# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:24 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1N8P |
| Title | : | Crystal Structure of cystathionine gamma-lyase from yeast |
| Authors | : | Messerschmidt, A.; Worbs, M.; Steegborn, C.; Wahl, M.C.; Huber, R.; Clausen, T. |
| Deposited on | : | 2002-11-21 |
| 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

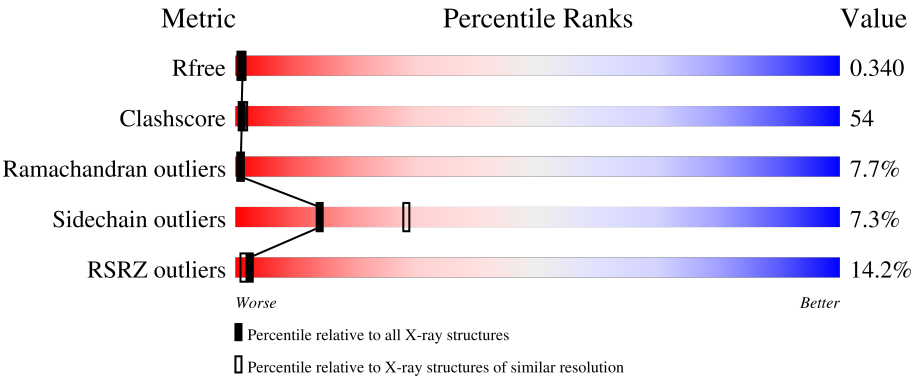
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 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 2.60 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 3163 (2.60-2.60) |
| Clashscore | 141614 | 3518 (2.60-2.60) |
| Ramachandran outliers | 138981 | 3455 (2.60-2.60) |
| Sidechain outliers | 138945 | 3455 (2.60-2.60) |
| RSRZ outliers | 127900 | 3104 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 393 | 12% 35% 55% 8% |
| 1 | B | 393 | 15% 35% 53% 11% |
| 1 | C | 393 | 17% 30% 61% 9% |
| 1 | D | 393 | 13% 40% 50% 10% |

## 2 Entry composition

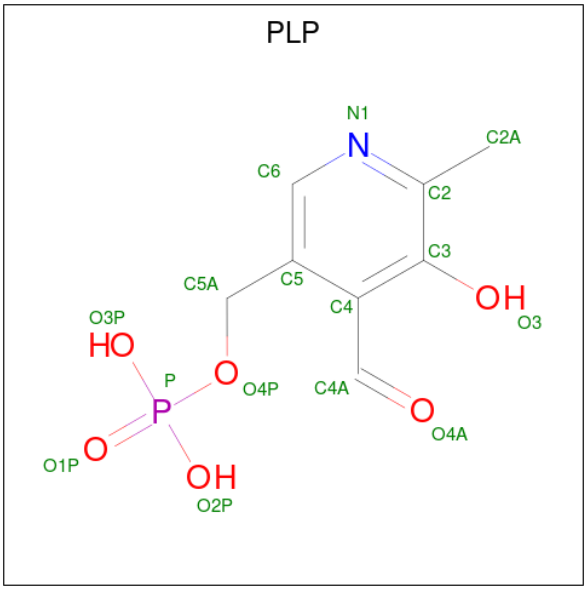
There are 3 unique types of molecules in this entry. The entry contains 12287 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cystathionine gamma-lyase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 393 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2969 | 1871 | 518 | 578 | 2 | | | |
| 1 | B | 393 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2969 | 1871 | 518 | 578 | 2 | | | |
| 1 | C | 393 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2969 | 1871 | 518 | 578 | 2 | | | |
| 1 | D | 393 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 2969 | 1871 | 518 | 578 | 2 | | | |

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).




| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 15 | 8 | 1 | 5 | 1 | | |
| 2 | B | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 15 | 8 | 1 | 5 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 15 | 8 | 1 | 5 | 1 | | |
| 2 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 15 | 8 | 1 | 5 | 1 | | |

- Molecule 3 is water.

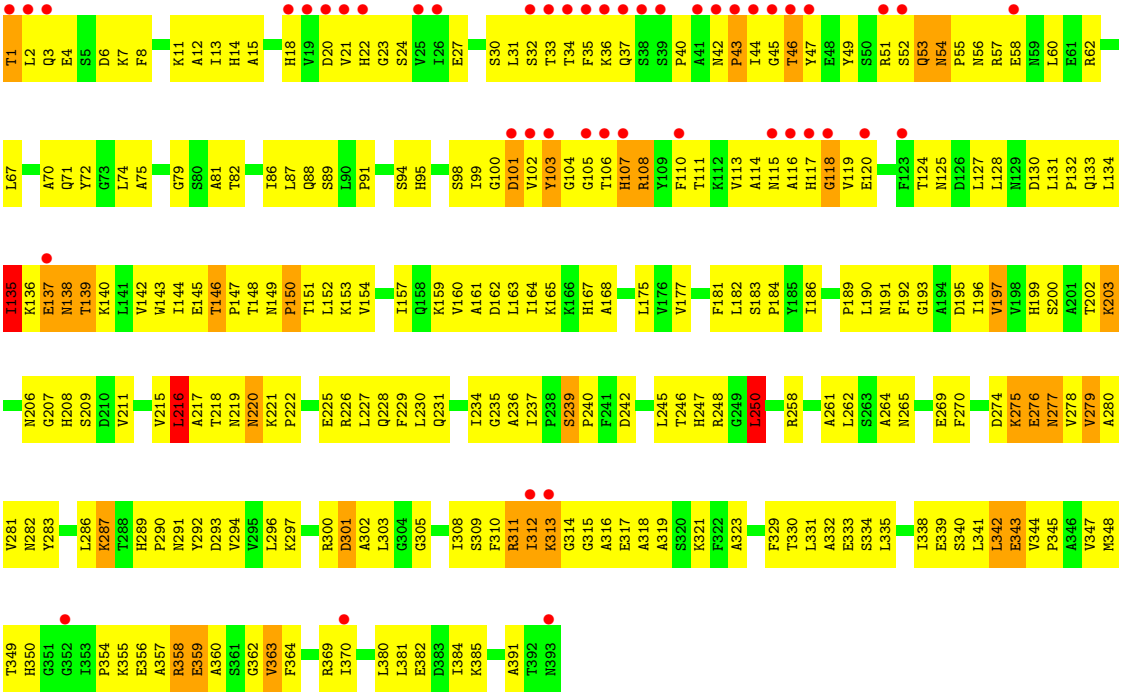
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 3 | A | 74 | Total | O | 0 | 0 |
| | | | 74 | 74 | | |
| 3 | B | 94 | Total | O | 0 | 0 |
| | | | 94 | 94 | | |
| 3 | C | 95 | Total | O | 0 | 0 |
| | | | 95 | 95 | | |
| 3 | D | 88 | Total | O | 0 | 0 |
| | | | 88 | 88 | | |

# 3 Residue-property plots (i)

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

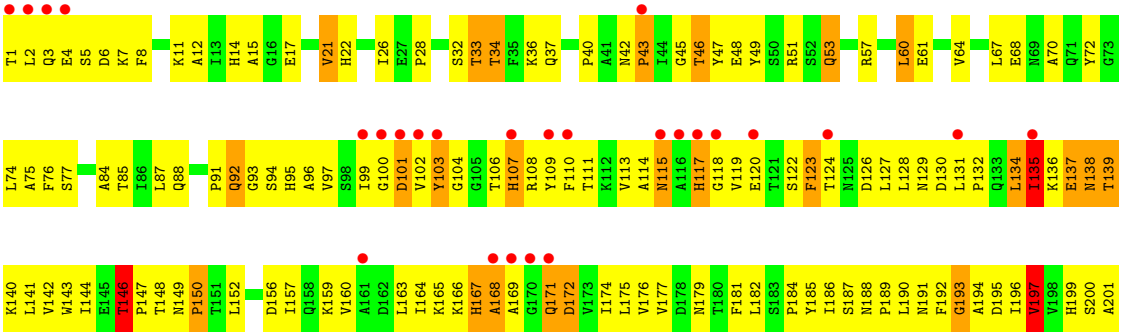
• Molecule 1: Cystathionine gamma-lyase

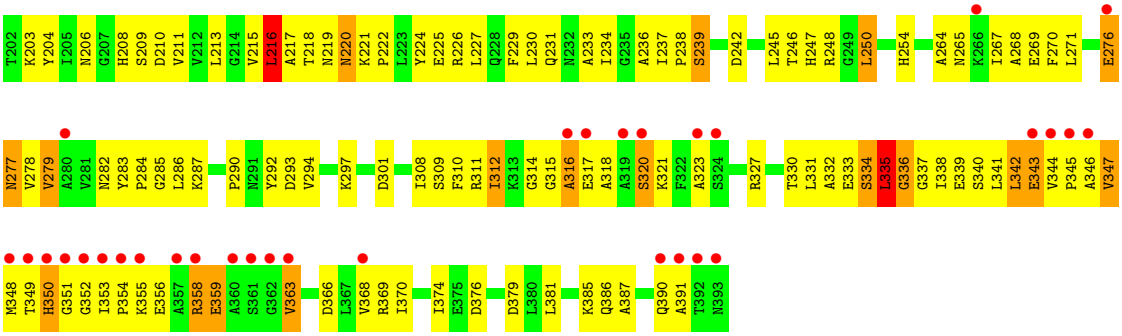
Chain A:

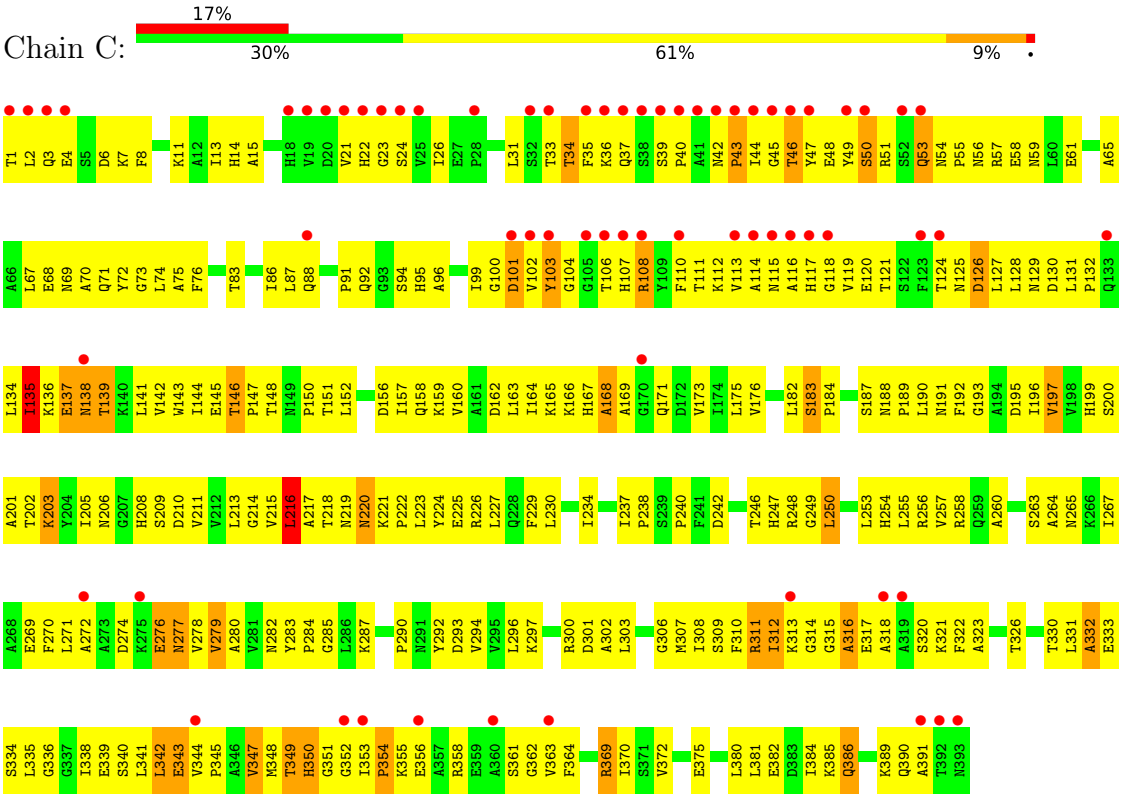

• Molecule 1: Cystathionine gamma-lyase

Chain B:

