |
| 1 | B | 1343 | SER |
| 1 | A | 233 | SER |
| 1 | B | 1197 | PRO |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 335/335 (100%) | 294 (88%) | 41 (12%) | 5 6 |
| 1 | B | 335/335 (100%) | 301 (90%) | 34 (10%) | 7 11 |
| All | All | 670/670 (100%) | 595 (89%) | 75 (11%) | 6 8 |

All (75) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 20 | LEU |
| 1 | A | 21 | ARG |
| 1 | A | 26 | ASN |
| 1 | A | 30 | VAL |
| 1 | A | 41 | GLU |
| 1 | A | 44 | VAL |
| 1 | A | 49 | LEU |
| 1 | A | 65 | ARG |
| 1 | A | 68 | LEU |
| 1 | A | 75 | LYS |
| 1 | A | 79 | CYS |
| 1 | A | 90 | ASN |
| 1 | A | 91 | SER |
| 1 | A | 98 | THR |
| 1 | A | 128 | ASN |
| 1 | A | 150 | LEU |
| 1 | A | 154 | GLN |
| 1 | A | 155 | LEU |
| 1 | A | 161 | LEU |
| 1 | A | 162 | LEU |
| 1 | A | 167 | ASN |
| 1 | A | 182 | LEU |
| 1 | A | 186 | LYS |
| 1 | A | 188 | THR |
| 1 | A | 192 | LYS |
| 1 | A | 199 | VAL |
| 1 | A | 205 | VAL |
| 1 | A | 215 | LEU |
| 1 | A | 225 | GLN |
| 1 | A | 237 | TRP |
| 1 | A | 238 | LYS |
| 1 | A | 265 | LEU |
| 1 | A | 277 | ARG |
| 1 | A | 286 | LEU |
| 1 | A | 303 | LYS |
| 1 | A | 307 | LEU |
| 1 | A | 321 | VAL |
| 1 | A | 331 | ASN |
| 1 | A | 339 | TYR |
| 1 | A | 345 | GLU |
| 1 | A | 369 | CYS |
| 1 | B | 1005 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1011 | GLN |
| 1 | B | 1019 | ASN |
| 1 | B | 1024 | LEU |
| 1 | B | 1049 | LEU |
| 1 | B | 1074 | VAL |
| 1 | B | 1075 | LYS |
| 1 | B | 1082 | PRO |
| 1 | B | 1088 | TYR |
| 1 | B | 1128 | ASN |
| 1 | B | 1150 | LEU |
| 1 | B | 1153 | LEU |
| 1 | B | 1156 | THR |
| 1 | B | 1161 | LEU |
| 1 | B | 1162 | LEU |
| 1 | B | 1167 | ASN |
| 1 | B | 1186 | LYS |
| 1 | B | 1192 | LYS |
| 1 | B | 1205 | VAL |
| 1 | B | 1209 | LEU |
| 1 | B | 1215 | LEU |
| 1 | B | 1231 | ILE |
| 1 | B | 1237 | TRP |
| 1 | B | 1265 | LEU |
| 1 | B | 1274 | VAL |
| 1 | B | 1286 | LEU |
| 1 | B | 1297 | LEU |
| 1 | B | 1306 | GLN |
| 1 | B | 1307 | LEU |
| 1 | B | 1309 | ASP |
| 1 | B | 1339 | TYR |
| 1 | B | 1348 | ARG |
| 1 | B | 1363 | THR |
| 1 | B | 1369 | CYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 11 | GLN |
| 1 | A | 19 | ASN |
| 1 | A | 26 | ASN |
| 1 | A | 71 | GLN |
| 1 | A | 90 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 117 | GLN |
| 1 | A | 128 | ASN |
| 1 | A | 141 | GLN |
| 1 | A | 167 | ASN |
| 1 | A | 194 | GLN |
| 1 | A | 236 | GLN |
| 1 | A | 248 | GLN |
| 1 | A | 260 | ASN |
| 1 | A | 306 | GLN |
| 1 | A | 308 | HIS |
| 1 | A | 310 | GLN |
| 1 | A | 311 | ASN |
| 1 | A | 331 | ASN |
| 1 | A | 346 | GLN |
| 1 | A | 349 | ASN |
| 1 | A | 360 | GLN |
| 1 | A | 387 | ASN |
| 1 | B | 1008 | GLN |
| 1 | B | 1011 | GLN |
| 1 | B | 1019 | ASN |
| 1 | B | 1033 | GLN |
| 1 | B | 1062 | HIS |
| 1 | B | 1071 | GLN |
| 1 | B | 1116 | HIS |
| 1 | B | 1128 | ASN |
| 1 | B | 1141 | GLN |
| 1 | B | 1167 | ASN |
| 1 | B | 1195 | GLN |
| 1 | B | 1260 | ASN |
| 1 | B | 1306 | GLN |
| 1 | B | 1310 | GLN |
| 1 | B | 1311 | ASN |
| 1 | B | 1331 | ASN |
| 1 | B | 1342 | GLN |
| 1 | B | 1346 | GLN |
| 1 | B | 1349 | 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 monosaccharides in this entry.