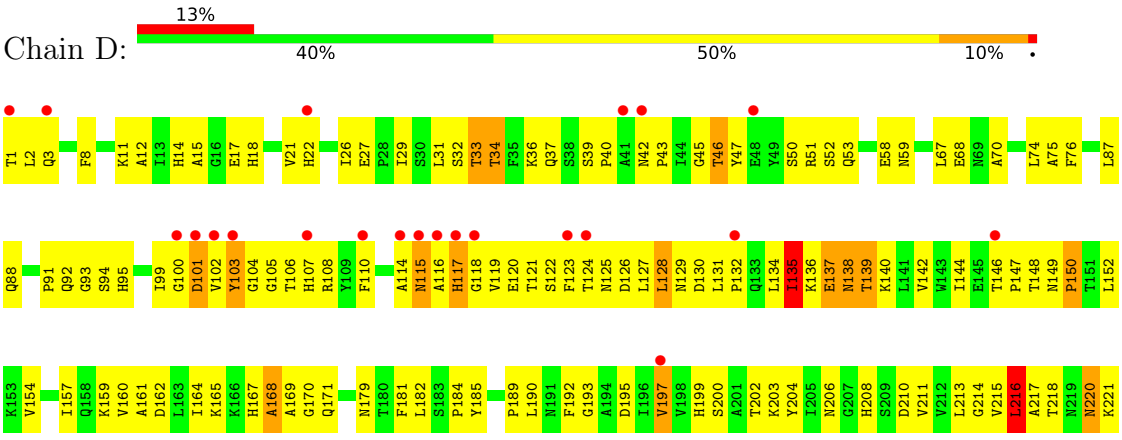



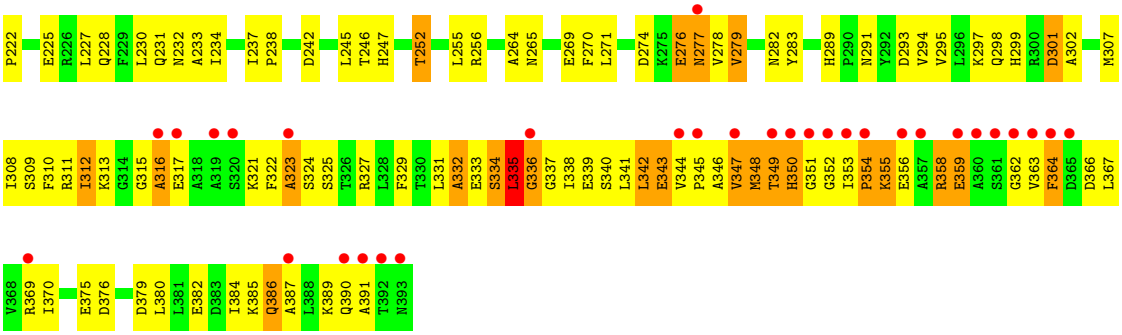


• Molecule 1: Cystathionine gamma-lyase




• Molecule 1: Cystathionine gamma-lyase




P222
E225
R226
L227
Q228
F229
L230
Q231
N232
A233
I234
I237
P238
D242
L245
T246
H247
T252
L255
R256
A264
N265
E269
F270
L271
D274
K275
E276
N277
V278
V279
N282
Y283
H289
P290
N291
Y292
D293
V294
V295
L296
K297
Q298
H299
R300
D301
A302
M307
I308
S309
F310
R311
I312
K313
G314
G315
A316
E317
A318
A319
S320
K321
F322
A323
S324
S325
T326
R327
L328
F329
T330
L331
A332
E333
S334
L335
G336
G337
I338
E339
S340
L341
L342
E343
V344
P345
A346
V347
M348
T349
H350
G351
G352
I353
P354
K355
E356
A357
R358
E359
A360
S361
G362
V363
F364
D365
D366
L367
V368
R369
I370
E375
D376
D379
L380
L381
E382
D383
I384
K385
Q386
A387
L388
K389
Q390
A391
T392
N393

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 153.82Å 62.16Å 160.84Å<br>90.00° 105.42° 90.00° | Depositor |
| Resolution (Å) | 6.00 – 2.60<br>19.90 – 2.60 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.1 (6.00-2.60)<br>98.9 (19.90-2.60) | Depositor<br>EDS |
| $R_{merge}$ | 0.05 | Depositor |
| $R_{sym}$ | 0.05 | Depositor |
| $< I/\sigma(I) >$ [1] | 1.21 (at 2.59Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.253 , 0.346<br>0.261 , 0.340 | Depositor<br>DCC |
| $R_{free}$ test set | 2253 reflections (5.01%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 54.6 | Xtriage |
| Anisotropy | 0.556 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 72.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.90 | EDS |
| Total number of atoms | 12287 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

# 5 Model quality

## 5.1 Standard geometry

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

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 | 0.54 | 0/3026 | 0.80 | 3/4121 (0.1%) |
| 1 | B | 0.52 | 0/3026 | 0.80 | 5/4121 (0.1%) |
| 1 | C | 0.50 | 0/3026 | 0.78 | 2/4121 (0.0%) |
| 1 | D | 0.56 | 0/3026 | 0.79 | 2/4121 (0.0%) |
| All | All | 0.53 | 0/12104 | 0.79 | 12/16484 (0.1%) |

There are no bond length outliers.

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 216 | LEU | CA-CB-CG | 8.30 | 134.38 | 115.30 |
| 1 | A | 216 | LEU | CA-CB-CG | 6.59 | 130.45 | 115.30 |
| 1 | B | 200 | SER | N-CA-C | -6.49 | 93.47 | 111.00 |
| 1 | D | 216 | LEU | CA-CB-CG | 6.44 | 130.11 | 115.30 |
| 1 | D | 200 | SER | N-CA-C | -6.33 | 93.89 | 111.00 |
| 1 | C | 216 | LEU | CA-CB-CG | 6.20 | 129.57 | 115.30 |
| 1 | A | 250 | LEU | CA-CB-CG | 6.11 | 129.35 | 115.30 |
| 1 | B | 250 | LEU | CA-CB-CG | 5.93 | 128.93 | 115.30 |
| 1 | A | 200 | SER | N-CA-C | -5.80 | 95.33 | 111.00 |
| 1 | B | 194 | ALA | N-CA-C | -5.43 | 96.33 | 111.00 |
| 1 | B | 197 | VAL | CB-CA-C | -5.30 | 101.33 | 111.40 |
| 1 | C | 200 | SER | N-CA-C | -5.08 | 97.28 | 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 | 2969 | 0 | 2939 | 345 | 0 |
| 1 | B | 2969 | 0 | 2939 | 323 | 0 |
| 1 | C | 2969 | 0 | 2939 | 373 | 0 |
| 1 | D | 2969 | 0 | 2939 | 333 | 0 |
| 2 | A | 15 | 0 | 6 | 0 | 0 |
| 2 | B | 15 | 0 | 6 | 1 | 0 |
| 2 | C | 15 | 0 | 6 | 0 | 0 |
| 2 | D | 15 | 0 | 6 | 0 | 0 |
| 3 | A | 74 | 0 | 0 | 3 | 0 |
| 3 | B | 94 | 0 | 0 | 20 | 0 |
| 3 | C | 95 | 0 | 0 | 17 | 0 |
| 3 | D | 88 | 0 | 0 | 18 | 0 |
| All | All | 12287 | 0 | 11780 | 1281 | 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 54.

All (1281) 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:B:321:LYS:HG2 | 1:B:391:ALA:HA | 1.21 | 1.20 |
| 1:C:321:LYS:HG2 | 1:C:391:ALA:HA | 1.28 | 1.16 |
| 1:A:36:LYS:H | 1:C:23:GLY:HA3 | 1.17 | 1.09 |
| 1:D:321:LYS:HG2 | 1:D:391:ALA:HA | 1.35 | 1.08 |
| 1:C:95:HIS:ND1 | 1:C:139:THR:HG22 | 1.69 | 1.08 |
| 1:A:95:HIS:ND1 | 1:A:139:THR:HG22 | 1.68 | 1.08 |
| 1:D:220:ASN:ND2 | 1:D:222:PRO:HD2 | 1.70 | 1.06 |
| 1:D:279:VAL:HB | 1:D:311:ARG:HG3 | 1.36 | 1.06 |
| 1:D:95:HIS:ND1 | 1:D:139:THR:HG22 | 1.69 | 1.06 |
| 1:A:348:MET:HG2 | 1:B:40:PRO:O | 1.55 | 1.05 |
| 1:C:37:GLN:HE21 | 1:C:43:PRO:HG3 | 1.13 | 1.05 |
| 1:B:347:VAL:HG23 | 1:B:348:MET:H | 1.23 | 1.03 |
| 1:A:321:LYS:HG2 | 1:A:391:ALA:HA | 1.42 | 1.01 |
| 1:C:115:ASN:O | 1:D:92:GLN:HB2 | 1.59 | 1.01 |
| 1:B:95:HIS:ND1 | 1:B:139:THR:HG22 | 1.76 | 1.00 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:279:VAL:HB | 1:B:311:ARG:HG3 | 1.42 | 1.00 |
| 1:A:220:ASN:ND2 | 1:A:222:PRO:HD2 | 1.77 | 0.98 |
| 1:A:3:GLN:HE22 | 1:A:15:ALA:HB2 | 1.28 | 0.98 |
| 1:A:37:GLN:HE21 | 1:A:43:PRO:HG3 | 1.25 | 0.98 |
| 1:B:323:ALA:HB1 | 1:B:331:LEU:HD13 | 1.46 | 0.97 |
| 1:A:136:LYS:HG3 | 1:A:137:GLU:H | 1.27 | 0.96 |
| 1:A:206:ASN:HB2 | 1:A:246:THR:HG23 | 1.47 | 0.96 |
| 1:D:75:ALA:HA | 1:D:215:VAL:HG12 | 1.46 | 0.95 |
| 1:B:342:LEU:HB2 | 1:B:370:ILE:HG22 | 1.45 | 0.95 |
| 1:B:195:ASP:O | 1:B:218:THR:HG22 | 1.64 | 0.95 |
| 1:C:323:ALA:HB1 | 1:C:331:LEU:HD13 | 1.48 | 0.94 |
| 1:D:347:VAL:HG23 | 1:D:348:MET:H | 1.33 | 0.94 |
| 1:C:279:VAL:HB | 1:C:311:ARG:HG3 | 1.48 | 0.94 |
| 1:D:136:LYS:HG3 | 1:D:137:GLU:H | 1.33 | 0.94 |
| 1:A:347:VAL:HG23 | 1:A:348:MET:H | 1.35 | 0.92 |
| 1:C:347:VAL:HG23 | 1:C:348:MET:H | 1.32 | 0.92 |
| 1:A:36:LYS:H | 1:C:23:GLY:CA | 1.82 | 0.92 |
| 1:B:335:LEU:O | 1:B:337:GLY:N | 2.04 | 0.91 |
| 1:A:323:ALA:HB1 | 1:A:331:LEU:HD13 | 1.54 | 0.89 |
| 1:A:23:GLY:HA3 | 1:C:36:LYS:H | 1.34 | 0.89 |
| 1:A:279:VAL:HB | 1:A:311:ARG:HG3 | 1.54 | 0.89 |
| 1:C:68:GLU:OE1 | 1:C:184:PRO:HG3 | 1.72 | 0.89 |
| 1:D:317:GLU:HB3 | 3:D:448:HOH:O | 1.70 | 0.89 |
| 1:B:342:LEU:HD23 | 1:B:342:LEU:O | 1.73 | 0.89 |
| 1:A:342:LEU:HB2 | 1:A:370:ILE:HG22 | 1.52 | 0.89 |
| 1:C:87:LEU:HD13 | 1:C:110:PHE:HA | 1.55 | 0.88 |
| 1:A:23:GLY:CA | 1:C:36:LYS:H | 1.88 | 0.87 |
| 1:C:265:ASN:O | 1:C:269:GLU:HG3 | 1.75 | 0.86 |
| 1:C:137:GLU:O | 1:C:138:ASN:HB2 | 1.76 | 0.86 |
| 1:C:340:SER:O | 1:C:341:LEU:HD23 | 1.75 | 0.86 |
| 1:C:144:ILE:HD11 | 1:C:160:VAL:HG11 | 1.58 | 0.86 |
| 1:A:36:LYS:N | 1:C:23:GLY:HA3 | 1.90 | 0.86 |
| 1:B:99:ILE:O | 1:B:102:VAL:HG23 | 1.76 | 0.85 |
| 1:C:37:GLN:NE2 | 1:C:43:PRO:HG3 | 1.91 | 0.85 |
| 1:A:71:GLN:H | 1:A:219:ASN:ND2 | 1.75 | 0.84 |
| 1:B:277:ASN:N | 1:B:277:ASN:HD22 | 1.76 | 0.84 |
| 1:A:340:SER:O | 1:A:341:LEU:HD23 | 1.77 | 0.84 |
| 1:A:1:THR:HG21 | 1:A:14:HIS:CG | 2.12 | 0.84 |
| 1:B:149:ASN:HB2 | 1:B:181:PHE:HE2 | 1.42 | 0.84 |
| 1:C:344:VAL:H | 1:C:348:MET:CE | 1.90 | 0.83 |
| 1:A:35:PHE:HB3 | 1:C:22:HIS:O | 1.76 | 0.83 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:206:ASN:HD22 | 1:C:246:THR:HA | 1.42 | 0.83 |
| 1:C:277:ASN:HD22 | 1:C:277:ASN:N | 1.77 | 0.83 |
| 1:B:346:ALA:HB3 | 3:B:492:HOH:O | 1.79 | 0.82 |
| 1:B:220:ASN:ND2 | 1:B:222:PRO:HD2 | 1.95 | 0.82 |
| 1:A:338:ILE:HG22 | 3:A:416:HOH:O | 1.79 | 0.82 |
| 1:D:349:THR:HG22 | 1:D:350:HIS:N | 1.93 | 0.82 |
| 1:B:95:HIS:HD2 | 1:B:120:GLU:HB3 | 1.45 | 0.81 |
| 1:A:118:GLY:HA3 | 3:B:424:HOH:O | 1.79 | 0.81 |
| 1:A:136:LYS:O | 1:A:137:GLU:HB3 | 1.77 | 0.81 |
| 1:C:220:ASN:ND2 | 1:C:222:PRO:HD2 | 1.96 | 0.81 |
| 1:C:1:THR:HG21 | 1:C:14:HIS:CG | 2.16 | 0.81 |
| 1:C:3:GLN:HE21 | 1:C:11:LYS:HG2 | 1.45 | 0.80 |
| 1:C:342:LEU:HD23 | 1:C:342:LEU:O | 1.82 | 0.80 |
| 1:D:344:VAL:H | 1:D:348:MET:HE3 | 1.45 | 0.80 |
| 1:A:95:HIS:HB3 | 1:A:138:ASN:C | 2.02 | 0.80 |
| 1:D:51:ARG:HG3 | 1:D:237:ILE:HD13 | 1.63 | 0.79 |
| 1:D:75:ALA:CA | 1:D:215:VAL:HG12 | 2.11 | 0.79 |
| 1:B:150:PRO:O | 1:B:152:LEU:HG | 1.82 | 0.78 |
| 1:A:23:GLY:HA3 | 1:C:36:LYS:N | 1.97 | 0.78 |
| 1:A:343:GLU:HA | 1:A:348:MET:HE1 | 1.65 | 0.78 |
| 1:C:206:ASN:HB2 | 1:C:246:THR:HG23 | 1.66 | 0.78 |
| 1:D:146:THR:OG1 | 1:D:147:PRO:HD3 | 1.84 | 0.78 |
| 1:B:70:ALA:HB2 | 1:B:190:LEU:HD12 | 1.65 | 0.78 |
| 1:D:344:VAL:H | 1:D:348:MET:CE | 1.96 | 0.78 |
| 1:B:135:ILE:HG21 | 1:B:167:HIS:O | 1.84 | 0.78 |
| 1:B:114:ALA:CB | 1:B:119:VAL:H | 1.97 | 0.78 |
| 1:B:379:ASP:OD1 | 1:C:7:LYS:HG2 | 1.83 | 0.78 |
| 1:A:242:ASP:OD1 | 1:B:239:SER:HB2 | 1.82 | 0.78 |
| 1:B:149:ASN:HB2 | 1:B:181:PHE:CE2 | 2.19 | 0.78 |
| 1:C:95:HIS:O | 1:C:139:THR:HA | 1.84 | 0.77 |
| 1:A:3:GLN:HE21 | 1:A:11:LYS:HG2 | 1.48 | 0.77 |
| 1:A:382:GLU:HG3 | 3:A:420:HOH:O | 1.83 | 0.77 |
| 1:B:95:HIS:HB3 | 1:B:139:THR:N | 1.99 | 0.77 |
| 1:C:95:HIS:HB3 | 1:C:139:THR:N | 2.00 | 0.77 |
| 1:D:114:ALA:HA | 1:D:119:VAL:H | 1.49 | 0.77 |
| 1:A:23:GLY:C | 1:C:36:LYS:H | 1.87 | 0.77 |
| 1:A:95:HIS:HB3 | 1:A:139:THR:N | 1.99 | 0.77 |
| 1:A:136:LYS:HA | 1:A:139:THR:HG23 | 1.65 | 0.77 |
| 1:D:3:GLN:HE21 | 1:D:11:LYS:HG2 | 1.50 | 0.77 |
| 1:A:137:GLU:O | 1:A:138:ASN:HB2 | 1.83 | 0.77 |
| 1:D:335:LEU:O | 1:D:337:GLY:N | 2.18 | 0.77 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:165:LYS:O | 1:B:169:ALA:HB2 | 1.85 | 0.76 |
| 1:C:293:ASP:O | 1:C:297:LYS:HG2 | 1.84 | 0.76 |
| 1:D:220:ASN:C | 1:D:220:ASN:HD22 | 1.88 | 0.76 |
| 1:C:146:THR:OG1 | 1:C:147:PRO:HD3 | 1.85 | 0.76 |
| 1:B:143:TRP:CZ3 | 1:B:176:VAL:HG11 | 2.21 | 0.75 |
| 1:D:342:LEU:O | 1:D:342:LEU:HD23 | 1.87 | 0.75 |
| 1:D:95:HIS:HB3 | 1:D:138:ASN:C | 2.06 | 0.75 |
| 1:A:87:LEU:HD13 | 1:A:110:PHE:HA | 1.67 | 0.75 |
| 1:C:220:ASN:C | 1:C:220:ASN:HD22 | 1.89 | 0.75 |
| 1:D:136:LYS:CG | 1:D:137:GLU:H | 1.98 | 0.75 |
| 1:A:142:VAL:HG21 | 1:A:164:ILE:HD11 | 1.69 | 0.75 |
| 1:B:157:ILE:HG22 | 1:B:192:PHE:O | 1.87 | 0.75 |
| 1:B:70:ALA:HA | 1:B:219:ASN:HD21 | 1.50 | 0.75 |
| 1:B:95:HIS:HB3 | 1:B:138:ASN:C | 2.07 | 0.74 |
| 1:D:323:ALA:HA | 1:D:342:LEU:HD11 | 1.67 | 0.74 |
| 1:C:142:VAL:HG21 | 1:C:164:ILE:HD11 | 1.69 | 0.74 |
| 1:A:22:HIS:O | 1:C:35:PHE:HB3 | 1.87 | 0.74 |
| 1:B:344:VAL:HG21 | 3:B:443:HOH:O | 1.86 | 0.74 |
| 1:D:195:ASP:O | 1:D:218:THR:HG22 | 1.87 | 0.74 |
| 1:A:135:ILE:HD12 | 1:A:167:HIS:HB2 | 1.69 | 0.74 |
| 1:A:206:ASN:HD22 | 1:A:246:THR:HA | 1.51 | 0.74 |
| 1:A:220:ASN:HD22 | 1:A:222:PRO:HD2 | 1.52 | 0.74 |
| 1:C:3:GLN:HE22 | 1:C:15:ALA:HB2 | 1.52 | 0.74 |
| 1:D:68:GLU:HG3 | 3:D:439:HOH:O | 1.86 | 0.74 |
| 1:A:75:ALA:HA | 1:A:215:VAL:HG12 | 1.69 | 0.74 |
| 1:B:74:LEU:HB2 | 1:B:216:LEU:HD22 | 1.70 | 0.74 |
| 1:C:114:ALA:CB | 1:C:119:VAL:H | 2.01 | 0.74 |
| 1:D:136:LYS:O | 1:D:137:GLU:HB3 | 1.85 | 0.74 |
| 3:C:458:HOH:O | 1:D:33:THR:HG21 | 1.88 | 0.73 |
| 1:D:114:ALA:CB | 1:D:119:VAL:H | 1.99 | 0.73 |
| 1:C:150:PRO:HG3 | 1:C:345:PRO:HG3 | 1.70 | 0.73 |
| 1:C:150:PRO:O | 1:C:152:LEU:HG | 1.88 | 0.73 |
| 1:C:116:ALA:HB3 | 1:D:92:GLN:CB | 2.18 | 0.73 |
| 1:C:282:ASN:HB2 | 1:C:309:SER:HB3 | 1.70 | 0.73 |
| 1:A:99:ILE:O | 1:A:102:VAL:HG23 | 1.88 | 0.73 |
| 1:D:347:VAL:HA | 3:D:438:HOH:O | 1.86 | 0.73 |
| 1:A:71:GLN:H | 1:A:219:ASN:HD22 | 1.35 | 0.73 |
| 1:D:230:LEU:O | 1:D:234:ILE:HG12 | 1.89 | 0.73 |
| 1:A:277:ASN:N | 1:A:277:ASN:HD22 | 1.87 | 0.72 |
| 1:D:3:GLN:HE22 | 1:D:15:ALA:HB2 | 1.54 | 0.72 |