## 5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | XGP | B | 2001 | - | 15,16,16 | 1.34 | 2 (13%) | 23,24,24 | 0.82 | 1 (4%) |
| 2 | XGP | A | 2000 | - | 15,16,16 | 1.11 | 1 (6%) | 23,24,24 | 0.82 | 1 (4%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | XGP | B | 2001 | - | - | 1/7/27/27 | 0/1/1/1 |
| 2 | XGP | A | 2000 | - | - | 1/7/27/27 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 2001 | XGP | P-OP2 | 2.76 | 1.59 | 1.50 |
| 2 | B | 2001 | XGP | C4-C3 | 2.07 | 1.57 | 1.52 |
| 2 | A | 2000 | XGP | C4-C3 | 2.06 | 1.57 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 2001 | XGP | O5-C1-O1 | -2.71 | 107.82 | 111.36 |
| 2 | A | 2000 | XGP | O5-C1-O1 | -2.70 | 107.83 | 111.36 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 2000 | XGP | C2-C1-O1-P |
| 2 | B | 2001 | XGP | C2-C1-O1-P |

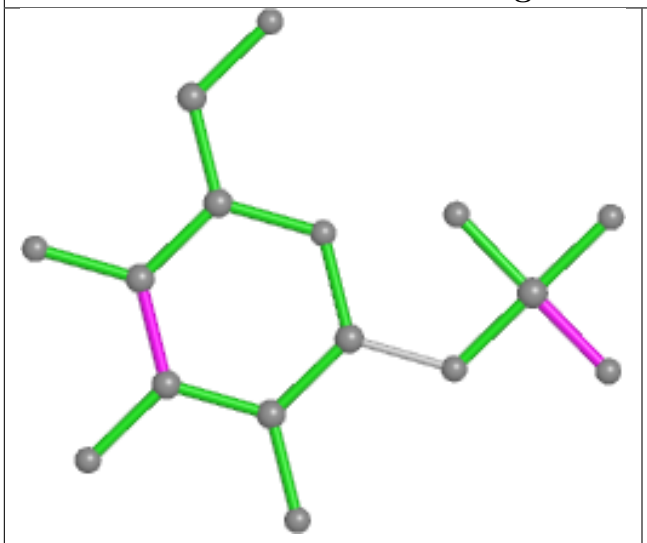
There are no ring outliers.

2 monomers are involved in 12 short contacts:

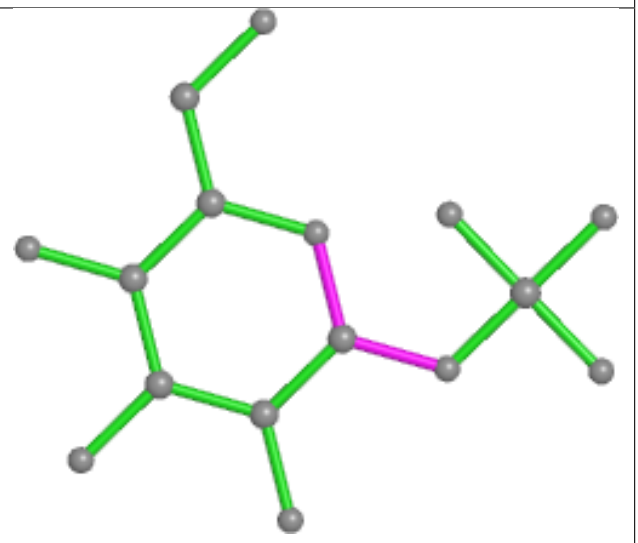
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 2001 | XGP | 6 | 0 |
| 2 | A | 2000 | XGP | 6 | 0 |