| 1:D:88:GLN:OE1 | 1:D:234:ILE:HD13 | 1.88 | 0.72 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:220:ASN:HD21 | 1:D:222:PRO:HD2 | 1.53 | 0.72 |
| 1:D:349:THR:HG22 | 1:D:350:HIS:H | 1.55 | 0.72 |
| 1:D:106:THR:HG22 | 1:D:110:PHE:CE1 | 2.24 | 0.72 |
| 1:D:342:LEU:HB2 | 1:D:370:ILE:HG22 | 1.71 | 0.72 |
| 1:B:26:ILE:HB | 1:D:32:SER:HB3 | 1.71 | 0.72 |
| 1:D:95:HIS:NE2 | 1:D:122:SER:OG | 2.22 | 0.72 |
| 1:C:31:LEU:HD23 | 1:C:240:PRO:HB2 | 1.72 | 0.72 |
| 1:D:220:ASN:HD22 | 1:D:222:PRO:HD2 | 1.50 | 0.72 |
| 1:C:87:LEU:HD11 | 1:C:110:PHE:CD1 | 2.25 | 0.72 |
| 1:B:321:LYS:HG2 | 1:B:391:ALA:CA | 2.11 | 0.71 |
| 1:D:149:ASN:HB2 | 1:D:181:PHE:HE2 | 1.55 | 0.71 |
| 1:A:162:ASP:HA | 1:A:165:LYS:NZ | 2.05 | 0.71 |
| 1:D:317:GLU:HB2 | 3:D:442:HOH:O | 1.91 | 0.71 |
| 1:A:347:VAL:HG23 | 1:A:348:MET:N | 2.04 | 0.71 |
| 1:B:136:LYS:HA | 1:B:139:THR:HG23 | 1.71 | 0.71 |
| 1:C:102:VAL:HG12 | 1:C:103:TYR:O | 1.91 | 0.71 |
| 1:D:277:ASN:N | 1:D:277:ASN:HD22 | 1.89 | 0.71 |
| 1:C:348:MET:HE2 | 1:D:40:PRO:HB3 | 1.72 | 0.71 |
| 1:B:293:ASP:O | 1:B:297:LYS:HG2 | 1.90 | 0.71 |
| 1:C:95:HIS:HB3 | 1:C:138:ASN:C | 2.11 | 0.71 |
| 1:A:220:ASN:HD21 | 1:A:222:PRO:HD2 | 1.55 | 0.71 |
| 1:A:258:ARG:NH1 | 1:A:303:LEU:HD11 | 2.06 | 0.70 |
| 1:D:3:GLN:NE2 | 1:D:11:LYS:HG2 | 2.05 | 0.70 |
| 1:B:100:GLY:O | 1:B:102:VAL:N | 2.24 | 0.70 |
| 1:C:75:ALA:HA | 1:C:215:VAL:HG12 | 1.74 | 0.70 |
| 1:C:342:LEU:HB2 | 1:C:370:ILE:HG22 | 1.72 | 0.70 |
| 1:B:344:VAL:H | 1:B:348:MET:CE | 2.05 | 0.70 |
| 1:A:146:THR:OG1 | 1:A:147:PRO:HD3 | 1.92 | 0.70 |
| 1:A:150:PRO:HB3 | 1:A:369:ARG:HD2 | 1.72 | 0.70 |
| 1:D:315:GLY:O | 1:D:317:GLU:N | 2.25 | 0.70 |
| 1:D:362:GLY:O | 1:D:364:PHE:N | 2.24 | 0.70 |
| 1:C:254:HIS:CE1 | 1:C:255:LEU:HG | 2.26 | 0.70 |
| 1:C:349:THR:HG22 | 1:C:350:HIS:N | 2.07 | 0.70 |
| 1:D:106:THR:HA | 1:D:110:PHE:CD1 | 2.27 | 0.70 |
| 1:A:37:GLN:NE2 | 1:A:43:PRO:HG3 | 2.03 | 0.70 |
| 1:A:95:HIS:O | 1:A:139:THR:HA | 1.92 | 0.70 |
| 1:B:127:LEU:HD23 | 1:B:160:VAL:HG21 | 1.74 | 0.70 |
| 1:B:220:ASN:C | 1:B:220:ASN:HD22 | 1.94 | 0.70 |
| 1:B:390:GLN:HA | 3:B:465:HOH:O | 1.91 | 0.70 |
| 1:B:45:GLY:O | 1:B:47:TYR:N | 2.24 | 0.70 |
| 1:D:53:GLN:NE2 | 1:D:58:GLU:HB2 | 2.06 | 0.70 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:146:THR:OG1 | 1:B:147:PRO:HD3 | 1.91 | 0.69 |
| 1:B:152:LEU:HD12 | 1:B:282:ASN:O | 1.92 | 0.69 |
| 1:C:277:ASN:HD22 | 1:C:277:ASN:H | 1.38 | 0.69 |
| 1:B:128:LEU:HD22 | 3:B:413:HOH:O | 1.91 | 0.69 |
| 1:B:206:ASN:HB2 | 1:B:246:THR:HG23 | 1.74 | 0.69 |
| 1:C:196:ILE:HG12 | 1:C:218:THR:HG21 | 1.74 | 0.69 |
| 1:D:279:VAL:CB | 1:D:311:ARG:HG3 | 2.20 | 0.69 |
| 1:D:102:VAL:HG12 | 1:D:103:TYR:O | 1.92 | 0.69 |
| 1:D:206:ASN:HB2 | 1:D:246:THR:HG23 | 1.73 | 0.69 |
| 1:D:1:THR:HG21 | 1:D:14:HIS:CB | 2.23 | 0.69 |
| 1:C:116:ALA:HB3 | 1:D:92:GLN:HB2 | 1.75 | 0.69 |
| 1:D:99:ILE:O | 1:D:102:VAL:HG23 | 1.93 | 0.69 |
| 1:B:347:VAL:HG23 | 1:B:348:MET:N | 2.05 | 0.69 |
| 1:D:45:GLY:O | 1:D:47:TYR:N | 2.25 | 0.69 |
| 1:B:182:LEU:HD22 | 1:B:186:ILE:HG21 | 1.74 | 0.68 |
| 1:D:1:THR:HG21 | 1:D:14:HIS:CG | 2.28 | 0.68 |
| 1:C:137:GLU:O | 1:C:138:ASN:CB | 2.41 | 0.68 |
| 1:B:184:PRO:HD3 | 1:B:199:HIS:CE1 | 2.28 | 0.68 |
| 1:D:87:LEU:HD13 | 1:D:110:PHE:HA | 1.74 | 0.68 |
| 1:D:220:ASN:ND2 | 1:D:222:PRO:CD | 2.54 | 0.68 |
| 1:B:131:LEU:N | 1:B:132:PRO:HD2 | 2.07 | 0.68 |
| 1:B:315:GLY:O | 1:B:317:GLU:N | 2.27 | 0.68 |
| 1:C:165:LYS:O | 1:C:169:ALA:HB2 | 1.93 | 0.68 |
| 1:A:33:THR:HG22 | 1:A:34:THR:HG23 | 1.76 | 0.68 |
| 1:A:102:VAL:HG12 | 1:A:103:TYR:N | 2.09 | 0.68 |
| 1:B:3:GLN:HE22 | 1:B:15:ALA:HB2 | 1.58 | 0.68 |
| 1:C:106:THR:O | 1:C:110:PHE:HB2 | 1.93 | 0.68 |
| 1:D:208:HIS:CE1 | 1:D:338:ILE:HD12 | 2.28 | 0.68 |
| 1:B:323:ALA:HA | 1:B:342:LEU:HD11 | 1.75 | 0.68 |
| 1:A:137:GLU:O | 1:A:138:ASN:CB | 2.42 | 0.67 |
| 1:A:208:HIS:CE1 | 1:A:338:ILE:HD12 | 2.28 | 0.67 |
| 1:C:136:LYS:HA | 1:C:139:THR:HG23 | 1.76 | 0.67 |
| 1:C:344:VAL:H | 1:C:348:MET:HE3 | 1.57 | 0.67 |
| 1:D:126:ASP:OD2 | 1:D:129:ASN:HB2 | 1.93 | 0.67 |
| 1:A:95:HIS:ND1 | 1:A:139:THR:CG2 | 2.55 | 0.67 |
| 1:C:53:GLN:CD | 1:C:58:GLU:HB2 | 2.14 | 0.67 |
| 1:C:115:ASN:H | 1:C:115:ASN:HD22 | 1.41 | 0.67 |
| 1:C:310:PHE:HE1 | 1:C:312:ILE:HG23 | 1.59 | 0.67 |
| 1:D:114:ALA:CA | 1:D:119:VAL:H | 2.07 | 0.67 |
| 1:D:340:SER:O | 1:D:341:LEU:HD23 | 1.93 | 0.67 |
| 1:A:91:PRO:HG2 | 1:A:94:SER:OG | 1.94 | 0.67 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:270:PHE:CZ | 1:C:385:LYS:HG2 | 2.29 | 0.67 |
| 1:D:70:ALA:HB2 | 1:D:190:LEU:HD12 | 1.75 | 0.67 |
| 1:A:3:GLN:NE2 | 1:A:11:LYS:HG2 | 2.09 | 0.67 |
| 1:A:128:LEU:HD13 | 1:A:159:LYS:HD3 | 1.76 | 0.67 |
| 1:B:343:GLU:OE1 | 1:B:369:ARG:HD3 | 1.95 | 0.67 |
| 1:D:136:LYS:O | 1:D:137:GLU:CB | 2.42 | 0.67 |
| 1:A:344:VAL:H | 1:A:348:MET:CE | 2.07 | 0.67 |
| 1:C:3:GLN:NE2 | 1:C:11:LYS:HG2 | 2.09 | 0.67 |
| 1:D:347:VAL:HG23 | 1:D:348:MET:N | 2.09 | 0.67 |
| 1:B:106:THR:HG22 | 1:B:110:PHE:CE1 | 2.30 | 0.67 |
| 1:B:114:ALA:HB2 | 1:B:119:VAL:HB | 1.77 | 0.67 |
| 1:B:379:ASP:OD2 | 1:C:6:ASP:HB3 | 1.95 | 0.67 |
| 1:D:147:PRO:HG2 | 1:D:182:LEU:HG | 1.76 | 0.67 |
| 1:A:248:ARG:NE | 1:D:210:ASP:OD1 | 2.25 | 0.66 |
| 1:C:37:GLN:HG2 | 1:C:43:PRO:HA | 1.77 | 0.66 |
| 1:B:142:VAL:HG21 | 1:B:164:ILE:HD11 | 1.78 | 0.66 |
| 1:C:53:GLN:OE1 | 1:C:58:GLU:HB2 | 1.95 | 0.66 |
| 1:A:310:PHE:HE1 | 1:A:312:ILE:HG23 | 1.58 | 0.66 |
| 1:A:315:GLY:O | 1:A:317:GLU:N | 2.28 | 0.66 |
| 1:C:87:LEU:CD1 | 1:C:110:PHE:HA | 2.25 | 0.66 |
| 1:C:369:ARG:HG2 | 1:C:369:ARG:HH11 | 1.58 | 0.66 |
| 1:C:331:LEU:HD21 | 1:D:40:PRO:N | 2.10 | 0.66 |
| 1:D:3:GLN:HE21 | 1:D:11:LYS:HA | 1.60 | 0.66 |
| 1:C:344:VAL:H | 1:C:348:MET:HE1 | 1.61 | 0.66 |
| 1:C:53:GLN:HA | 1:C:57:ARG:NH2 | 2.11 | 0.66 |
| 1:B:282:ASN:HB2 | 1:B:309:SER:HB3 | 1.78 | 0.65 |
| 1:C:375:GLU:OE2 | 1:C:375:GLU:N | 2.26 | 0.65 |
| 1:C:258:ARG:HH11 | 1:C:303:LEU:HD11 | 1.60 | 0.65 |
| 1:D:204:TYR:CE2 | 1:D:336:GLY:HA2 | 2.31 | 0.65 |
| 1:A:106:THR:HA | 1:A:110:PHE:CD1 | 2.32 | 0.65 |
| 1:A:134:LEU:O | 1:A:136:LYS:N | 2.30 | 0.65 |
| 1:D:137:GLU:O | 1:D:138:ASN:CB | 2.44 | 0.65 |
| 1:B:147:PRO:HG2 | 1:B:182:LEU:HG | 1.79 | 0.65 |
| 1:A:35:PHE:HA | 1:C:23:GLY:C | 2.17 | 0.65 |
| 1:C:106:THR:HA | 1:C:110:PHE:CD1 | 2.32 | 0.65 |
| 1:A:6:ASP:HB3 | 1:D:379:ASP:OD2 | 1.97 | 0.65 |
| 1:C:131:LEU:N | 1:C:132:PRO:HD2 | 2.12 | 0.65 |
| 1:A:95:HIS:HB2 | 1:A:138:ASN:HB3 | 1.79 | 0.65 |
| 1:B:26:ILE:HB | 1:D:32:SER:CB | 2.26 | 0.65 |
| 1:C:143:TRP:CZ3 | 1:C:176:VAL:HG11 | 2.31 | 0.65 |
| 1:C:355:LYS:HB2 | 1:C:358:ARG:NH2 | 2.11 | 0.65 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:37:GLN:HA | 1:A:43:PRO:HA | 1.77 | 0.64 |
| 1:A:136:LYS:CA | 1:A:139:THR:HG23 | 2.27 | 0.64 |
| 1:D:197:VAL:O | 1:D:216:LEU:HA | 1.97 | 0.64 |
| 1:B:210:ASP:OD1 | 1:C:248:ARG:NE | 2.19 | 0.64 |
| 1:D:265:ASN:O | 1:D:269:GLU:HG3 | 1.97 | 0.64 |
| 1:A:23:GLY:O | 1:C:36:LYS:N | 2.30 | 0.64 |
| 1:A:196:ILE:HG23 | 1:A:218:THR:CG2 | 2.28 | 0.64 |
| 1:C:351:GLY:O | 1:C:353:ILE:N | 2.29 | 0.64 |
| 1:A:23:GLY:O | 1:C:36:LYS:HG3 | 1.98 | 0.64 |
| 1:B:21:VAL:HG23 | 1:D:21:VAL:HG21 | 1.80 | 0.64 |
| 1:C:88:GLN:OE1 | 1:C:234:ILE:HD13 | 1.97 | 0.64 |
| 1:C:100:GLY:O | 1:C:102:VAL:N | 2.31 | 0.64 |
| 1:D:271:LEU:O | 1:D:278:VAL:HG11 | 1.97 | 0.64 |
| 1:A:3:GLN:NE2 | 1:A:15:ALA:HB2 | 2.08 | 0.64 |
| 1:B:333:GLU:OE1 | 1:B:343:GLU:HG3 | 1.97 | 0.64 |
| 1:B:358:ARG:HH11 | 1:B:358:ARG:HB3 | 1.62 | 0.64 |
| 1:D:331:LEU:HA | 1:D:342:LEU:HD23 | 1.79 | 0.64 |
| 1:A:144:ILE:HD11 | 1:A:160:VAL:HG11 | 1.79 | 0.64 |
| 1:D:350:HIS:HA | 3:D:421:HOH:O | 1.96 | 0.63 |
| 1:A:196:ILE:HA | 1:A:218:THR:HG22 | 1.80 | 0.63 |
| 1:C:95:HIS:HD2 | 1:C:120:GLU:HB3 | 1.61 | 0.63 |
| 1:C:71:GLN:H | 1:C:219:ASN:ND2 | 1.97 | 0.63 |
| 1:D:181:PHE:CD1 | 1:D:335:LEU:HD11 | 2.32 | 0.63 |
| 1:A:332:ALA:HA | 1:B:37:GLN:HG3 | 1.80 | 0.63 |
| 1:C:318:ALA:O | 1:C:321:LYS:HB3 | 1.97 | 0.63 |
| 1:D:310:PHE:HE1 | 1:D:312:ILE:HG23 | 1.64 | 0.63 |
| 1:A:146:THR:CB | 1:A:147:PRO:HD3 | 2.29 | 0.63 |
| 1:B:146:THR:CB | 1:B:147:PRO:HD3 | 2.29 | 0.63 |
| 1:C:101:ASP:CB | 1:C:148:THR:HB | 2.28 | 0.63 |
| 1:A:270:PHE:CZ | 1:A:385:LYS:HG2 | 2.34 | 0.63 |
| 1:D:1:THR:CG2 | 1:D:2:LEU:N | 2.62 | 0.63 |
| 1:B:1:THR:HG21 | 1:B:14:HIS:CG | 2.33 | 0.63 |
| 1:A:31:LEU:HD22 | 3:B:441:HOH:O | 1.98 | 0.62 |
| 1:A:349:THR:HG22 | 1:A:350:HIS:N | 2.14 | 0.62 |
| 1:C:333:GLU:O | 1:D:34:THR:HG21 | 1.99 | 0.62 |
| 1:D:27:GLU:OE1 | 1:D:59:ASN:ND2 | 2.28 | 0.62 |
| 1:A:136:LYS:O | 1:A:137:GLU:CB | 2.45 | 0.62 |
| 1:B:135:ILE:HD12 | 1:B:167:HIS:HB2 | 1.80 | 0.62 |
| 1:D:131:LEU:N | 1:D:132:PRO:HD2 | 2.14 | 0.62 |
| 1:B:265:ASN:O | 1:B:269:GLU:HG3 | 1.98 | 0.62 |
| 1:D:211:VAL:HG23 | 1:D:245:LEU:HD23 | 1.81 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:76:PHE:CA | 1:B:238:PRO:HD3 | 2.29 | 0.62 |
| 1:C:91:PRO:HG2 | 1:C:94:SER:OG | 1.99 | 0.62 |
| 1:C:315:GLY:O | 1:C:317:GLU:N | 2.32 | 0.62 |
| 1:D:87:LEU:CD1 | 1:D:110:PHE:HA | 2.28 | 0.62 |
| 1:A:46:THR:O | 1:A:46:THR:HG22 | 1.99 | 0.62 |
| 1:A:274:ASP:O | 1:A:274:ASP:OD1 | 2.17 | 0.62 |
| 1:B:99:ILE:O | 1:B:102:VAL:CG2 | 2.46 | 0.62 |
| 1:A:53:GLN:NE2 | 1:A:58:GLU:HB2 | 2.15 | 0.62 |
| 1:C:221:LYS:HG2 | 1:C:225:GLU:OE2 | 1.98 | 0.62 |
| 1:D:3:GLN:NE2 | 1:D:11:LYS:HA | 2.14 | 0.62 |
| 1:A:136:LYS:HG3 | 1:A:137:GLU:N | 2.09 | 0.62 |
| 1:B:70:ALA:HB2 | 1:B:190:LEU:CD1 | 2.29 | 0.62 |
| 1:D:75:ALA:HA | 1:D:215:VAL:CG1 | 2.26 | 0.62 |
| 1:D:171:GLN:HB3 | 3:D:457:HOH:O | 2.00 | 0.62 |
| 1:A:157:ILE:HG22 | 1:A:192:PHE:O | 1.99 | 0.62 |
| 1:B:264:ALA:O | 1:B:308:ILE:HD11 | 2.00 | 0.62 |
| 1:D:137:GLU:O | 1:D:138:ASN:HB2 | 1.97 | 0.62 |
| 1:D:149:ASN:HB2 | 1:D:181:PHE:CE2 | 2.35 | 0.62 |
| 1:A:51:ARG:HG3 | 1:A:237:ILE:HD13 | 1.81 | 0.62 |
| 1:C:369:ARG:HG2 | 1:C:369:ARG:NH1 | 2.15 | 0.62 |
| 1:C:104:GLY:O | 1:C:107:HIS:HB3 | 1.99 | 0.61 |
| 1:D:114:ALA:CB | 1:D:119:VAL:N | 2.63 | 0.61 |
| 1:A:381:LEU:HG | 1:A:385:LYS:HE3 | 1.81 | 0.61 |
| 1:A:124:THR:HG22 | 1:A:125:ASN:O | 2.00 | 0.61 |
| 1:B:168:ALA:O | 1:B:171:GLN:HG3 | 2.00 | 0.61 |
| 1:B:208:HIS:CE1 | 1:B:338:ILE:HD12 | 2.35 | 0.61 |
| 1:B:277:ASN:N | 1:B:277:ASN:ND2 | 2.48 | 0.61 |
| 1:C:74:LEU:HB2 | 1:C:216:LEU:HD22 | 1.82 | 0.61 |
| 1:C:292:TYR:CE2 | 1:C:296:LEU:HD21 | 2.35 | 0.61 |
| 1:D:135:ILE:HG23 | 1:D:135:ILE:O | 1.98 | 0.61 |
| 1:C:331:LEU:HA | 1:C:342:LEU:HD23 | 1.82 | 0.61 |
| 1:C:347:VAL:HG23 | 1:C:348:MET:N | 2.11 | 0.61 |
| 1:A:282:ASN:HB2 | 1:A:309:SER:HB3 | 1.82 | 0.61 |
| 1:B:95:HIS:HA | 1:B:120:GLU:HB2 | 1.82 | 0.61 |
| 1:B:128:LEU:HD13 | 1:B:159:LYS:HD3 | 1.83 | 0.61 |
| 1:B:163:LEU:O | 1:B:166:LYS:HB3 | 2.00 | 0.61 |
| 1:D:95:HIS:HA | 1:D:120:GLU:HB2 | 1.83 | 0.61 |
| 1:D:221:LYS:HG2 | 1:D:225:GLU:OE2 | 2.00 | 0.61 |
| 1:C:114:ALA:HA | 1:C:119:VAL:H | 1.65 | 0.61 |
| 1:D:349:THR:CG2 | 1:D:350:HIS:N | 2.64 | 0.61 |
| 1:A:24:SER:HA | 1:C:34:THR:O | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:131:LEU:N | 1:A:132:PRO:HD2 | 2.15 | 0.61 |
| 1:A:184:PRO:HD3 | 1:A:199:HIS:CE1 | 2.36 | 0.61 |
| 1:D:322:PHE:O | 1:D:324:SER:N | 2.34 | 0.61 |
| 1:A:310:PHE:CE1 | 1:A:312:ILE:HG23 | 2.36 | 0.61 |
| 1:C:210:ASP:HA | 1:D:31:LEU:O | 2.01 | 0.61 |
| 1:D:321:LYS:CG | 1:D:391:ALA:HA | 2.21 | 0.61 |
| 1:A:124:THR:HG21 | 1:A:130:ASP:HB2 | 1.83 | 0.60 |
| 1:A:131:LEU:HG | 1:A:135:ILE:HG13 | 1.83 | 0.60 |
| 1:B:72:TYR:O | 1:B:217:ALA:HA | 2.01 | 0.60 |
| 1:C:101:ASP:HB2 | 1:C:148:THR:HB | 1.82 | 0.60 |
| 1:C:136:LYS:HG3 | 1:C:137:GLU:H | 1.67 | 0.60 |
| 1:D:343:GLU:OE2 | 1:D:345:PRO:HA | 2.00 | 0.60 |
| 1:C:37:GLN:CB | 1:C:43:PRO:HA | 2.30 | 0.60 |
| 1:B:60:LEU:HD12 | 1:B:64:VAL:HG23 | 1.82 | 0.60 |
| 1:C:196:ILE:HG12 | 1:C:218:THR:CG2 | 2.31 | 0.60 |
| 1:A:358:ARG:HB3 | 1:A:358:ARG:HH11 | 1.65 | 0.60 |
| 1:B:104:GLY:O | 1:B:107:HIS:HB3 | 2.02 | 0.60 |
| 1:C:330:THR:HG21 | 1:D:36:LYS:HG2 | 1.84 | 0.60 |
| 1:A:102:VAL:HG12 | 1:A:103:TYR:O | 2.02 | 0.60 |
| 1:A:258:ARG:HH11 | 1:A:303:LEU:HD11 | 1.67 | 0.60 |
| 1:D:135:ILE:HG21 | 1:D:168:ALA:HB2 | 1.83 | 0.60 |
| 1:D:211:VAL:CG2 | 1:D:245:LEU:HD23 | 2.32 | 0.60 |
| 1:A:45:GLY:O | 1:A:47:TYR:N | 2.35 | 0.60 |
| 1:A:103:TYR:C | 1:A:105:GLY:H | 2.04 | 0.60 |
| 1:A:110:PHE:O | 1:A:114:ALA:HB2 | 2.02 | 0.60 |
| 1:C:349:THR:O | 1:C:351:GLY:N | 2.34 | 0.60 |
| 1:D:128:LEU:HD21 | 1:D:159:LYS:HB3 | 1.84 | 0.60 |
| 1:D:136:LYS:HA | 1:D:139:THR:HG23 | 1.82 | 0.60 |
| 1:A:220:ASN:HD22 | 1:A:220:ASN:C | 2.05 | 0.60 |
| 1:A:344:VAL:H | 1:A:348:MET:HE3 | 1.66 | 0.60 |
| 1:C:264:ALA:O | 1:C:308:ILE:HD11 | 2.02 | 0.60 |
| 1:C:386:GLN:HG2 | 3:C:413:HOH:O | 2.02 | 0.60 |
| 1:D:165:LYS:O | 1:D:169:ALA:HB2 | 2.01 | 0.60 |
| 1:D:277:ASN:O | 1:D:313:LYS:N | 2.35 | 0.60 |
| 1:C:134:LEU:O | 1:C:136:LYS:N | 2.35 | 0.60 |
| 1:B:150:PRO:HB3 | 1:B:369:ARG:HD2 | 1.83 | 0.59 |
| 1:B:354:PRO:C | 1:B:356:GLU:H | 2.04 | 0.59 |
| 1:C:277:ASN:N | 1:C:277:ASN:ND2 | 2.50 | 0.59 |
| 1:A:53:GLN:CD | 1:A:58:GLU:HB2 | 2.22 | 0.59 |
| 1:A:74:LEU:HB2 | 1:A:216:LEU:HD22 | 1.82 | 0.59 |
| 1:C:116:ALA:HB3 | 1:D:92:GLN:HB3 | 1.83 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:132:PRO:CB | 1:C:167:HIS:CD2 | 2.85 | 0.59 |
| 1:D:135:ILE:CG2 | 1:D:168:ALA:HB2 | 2.32 | 0.59 |
| 1:A:265:ASN:O | 1:A:269:GLU:HG3 | 2.01 | 0.59 |
| 1:B:3:GLN:HE22 | 1:B:15:ALA:CB | 2.16 | 0.59 |
| 1:B:156:ASP:HB3 | 1:B:159:LYS:HB2 | 1.84 | 0.59 |
| 1:A:12:ALA:HA | 1:A:67:LEU:HD21 | 1.85 | 0.59 |
| 1:A:36:LYS:H | 1:C:23:GLY:C | 2.06 | 0.59 |
| 1:D:170:GLY:N | 3:D:465:HOH:O | 2.34 | 0.59 |
| 1:A:242:ASP:O | 1:A:246:THR:OG1 | 2.16 | 0.59 |
| 1:A:230:LEU:O | 1:A:234:ILE:HG12 | 2.01 | 0.59 |
| 1:D:102:VAL:HG12 | 1:D:103:TYR:N | 2.17 | 0.59 |
| 1:D:335:LEU:C | 1:D:337:GLY:H | 2.05 | 0.59 |
| 1:A:209:SER:O | 1:B:33:THR:N | 2.35 | 0.59 |
| 1:C:2:LEU:HD23 | 1:C:2:LEU:O | 2.01 | 0.59 |
| 1:D:270:PHE:CZ | 1:D:385:LYS:HG2 | 2.37 | 0.59 |
| 1:B:76:PHE:C | 1:B:238:PRO:HD3 | 2.23 | 0.59 |
| 1:C:53:GLN:HE22 | 1:C:58:GLU:HG3 | 1.68 | 0.59 |
| 1:C:258:ARG:NH1 | 1:C:303:LEU:HD11 | 2.17 | 0.59 |
| 1:D:339:GLU:HG2 | 1:D:341:LEU:HD21 | 1.85 | 0.59 |
| 1:B:114:ALA:HA | 1:B:119:VAL:H | 1.66 | 0.59 |
| 1:B:128:LEU:HB3 | 3:B:413:HOH:O | 2.01 | 0.59 |
| 1:B:134:LEU:O | 1:B:136:LYS:N | 2.36 | 0.59 |
| 1:A:190:LEU:C | 1:A:192:PHE:H | 2.06 | 0.58 |
| 1:B:95:HIS:CD2 | 1:B:120:GLU:HB3 | 2.33 | 0.58 |
| 1:B:137:GLU:O | 1:B:138:ASN:CB | 2.50 | 0.58 |
| 1:D:204:TYR:CZ | 1:D:336:GLY:HA2 | 2.38 | 0.58 |
| 1:A:70:ALA:HA | 1:A:219:ASN:HD21 | 1.67 | 0.58 |
| 1:C:144:ILE:CD1 | 1:C:175:LEU:HD11 | 2.34 | 0.58 |