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

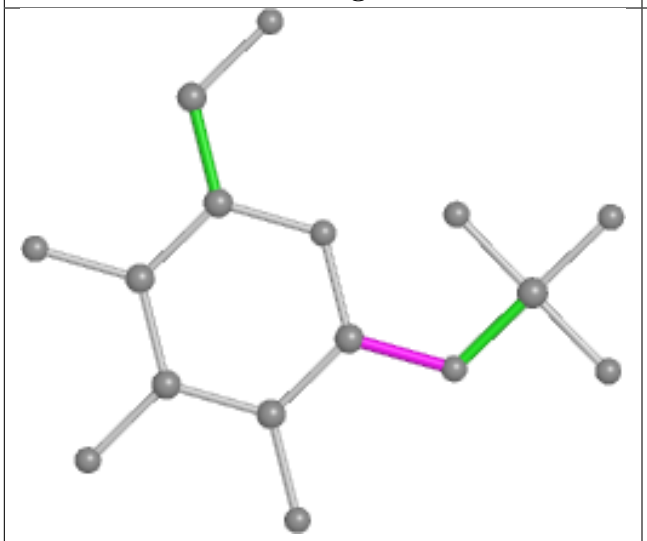
**Ligand XGP B 2001**



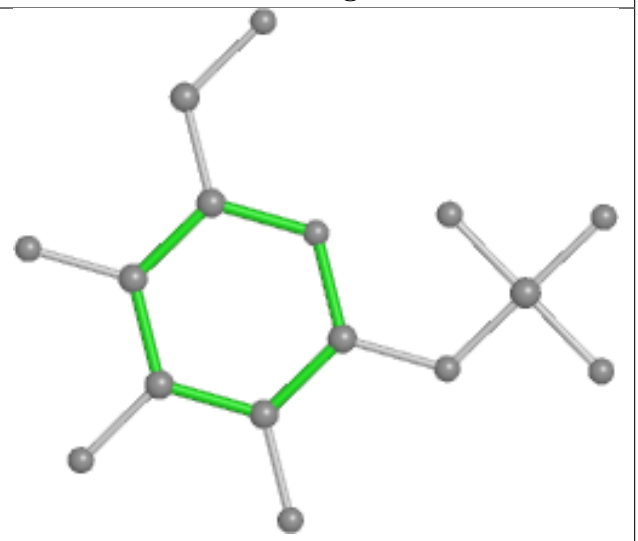
**Bond lengths**



**Bond angles**

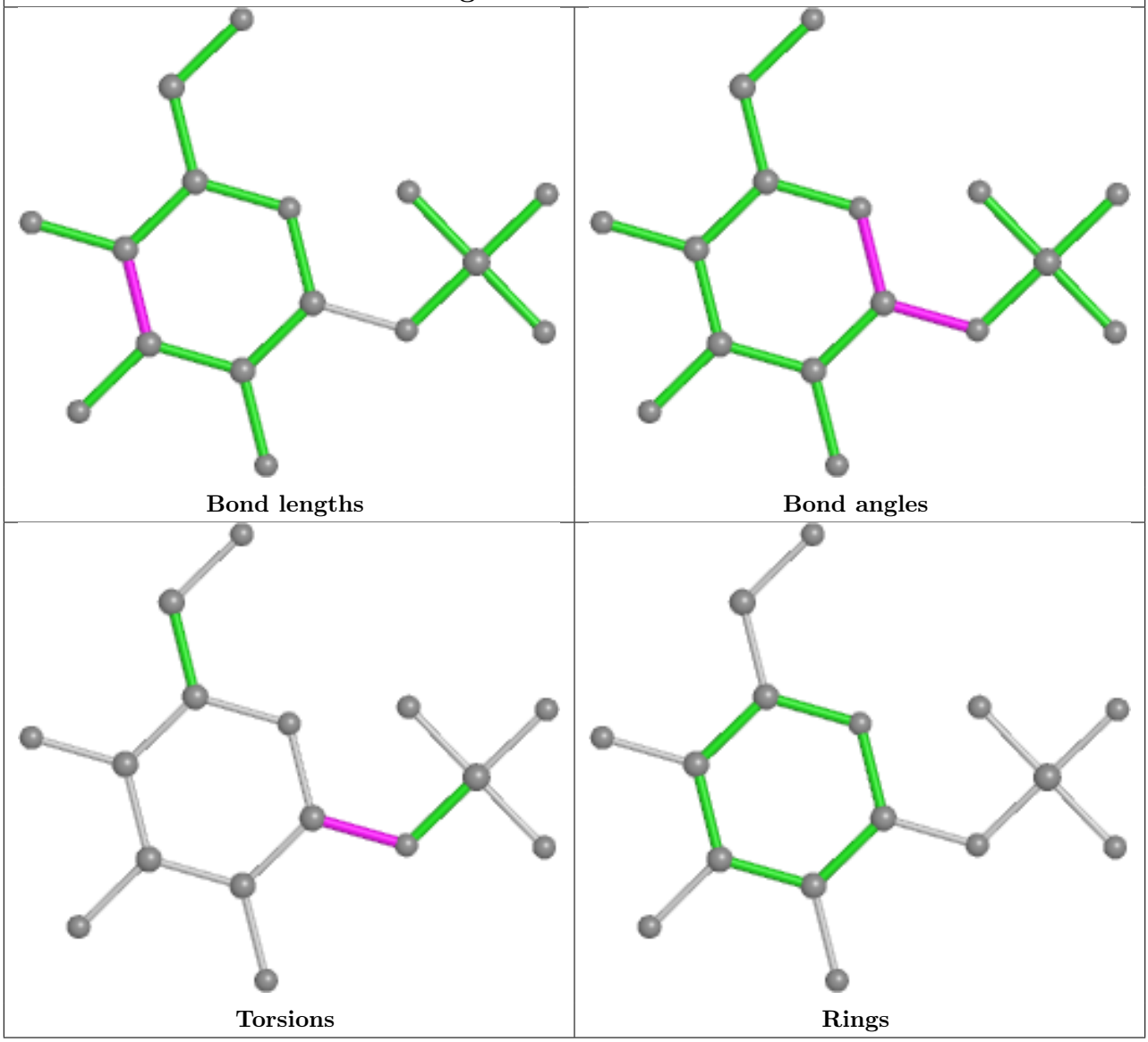


**Torsions**



**Rings**

**Ligand XGP A 2000**




## 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 (i)

## 6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.