| 1:A:264:ALA:O | 1:A:308:ILE:HD11 | 2.02 | 0.58 |
| 1:A:131:LEU:O | 1:A:135:ILE:HG13 | 2.03 | 0.58 |
| 1:A:142:VAL:HG21 | 1:A:164:ILE:CD1 | 2.33 | 0.58 |
| 1:B:114:ALA:HB1 | 1:B:119:VAL:H | 1.68 | 0.58 |
| 1:D:1:THR:HG21 | 1:D:14:HIS:HB3 | 1.84 | 0.58 |
| 1:B:354:PRO:C | 1:B:356:GLU:N | 2.56 | 0.58 |
| 1:A:87:LEU:HD11 | 1:A:110:PHE:CD1 | 2.39 | 0.58 |
| 1:A:203:LYS:O | 1:A:207:GLY:HA2 | 2.03 | 0.58 |
| 1:D:46:THR:CG2 | 1:D:46:THR:O | 2.51 | 0.58 |
| 1:D:136:LYS:CG | 1:D:137:GLU:N | 2.67 | 0.58 |
| 1:A:22:HIS:H | 1:A:22:HIS:HD1 | 1.51 | 0.58 |
| 1:A:95:HIS:HD2 | 1:A:120:GLU:HB3 | 1.68 | 0.58 |
| 1:A:135:ILE:O | 1:A:139:THR:CG2 | 2.51 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:135:ILE:CD1 | 1:A:167:HIS:HB2 | 2.34 | 0.58 |
| 1:B:338:ILE:HG12 | 1:B:374:ILE:HD11 | 1.85 | 0.58 |
| 1:C:45:GLY:O | 1:C:47:TYR:N | 2.37 | 0.58 |
| 1:C:135:ILE:HD12 | 1:C:167:HIS:HB2 | 1.86 | 0.58 |
| 1:C:146:THR:CB | 1:C:147:PRO:HD3 | 2.34 | 0.58 |
| 1:C:187:SER:C | 1:C:188:ASN:HD22 | 2.07 | 0.58 |
| 1:A:35:PHE:HA | 1:C:23:GLY:O | 2.04 | 0.57 |
| 1:C:135:ILE:CG2 | 1:C:168:ALA:HB2 | 2.34 | 0.57 |
| 1:D:135:ILE:HG21 | 1:D:167:HIS:O | 2.03 | 0.57 |
| 1:D:385:LYS:C | 1:D:387:ALA:H | 2.07 | 0.57 |
| 1:B:68:GLU:OE1 | 1:B:184:PRO:HG3 | 2.03 | 0.57 |
| 1:C:102:VAL:N | 3:C:435:HOH:O | 2.30 | 0.57 |
| 1:D:150:PRO:HG3 | 1:D:345:PRO:HG3 | 1.86 | 0.57 |
| 1:B:51:ARG:HG3 | 1:B:237:ILE:HD13 | 1.86 | 0.57 |
| 1:C:37:GLN:HE21 | 1:C:43:PRO:CG | 2.03 | 0.57 |
| 1:B:87:LEU:HD13 | 1:B:110:PHE:HA | 1.86 | 0.57 |
| 1:C:96:ALA:CB | 1:C:141:LEU:HB3 | 2.35 | 0.57 |
| 1:A:150:PRO:CB | 1:A:369:ARG:HD2 | 2.33 | 0.57 |
| 1:B:206:ASN:HD22 | 1:B:246:THR:HA | 1.69 | 0.57 |
| 1:D:157:ILE:HD12 | 1:D:298:GLN:OE1 | 2.04 | 0.57 |
| 1:A:127:LEU:HD23 | 1:A:160:VAL:HG21 | 1.86 | 0.57 |
| 1:B:343:GLU:HG2 | 1:B:344:VAL:N | 2.19 | 0.57 |
| 1:C:37:GLN:CG | 1:C:43:PRO:HA | 2.34 | 0.57 |
| 1:D:150:PRO:HB3 | 1:D:369:ARG:HD2 | 1.87 | 0.57 |
| 1:A:190:LEU:HD21 | 1:A:197:VAL:HG22 | 1.85 | 0.57 |
| 1:B:114:ALA:CA | 1:B:119:VAL:H | 2.17 | 0.57 |
| 1:A:362:GLY:O | 1:A:364:PHE:N | 2.37 | 0.57 |
| 1:B:221:LYS:HG2 | 1:B:225:GLU:OE2 | 2.03 | 0.57 |
| 1:D:317:GLU:O | 1:D:321:LYS:N | 2.37 | 0.57 |
| 1:A:102:VAL:HG11 | 1:A:106:THR:HG23 | 1.86 | 0.57 |
| 1:B:221:LYS:HB3 | 1:B:222:PRO:HD3 | 1.87 | 0.57 |
| 1:B:234:ILE:HG13 | 1:B:236:ALA:H | 1.68 | 0.57 |
| 1:B:369:ARG:HG2 | 1:B:369:ARG:HH11 | 1.70 | 0.57 |
| 1:D:333:GLU:OE1 | 1:D:343:GLU:HG3 | 2.04 | 0.57 |
| 1:A:358:ARG:HH11 | 1:A:358:ARG:CB | 2.18 | 0.57 |
| 1:B:3:GLN:HE22 | 1:B:15:ALA:CA | 2.17 | 0.57 |
| 1:C:108:ARG:CZ | 1:D:233:ALA:HA | 2.34 | 0.57 |
| 1:D:335:LEU:C | 1:D:337:GLY:N | 2.56 | 0.57 |
| 1:C:95:HIS:HB2 | 1:C:138:ASN:HB3 | 1.87 | 0.56 |
| 1:D:136:LYS:NZ | 1:D:138:ASN:HA | 2.20 | 0.56 |
| 1:C:132:PRO:HB3 | 1:C:167:HIS:CD2 | 2.39 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:203:LYS:N | 1:C:203:LYS:HD2 | 2.19 | 0.56 |
| 1:C:280:ALA:HB3 | 1:C:311:ARG:HD3 | 1.86 | 0.56 |
| 1:A:114:ALA:HA | 1:A:119:VAL:H | 1.69 | 0.56 |
| 1:A:248:ARG:HH11 | 1:A:248:ARG:HG2 | 1.70 | 0.56 |
| 1:B:128:LEU:CD1 | 1:B:159:LYS:HD3 | 2.35 | 0.56 |
| 1:C:70:ALA:HB2 | 1:C:190:LEU:HD12 | 1.88 | 0.56 |
| 1:C:280:ALA:H | 1:C:311:ARG:HG3 | 1.71 | 0.56 |
| 1:C:294:VAL:O | 1:C:297:LYS:HG3 | 2.04 | 0.56 |
| 1:D:152:LEU:HD12 | 1:D:282:ASN:O | 2.05 | 0.56 |
| 1:C:13:ILE:CG2 | 1:C:13:ILE:O | 2.54 | 0.56 |
| 1:D:276:GLU:HA | 3:D:461:HOH:O | 2.04 | 0.56 |
| 1:B:61:GLU:OE2 | 1:B:74:LEU:HA | 2.05 | 0.56 |
| 1:D:192:PHE:HE2 | 3:D:480:HOH:O | 1.87 | 0.56 |
| 1:B:75:ALA:HA | 1:B:215:VAL:HG12 | 1.87 | 0.56 |
| 1:C:196:ILE:HA | 1:C:218:THR:HG22 | 1.88 | 0.56 |
| 1:C:354:PRO:C | 1:C:356:GLU:N | 2.56 | 0.56 |
| 1:B:179:ASN:ND2 | 1:B:199:HIS:CE1 | 2.73 | 0.56 |
| 1:B:187:SER:O | 1:B:188:ASN:ND2 | 2.35 | 0.56 |
| 1:C:131:LEU:HG | 1:C:135:ILE:HG13 | 1.87 | 0.56 |
| 1:C:201:ALA:HB3 | 1:C:213:LEU:O | 2.05 | 0.56 |
| 1:D:95:HIS:HD2 | 1:D:120:GLU:HB3 | 1.71 | 0.56 |
| 1:D:102:VAL:HG11 | 1:D:106:THR:HG23 | 1.87 | 0.56 |
| 1:D:277:ASN:N | 1:D:277:ASN:ND2 | 2.54 | 0.56 |
| 1:C:116:ALA:HB2 | 1:D:92:GLN:H | 1.71 | 0.56 |
| 1:B:101:ASP:HA | 3:B:491:HOH:O | 2.05 | 0.56 |
| 1:B:102:VAL:HG11 | 1:B:106:THR:CG2 | 2.36 | 0.56 |
| 1:B:150:PRO:HG3 | 1:B:345:PRO:HG3 | 1.88 | 0.56 |
| 1:A:343:GLU:HG2 | 1:A:344:VAL:N | 2.21 | 0.55 |
| 1:A:358:ARG:HB2 | 1:A:358:ARG:NH1 | 2.21 | 0.55 |
| 1:B:187:SER:C | 1:B:188:ASN:HD22 | 2.09 | 0.55 |
| 1:B:312:ILE:HD12 | 1:B:318:ALA:HB1 | 1.87 | 0.55 |
| 1:B:343:GLU:OE1 | 1:B:345:PRO:HD3 | 2.06 | 0.55 |
| 1:C:128:LEU:HD13 | 1:C:159:LYS:HD3 | 1.88 | 0.55 |
| 1:D:95:HIS:CE1 | 1:D:139:THR:HG22 | 2.37 | 0.55 |
| 1:A:1:THR:HG21 | 1:A:14:HIS:CB | 2.35 | 0.55 |
| 1:B:32:SER:CB | 1:D:26:ILE:HB | 2.36 | 0.55 |
| 1:B:102:VAL:HG12 | 1:B:103:TYR:O | 2.07 | 0.55 |
| 1:C:102:VAL:HG12 | 1:C:103:TYR:N | 2.21 | 0.55 |
| 1:A:102:VAL:CG1 | 1:A:103:TYR:N | 2.69 | 0.55 |
| 1:A:333:GLU:O | 1:B:34:THR:HG21 | 2.05 | 0.55 |
| 1:A:358:ARG:CB | 1:A:358:ARG:NH1 | 2.69 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:191:ASN:HA | 3:B:461:HOH:O | 2.06 | 0.55 |
| 1:B:204:TYR:CE1 | 1:B:336:GLY:HA3 | 2.42 | 0.55 |
| 1:D:277:ASN:HD22 | 1:D:277:ASN:H | 1.55 | 0.55 |
| 1:A:71:GLN:N | 1:A:219:ASN:ND2 | 2.52 | 0.55 |
| 1:A:153:LYS:HB2 | 1:A:153:LYS:NZ | 2.21 | 0.55 |
| 1:B:196:ILE:HG12 | 1:B:218:THR:CG2 | 2.37 | 0.55 |
| 1:B:358:ARG:NH1 | 1:B:358:ARG:CB | 2.70 | 0.55 |
| 1:C:69:ASN:ND2 | 1:C:191:ASN:OD1 | 2.38 | 0.55 |
| 1:D:279:VAL:HG23 | 1:D:312:ILE:O | 2.07 | 0.55 |
| 1:D:316:ALA:HA | 3:D:488:HOH:O | 2.05 | 0.55 |
| 1:A:106:THR:HG22 | 1:A:110:PHE:CE1 | 2.41 | 0.55 |
| 1:C:67:LEU:HD12 | 1:C:250:LEU:HD11 | 1.88 | 0.55 |
| 1:C:343:GLU:HA | 1:C:348:MET:HE1 | 1.88 | 0.55 |
| 1:D:127:LEU:HD23 | 1:D:160:VAL:HG21 | 1.88 | 0.55 |
| 1:D:134:LEU:O | 1:D:136:LYS:N | 2.40 | 0.55 |
| 1:A:363:VAL:HG12 | 1:A:363:VAL:O | 2.06 | 0.55 |
| 1:B:106:THR:O | 1:B:110:PHE:HB2 | 2.06 | 0.55 |
| 1:A:3:GLN:HE21 | 1:A:11:LYS:CG | 2.19 | 0.55 |
| 1:B:3:GLN:HE21 | 1:B:11:LYS:HA | 1.72 | 0.55 |
| 1:B:123:PHE:HD1 | 1:B:123:PHE:H | 1.55 | 0.55 |
| 1:B:192:PHE:HD2 | 3:B:484:HOH:O | 1.90 | 0.55 |
| 1:B:196:ILE:HG23 | 1:B:218:THR:HG23 | 1.89 | 0.55 |
| 1:B:213:LEU:C | 1:B:213:LEU:HD23 | 2.27 | 0.55 |
| 1:C:331:LEU:HD11 | 1:C:348:MET:HE2 | 1.89 | 0.55 |
| 1:B:346:ALA:CB | 3:B:492:HOH:O | 2.46 | 0.55 |
| 1:B:95:HIS:O | 1:B:139:THR:HA | 2.07 | 0.54 |
| 1:B:327:ARG:NH2 | 1:C:6:ASP:OD1 | 2.27 | 0.54 |
| 1:C:187:SER:O | 1:C:188:ASN:ND2 | 2.38 | 0.54 |
| 1:C:311:ARG:HH11 | 1:C:311:ARG:HB3 | 1.72 | 0.54 |
| 1:A:7:LYS:HG3 | 1:D:376:ASP:OD2 | 2.06 | 0.54 |
| 1:A:95:HIS:HA | 1:A:120:GLU:HB2 | 1.89 | 0.54 |
| 1:A:323:ALA:HB1 | 1:A:331:LEU:CD1 | 2.32 | 0.54 |
| 1:A:348:MET:CE | 1:B:40:PRO:HB3 | 2.38 | 0.54 |
| 1:B:340:SER:O | 1:B:341:LEU:HD23 | 2.07 | 0.54 |
| 1:C:249:GLY:HA2 | 3:C:417:HOH:O | 2.08 | 0.54 |
| 1:C:294:VAL:HA | 1:C:297:LYS:CG | 2.38 | 0.54 |
| 1:D:68:GLU:HG2 | 1:D:197:VAL:HG21 | 1.89 | 0.54 |
| 1:A:103:TYR:C | 1:A:105:GLY:N | 2.60 | 0.54 |
| 1:B:76:PHE:CE2 | 1:B:231:GLN:HG3 | 2.42 | 0.54 |
| 1:B:363:VAL:HG12 | 1:B:363:VAL:O | 2.08 | 0.54 |
| 1:C:111:THR:O | 1:C:114:ALA:HB3 | 2.07 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:279:VAL:HG23 | 1:C:312:ILE:C | 2.27 | 0.54 |
| 1:C:280:ALA:H | 1:C:311:ARG:CG | 2.21 | 0.54 |
| 1:D:114:ALA:HB1 | 1:D:119:VAL:N | 2.22 | 0.54 |
| 1:D:323:ALA:HB1 | 1:D:331:LEU:HD13 | 1.90 | 0.54 |
| 1:A:136:LYS:CG | 1:A:137:GLU:H | 2.04 | 0.54 |
| 1:A:216:LEU:HD23 | 1:A:216:LEU:C | 2.28 | 0.54 |
| 1:B:131:LEU:N | 1:B:132:PRO:CD | 2.71 | 0.54 |
| 1:C:102:VAL:CG1 | 1:C:103:TYR:N | 2.70 | 0.54 |
| 1:C:142:VAL:HG21 | 1:C:164:ILE:CD1 | 2.37 | 0.54 |
| 1:C:196:ILE:HG23 | 1:C:218:THR:HG23 | 1.90 | 0.54 |
| 1:C:92:GLN:HB2 | 1:D:115:ASN:O | 2.08 | 0.54 |
| 1:D:242:ASP:O | 1:D:246:THR:OG1 | 2.23 | 0.54 |
| 1:B:137:GLU:O | 1:B:138:ASN:HB3 | 2.08 | 0.54 |
| 1:C:126:ASP:OD2 | 1:C:129:ASN:HB2 | 2.08 | 0.54 |
| 1:C:135:ILE:HG23 | 1:C:135:ILE:O | 2.08 | 0.54 |
| 1:C:137:GLU:O | 1:C:137:GLU:HG2 | 2.08 | 0.54 |
| 1:D:136:LYS:HD2 | 1:D:138:ASN:H | 1.72 | 0.54 |
| 1:D:220:ASN:ND2 | 1:D:220:ASN:C | 2.60 | 0.54 |
| 1:B:203:LYS:O | 1:B:336:GLY:O | 2.26 | 0.54 |
| 1:D:135:ILE:O | 1:D:135:ILE:CG2 | 2.55 | 0.54 |
| 1:A:3:GLN:HE21 | 1:A:11:LYS:HA | 1.72 | 0.54 |
| 1:A:7:LYS:HG2 | 1:D:379:ASP:OD1 | 2.07 | 0.54 |
| 1:A:331:LEU:HD11 | 1:A:348:MET:HE2 | 1.90 | 0.54 |
| 1:C:135:ILE:CG2 | 1:C:135:ILE:O | 2.56 | 0.54 |
| 1:C:182:LEU:O | 1:C:183:SER:CB | 2.56 | 0.54 |
| 1:D:136:LYS:HG3 | 1:D:137:GLU:N | 2.12 | 0.54 |
| 1:D:252:THR:O | 1:D:256:ARG:HG3 | 2.08 | 0.54 |
| 1:D:276:GLU:HB3 | 1:D:277:ASN:HD22 | 1.74 | 0.54 |
| 1:D:279:VAL:HG11 | 1:D:311:ARG:HE | 1.72 | 0.54 |
| 1:A:75:ALA:CA | 1:A:215:VAL:HG12 | 2.36 | 0.53 |
| 1:B:106:THR:HA | 1:B:110:PHE:CD1 | 2.42 | 0.53 |
| 1:C:136:LYS:O | 1:C:137:GLU:CB | 2.56 | 0.53 |
| 1:C:326:THR:HG21 | 1:C:342:LEU:HD13 | 1.89 | 0.53 |
| 1:C:108:ARG:HB3 | 1:D:233:ALA:HB1 | 1.90 | 0.53 |
| 1:A:101:ASP:CB | 1:A:148:THR:HB | 2.38 | 0.53 |
| 1:C:348:MET:HG2 | 1:D:40:PRO:O | 2.08 | 0.53 |
| 1:A:36:LYS:N | 1:C:23:GLY:O | 2.40 | 0.53 |
| 1:A:347:VAL:HG23 | 1:A:348:MET:HG3 | 1.90 | 0.53 |
| 1:B:344:VAL:H | 1:B:348:MET:HE3 | 1.73 | 0.53 |
| 1:D:70:ALA:HB2 | 1:D:190:LEU:CD1 | 2.38 | 0.53 |
| 1:A:31:LEU:HD23 | 1:A:240:PRO:HB2 | 1.90 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:114:ALA:CB | 1:A:119:VAL:H | 2.21 | 0.53 |
| 1:B:96:ALA:CB | 1:B:141:LEU:HB3 | 2.38 | 0.53 |
| 1:B:347:VAL:CG2 | 1:B:348:MET:H | 2.04 | 0.53 |
| 1:D:136:LYS:CA | 1:D:139:THR:HG23 | 2.39 | 0.53 |
| 1:D:354:PRO:O | 1:D:356:GLU:N | 2.41 | 0.53 |
| 1:A:357:ALA:O | 1:A:359:GLU:N | 2.38 | 0.53 |
| 1:C:39:SER:O | 1:C:40:PRO:C | 2.45 | 0.53 |
| 1:D:12:ALA:HA | 1:D:67:LEU:HD21 | 1.91 | 0.53 |
| 1:D:385:LYS:C | 1:D:387:ALA:N | 2.62 | 0.53 |
| 1:A:104:GLY:O | 1:A:107:HIS:HB3 | 2.08 | 0.53 |
| 1:A:226:ARG:O | 1:A:229:PHE:HB3 | 2.09 | 0.53 |
| 1:D:279:VAL:HB | 1:D:311:ARG:O | 2.07 | 0.53 |
| 1:C:136:LYS:HG3 | 1:C:137:GLU:N | 2.24 | 0.53 |
| 1:C:202:THR:HG22 | 3:C:458:HOH:O | 2.09 | 0.53 |
| 1:C:307:MET:SD | 1:C:335:LEU:HD13 | 2.49 | 0.53 |
| 1:C:343:GLU:HG2 | 1:C:348:MET:SD | 2.49 | 0.53 |
| 1:D:137:GLU:O | 1:D:137:GLU:HG2 | 2.08 | 0.53 |
| 1:D:162:ASP:HA | 1:D:165:LYS:NZ | 2.23 | 0.53 |
| 1:B:131:LEU:HG | 1:B:135:ILE:HG13 | 1.90 | 0.53 |
| 1:B:270:PHE:CZ | 1:B:385:LYS:HG2 | 2.44 | 0.53 |
| 1:D:37:GLN:HE21 | 1:D:43:PRO:HG3 | 1.74 | 0.53 |
| 1:B:211:VAL:HG23 | 1:B:245:LEU:HD23 | 1.90 | 0.53 |
| 1:C:102:VAL:HG11 | 1:C:106:THR:CG2 | 2.39 | 0.53 |
| 1:C:114:ALA:CA | 1:C:119:VAL:H | 2.20 | 0.53 |
| 1:D:221:LYS:HB3 | 1:D:222:PRO:HD3 | 1.91 | 0.53 |
| 1:A:261:ALA:HA | 1:A:305:GLY:O | 2.09 | 0.52 |
| 1:B:1:THR:CG2 | 1:B:2:LEU:N | 2.72 | 0.52 |
| 1:B:351:GLY:O | 1:B:353:ILE:N | 2.36 | 0.52 |
| 1:C:1:THR:HG21 | 1:C:14:HIS:CB | 2.39 | 0.52 |
| 1:D:346:ALA:O | 1:D:350:HIS:O | 2.26 | 0.52 |
| 1:B:21:VAL:CG2 | 1:D:21:VAL:HG21 | 2.39 | 0.52 |
| 1:B:46:THR:O | 1:B:46:THR:CG2 | 2.56 | 0.52 |
| 1:C:182:LEU:O | 1:C:183:SER:OG | 2.19 | 0.52 |
| 1:B:1:THR:HG21 | 1:B:14:HIS:CB | 2.40 | 0.52 |
| 1:B:277:ASN:HD22 | 1:B:277:ASN:H | 1.57 | 0.52 |
| 1:C:106:THR:HG22 | 1:C:110:PHE:CE1 | 2.44 | 0.52 |
| 1:C:354:PRO:C | 1:C:356:GLU:H | 2.12 | 0.52 |
| 1:D:74:LEU:HB2 | 1:D:216:LEU:HD22 | 1.91 | 0.52 |
| 1:D:179:ASN:ND2 | 1:D:199:HIS:CE1 | 2.77 | 0.52 |
| 1:A:22:HIS:HD2 | 1:C:47:TYR:CD1 | 2.28 | 0.52 |
| 1:C:13:ILE:O | 1:C:13:ILE:HG22 | 2.09 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:381:LEU:HG | 1:C:385:LYS:HE3 | 1.92 | 0.52 |
| 1:D:382:GLU:HA | 1:D:382:GLU:OE2 | 2.08 | 0.52 |
| 1:A:265:ASN:HA | 1:A:283:TYR:CE2 | 2.44 | 0.52 |
| 1:A:312:ILE:O | 1:A:314:GLY:N | 2.37 | 0.52 |
| 1:B:220:ASN:HD22 | 1:B:222:PRO:HD2 | 1.70 | 0.52 |
| 1:B:220:ASN:HD21 | 1:B:222:PRO:HD2 | 1.71 | 0.52 |
| 1:C:135:ILE:HG21 | 1:C:168:ALA:HB2 | 1.89 | 0.52 |
| 1:C:276:GLU:HB3 | 1:C:277:ASN:HD22 | 1.74 | 0.52 |
| 1:A:34:THR:O | 1:C:24:SER:HA | 2.10 | 0.52 |
| 1:C:114:ALA:HB1 | 1:C:119:VAL:H | 1.75 | 0.52 |
| 1:A:333:GLU:HG3 | 3:B:474:HOH:O | 2.10 | 0.52 |
| 1:D:46:THR:O | 1:D:46:THR:HG22 | 2.09 | 0.52 |
| 1:D:216:LEU:C | 1:D:216:LEU:HD23 | 2.30 | 0.52 |
| 1:D:307:MET:HE1 | 1:D:369:ARG:NH2 | 2.25 | 0.52 |
| 1:B:28:PRO:HA | 3:D:417:HOH:O | 2.09 | 0.52 |
| 1:B:114:ALA:HB1 | 1:B:119:VAL:N | 2.24 | 0.52 |
| 1:C:95:HIS:HA | 1:C:120:GLU:HB2 | 1.92 | 0.52 |
| 1:C:131:LEU:O | 1:C:135:ILE:N | 2.39 | 0.52 |
| 1:D:310:PHE:C | 1:D:367:LEU:HD12 | 2.29 | 0.52 |
| 1:A:72:TYR:O | 1:A:217:ALA:HA | 2.10 | 0.52 |
| 1:A:102:VAL:HG11 | 1:A:106:THR:CG2 | 2.40 | 0.52 |
| 1:B:46:THR:O | 1:B:46:THR:HG22 | 2.10 | 0.52 |
| 1:B:314:GLY:CA | 3:B:419:HOH:O | 2.57 | 0.52 |
| 1:B:181:PHE:CD1 | 1:B:335:LEU:HD11 | 2.45 | 0.52 |
| 1:D:142:VAL:HG21 | 1:D:164:ILE:HD11 | 1.92 | 0.52 |
| 1:A:99:ILE:O | 1:A:102:VAL:CG2 | 2.58 | 0.51 |
| 1:C:110:PHE:O | 1:C:114:ALA:HB2 | 2.10 | 0.51 |
| 1:D:135:ILE:HD11 | 1:D:164:ILE:HA | 1.92 | 0.51 |
| 1:A:22:HIS:HD2 | 1:C:47:TYR:HD1 | 1.58 | 0.51 |
| 1:A:82:THR:O | 1:A:86:ILE:HG13 | 2.10 | 0.51 |
| 1:B:137:GLU:O | 1:B:137:GLU:CG | 2.58 | 0.51 |
| 1:B:97:VAL:O | 1:B:142:VAL:HA | 2.11 | 0.51 |
| 1:B:310:PHE:CE2 | 1:B:368:VAL:HB | 2.45 | 0.51 |
| 1:C:136:LYS:CA | 1:C:139:THR:HG23 | 2.40 | 0.51 |
| 1:A:13:ILE:HG22 | 1:A:13:ILE:O | 2.10 | 0.51 |
| 1:B:354:PRO:O | 1:B:356:GLU:N | 2.43 | 0.51 |
| 1:C:326:THR:HG21 | 1:C:342:LEU:CD1 | 2.40 | 0.51 |
| 1:D:95:HIS:O | 1:D:139:THR:HA | 2.10 | 0.51 |
| 1:C:53:GLN:NE2 | 1:C:58:GLU:HG3 | 2.25 | 0.51 |
| 1:C:221:LYS:HB3 | 1:C:222:PRO:HD3 | 1.91 | 0.51 |
| 1:A:67:LEU:HD11 | 1:A:250:LEU:HD21 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:21:VAL:CG2 | 1:D:21:VAL:CG2 | 2.89 | 0.51 |
| 1:B:114:ALA:CB | 1:B:119:VAL:N | 2.71 | 0.51 |
| 1:C:102:VAL:HG11 | 1:C:106:THR:HG23 | 1.91 | 0.51 |
| 1:D:102:VAL:HG11 | 1:D:106:THR:CG2 | 2.41 | 0.51 |
| 1:D:131:LEU:O | 1:D:135:ILE:N | 2.42 | 0.51 |
| 1:A:1:THR:HG21 | 1:A:14:HIS:HB3 | 1.92 | 0.51 |
| 1:A:134:LEU:O | 1:A:136:LYS:O | 2.29 | 0.51 |
| 1:B:126:ASP:OD2 | 1:B:129:ASN:HB2 | 2.09 | 0.51 |
| 1:B:271:LEU:O | 1:B:278:VAL:HG11 | 2.11 | 0.51 |
| 1:C:220:ASN:HD21 | 1:C:222:PRO:HD2 | 1.75 | 0.51 |
| 1:D:3:GLN:HE21 | 1:D:11:LYS:CG | 2.19 | 0.51 |
| 1:D:106:THR:HG22 | 1:D:110:PHE:CZ | 2.46 | 0.51 |
| 1:D:106:THR:O | 1:D:107:HIS:C | 2.48 | 0.51 |
| 1:D:345:PRO:HA | 1:D:349:THR:HB | 1.91 | 0.51 |
| 1:A:124:THR:OG1 | 1:A:134:LEU:CD1 | 2.58 | 0.51 |
| 1:B:137:GLU:O | 1:B:137:GLU:HG2 | 2.10 | 0.51 |
| 1:D:91:PRO:HG3 | 1:D:140:LYS:HE2 | 1.93 | 0.51 |
| 1:D:102:VAL:CG1 | 1:D:103:TYR:N | 2.73 | 0.51 |
| 1:A:98:SER:HB3 | 1:A:143:TRP:HB3 | 1.93 | 0.51 |
| 1:A:348:MET:HE2 | 1:B:40:PRO:HB3 | 1.93 | 0.51 |
| 1:C:310:PHE:CE1 | 1:C:312:ILE:HG23 | 2.43 | 0.51 |
| 1:C:334:SER:HB3 | 1:D:34:THR:HG21 | 1.93 | 0.51 |
| 1:B:60:LEU:CD1 | 1:B:64:VAL:HG23 | 2.40 | 0.51 |
| 1:C:70:ALA:HA | 1:C:219:ASN:HD21 | 1.75 | 0.51 |
| 1:C:196:ILE:HG23 | 1:C:218:THR:CG2 | 2.41 | 0.50 |
| 1:C:311:ARG:HH11 | 1:C:311:ARG:CB | 2.24 | 0.50 |
| 1:A:51:ARG:HH11 | 1:A:51:ARG:HG2 | 1.75 | 0.50 |
| 1:D:220:ASN:HD22 | 1:D:222:PRO:CD | 2.23 | 0.50 |
| 1:D:276:GLU:HB3 | 1:D:277:ASN:ND2 | 2.27 | 0.50 |
| 1:B:46:THR:HB | 3:B:455:HOH:O | 2.12 | 0.50 |
| 1:B:331:LEU:HA | 1:B:342:LEU:HD23 | 1.93 | 0.50 |
| 1:D:213:LEU:HD23 | 1:D:214:GLY:N | 2.26 | 0.50 |
| 1:D:343:GLU:HB3 | 1:D:369:ARG:NH1 | 2.27 | 0.50 |
| 1:A:294:VAL:O | 1:A:297:LYS:HG3 | 2.11 | 0.50 |
| 1:B:70:ALA:HA | 1:B:219:ASN:ND2 | 2.22 | 0.50 |
| 1:B:358:ARG:HB3 | 1:B:358:ARG:NH1 | 2.25 | 0.50 |
| 1:C:3:GLN:HE21 | 1:C:11:LYS:HA | 1.74 | 0.50 |
| 1:C:51:ARG:HG3 | 1:C:237:ILE:HD13 | 1.92 | 0.50 |
| 1:C:230:LEU:O | 1:C:234:ILE:HG12 | 2.11 | 0.50 |
| 1:A:7:LYS:HB2 | 1:D:376:ASP:HB2 | 1.92 | 0.50 |
| 1:A:151:THR:O | 1:A:152:LEU:HB2 | 2.12 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:221:LYS:HE2 | 1:A:225:GLU:OE2 | 2.12 | 0.50 |
| 1:C:216:LEU:HD23 | 1:C:216:LEU:C | 2.32 | 0.50 |
| 1:C:330:THR:HB | 1:C:341:LEU:CD2 | 2.41 | 0.50 |
| 1:B:265:ASN:HA | 1:B:283:TYR:CE2 | 2.45 | 0.50 |
| 1:C:253:LEU:HD12 | 1:C:257:VAL:HG23 | 1.94 | 0.50 |
| 1:D:322:PHE:C | 1:D:324:SER:H | 2.14 | 0.50 |
| 1:C:53:GLN:NE2 | 1:C:58:GLU:CG | 2.75 | 0.50 |
| 1:C:369:ARG:HH11 | 1:C:369:ARG:CG | 2.23 | 0.50 |
| 1:D:274:ASP:O | 1:D:278:VAL:HB | 2.12 | 0.50 |
| 1:C:101:ASP:HB3 | 1:C:148:THR:HB | 1.94 | 0.50 |
| 1:D:37:GLN:NE2 | 1:D:43:PRO:HG3 | 2.26 | 0.50 |
| 1:A:3:GLN:NE2 | 1:A:11:LYS:HA | 2.26 | 0.50 |
| 1:B:135:ILE:O | 1:B:139:THR:CG2 | 2.60 | 0.50 |
| 1:C:220:ASN:ND2 | 1:C:220:ASN:C | 2.61 | 0.50 |
| 1:D:95:HIS:HB3 | 1:D:139:THR:N | 2.26 | 0.50 |
| 1:D:385:LYS:O | 1:D:387:ALA:N | 2.45 | 0.50 |
| 1:A:162:ASP:HA | 1:A:165:LYS:HZ1 | 1.75 | 0.49 |
| 1:A:47:TYR:CD1 | 1:C:22:HIS:HD2 | 2.30 | 0.49 |
| 1:C:61:GLU:OE2 | 1:C:74:LEU:HA | 2.12 | 0.49 |
| 1:C:206:ASN:O | 1:C:208:HIS:HD2 | 1.95 | 0.49 |
| 1:D:1:THR:HG22 | 1:D:2:LEU:N | 2.26 | 0.49 |
| 1:D:115:ASN:O | 1:D:116:ALA:HB3 | 2.12 | 0.49 |
| 1:A:2:LEU:O | 1:A:4:GLU:HG3 | 2.12 | 0.49 |
| 1:A:131:LEU:HD23 | 1:A:163:LEU:HD23 | 1.94 | 0.49 |
| 1:B:37:GLN:HE21 | 1:B:43:PRO:HG3 | 1.78 | 0.49 |
| 1:B:311:ARG:HH12 | 1:B:366:ASP:CG | 2.16 | 0.49 |
| 1:A:312:ILE:C | 1:A:314:GLY:H | 2.16 | 0.49 |
| 1:B:201:ALA:HB3 | 1:B:213:LEU:O | 2.12 | 0.49 |
| 1:B:294:VAL:HA | 1:B:297:LYS:CG | 2.43 | 0.49 |
| 1:C:96:ALA:HB2 | 1:C:141:LEU:HB3 | 1.93 | 0.49 |
| 1:C:253:LEU:HD12 | 1:C:257:VAL:CG2 | 2.42 | 0.49 |
| 1:C:382:GLU:OE2 | 1:C:382:GLU:HA | 2.13 | 0.49 |
| 1:D:181:PHE:CE1 | 1:D:335:LEU:HD11 | 2.48 | 0.49 |
| 1:C:184:PRO:HD3 | 1:C:199:HIS:CE1 | 2.47 | 0.49 |
| 1:D:334:SER:OG | 1:D:335:LEU:N | 2.44 | 0.49 |
| 1:A:312:ILE:HD11 | 1:A:319:ALA:HA | 1.94 | 0.49 |
| 1:C:126:ASP:OD2 | 1:C:129:ASN:ND2 | 2.45 | 0.49 |
| 1:C:330:THR:CG2 | 1:D:36:LYS:HG2 | 2.43 | 0.49 |
| 1:D:53:GLN:CD | 1:D:58:GLU:HB2 | 2.33 | 0.49 |
| 1:D:76:PHE:HA | 1:D:238:PRO:HD3 | 1.95 | 0.49 |
| 1:D:106:THR:O | 1:D:110:PHE:HB2 | 2.12 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:137:GLU:O | 1:A:137:GLU:HG2 | 2.12 | 0.49 |
| 1:B:135:ILE:C | 1:B:139:THR:HG21 | 2.33 | 0.49 |
| 1:B:343:GLU:OE2 | 1:B:345:PRO:HA | 2.13 | 0.49 |
| 1:D:321:LYS:O | 1:D:322:PHE:C | 2.50 | 0.49 |
| 1:A:18:HIS:NE2 | 1:A:27:GLU:HA | 2.27 | 0.49 |
| 1:A:52:SER:O | 1:A:53:GLN:HB2 | 2.12 | 0.49 |
| 1:A:103:TYR:O | 1:A:105:GLY:N | 2.45 | 0.49 |
| 1:A:13:ILE:O | 1:A:13:ILE:CG2 | 2.61 | 0.49 |
| 1:A:147:PRO:HG2 | 1:A:182:LEU:HG | 1.95 | 0.49 |
| 1:A:280:ALA:HB3 | 1:A:311:ARG:HD3 | 1.94 | 0.49 |
| 1:B:93:GLY:HA2 | 1:B:118:GLY:O | 2.13 | 0.49 |
| 1:C:151:THR:O | 1:C:152:LEU:HB2 | 2.11 | 0.49 |
| 1:C:209:SER:O | 1:D:33:THR:N | 2.45 | 0.49 |
| 1:C:211:VAL:HG13 | 1:C:242:ASP:HB3 | 1.95 | 0.49 |
| 1:B:349:THR:HG22 | 1:B:350:HIS:N | 2.28 | 0.49 |
| 1:D:197:VAL:HG23 | 1:D:217:ALA:HB3 | 1.94 | 0.49 |
| 1:A:144:ILE:HB | 1:A:177:VAL:HG22 | 1.95 | 0.48 |
| 1:C:101:ASP:OD1 | 1:C:361:SER:OG | 2.22 | 0.48 |
| 1:C:354:PRO:O | 1:C:356:GLU:N | 2.46 | 0.48 |
| 1:A:203:LYS:HD2 | 1:A:203:LYS:N | 2.28 | 0.48 |
| 1:B:210:ASP:O | 1:B:211:VAL:HG23 | 2.12 | 0.48 |
| 1:B:226:ARG:O | 1:B:229:PHE:HB3 | 2.12 | 0.48 |
| 1:C:265:ASN:HA | 1:C:283:TYR:CE2 | 2.48 | 0.48 |
| 1:A:18:HIS:CD2 | 1:A:27:GLU:HA | 2.48 | 0.48 |
| 1:B:287:LYS:HA | 1:B:292:TYR:CD1 | 2.48 | 0.48 |
| 1:D:307:MET:CE | 1:D:335:LEU:HD13 | 2.43 | 0.48 |
| 1:D:375:GLU:OE2 | 1:D:380:LEU:HD11 | 2.13 | 0.48 |
| 1:A:81:ALA:HA | 1:B:234:ILE:O | 2.12 | 0.48 |
| 1:B:95:HIS:HB3 | 1:B:139:THR:HA | 1.95 | 0.48 |
| 1:C:108:ARG:HH11 | 1:D:232:ASN:ND2 | 2.11 | 0.48 |
| 1:C:146:THR:HG21 | 1:C:157:ILE:HD11 | 1.95 | 0.48 |
| 1:A:131:LEU:N | 1:A:132:PRO:CD | 2.77 | 0.48 |
| 1:A:150:PRO:HG3 | 1:A:345:PRO:HG3 | 1.96 | 0.48 |
| 1:C:106:THR:O | 1:C:107:HIS:C | 2.51 | 0.48 |
| 1:C:287:LYS:NZ | 3:C:471:HOH:O | 2.45 | 0.48 |
| 1:D:354:PRO:C | 1:D:356:GLU:N | 2.67 | 0.48 |
| 1:A:277:ASN:N | 1:A:277:ASN:ND2 | 2.59 | 0.48 |
| 1:B:379:ASP:OD1 | 1:C:7:LYS:CG | 2.58 | 0.48 |
| 1:C:95:HIS:C | 1:C:139:THR:HA | 2.33 | 0.48 |
| 1:A:23:GLY:HA3 | 1:C:36:LYS:HB2 | 1.95 | 0.48 |
| 1:B:102:VAL:HG12 | 1:B:103:TYR:N | 2.28 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:179:ASN:O | 1:B:199:HIS:CE1 | 2.67 | 0.48 |
| 1:B:190:LEU:HD21 | 1:B:197:VAL:HG22 | 1.95 | 0.48 |
| 1:B:230:LEU:O | 1:B:234:ILE:HG12 | 2.14 | 0.48 |
| 1:B:335:LEU:C | 1:B:337:GLY:N | 2.67 | 0.48 |
| 1:C:124:THR:HG22 | 1:C:125:ASN:O | 2.13 | 0.48 |
| 1:D:106:THR:HA | 1:D:110:PHE:CE1 | 2.48 | 0.48 |
| 1:A:44:ILE:O | 1:C:21:VAL:O | 2.32 | 0.48 |
| 1:C:214:GLY:O | 1:C:215:VAL:HG13 | 2.14 | 0.48 |
| 1:C:263:SER:O | 1:C:267:ILE:HG13 | 2.13 | 0.48 |
| 1:D:358:ARG:HH11 | 1:D:358:ARG:HB3 | 1.79 | 0.48 |
| 1:A:311:ARG:HH11 | 1:A:311:ARG:HB3 | 1.78 | 0.48 |
| 1:B:220:ASN:ND2 | 1:B:220:ASN:C | 2.65 | 0.48 |
| 1:B:343:GLU:O | 1:B:369:ARG:HB3 | 2.14 | 0.48 |
| 1:C:44:ILE:HA | 3:C:462:HOH:O | 2.12 | 0.48 |
| 1:C:335:LEU:HD22 | 1:C:369:ARG:NH2 | 2.28 | 0.48 |
| 1:A:54:ASN:HD21 | 1:A:56:ASN:HB2 | 1.78 | 0.48 |
| 1:B:196:ILE:HG12 | 1:B:218:THR:HG21 | 1.95 | 0.48 |
| 1:C:282:ASN:HD22 | 1:C:309:SER:HB3 | 1.78 | 0.48 |
| 1:A:2:LEU:O | 1:A:2:LEU:HD23 | 2.14 | 0.47 |
| 1:A:101:ASP:HB3 | 1:A:148:THR:HB | 1.94 | 0.47 |
| 1:A:369:ARG:HG2 | 1:A:369:ARG:HH11 | 1.79 | 0.47 |
| 1:B:323:ALA:O | 1:B:331:LEU:HB2 | 2.14 | 0.47 |
| 1:A:150:PRO:O | 1:A:152:LEU:HG | 2.14 | 0.47 |
| 1:B:12:ALA:HA | 1:B:67:LEU:HD21 | 1.95 | 0.47 |
| 1:B:102:VAL:CG1 | 1:B:103:TYR:N | 2.77 | 0.47 |
| 1:B:286:LEU:O | 1:B:292:TYR:CD1 | 2.67 | 0.47 |
| 1:C:127:LEU:HD23 | 1:C:160:VAL:HG21 | 1.95 | 0.47 |
| 1:C:260:ALA:HB2 | 3:C:470:HOH:O | 2.13 | 0.47 |
| 1:D:321:LYS:HD3 | 3:D:484:HOH:O | 2.14 | 0.47 |
| 1:D:389:LYS:O | 1:D:390:GLN:C | 2.51 | 0.47 |
| 1:B:3:GLN:NE2 | 1:B:15:ALA:HB2 | 2.28 | 0.47 |
| 1:B:342:LEU:HD23 | 1:B:342:LEU:C | 2.35 | 0.47 |
| 1:D:114:ALA:HB2 | 1:D:119:VAL:HB | 1.94 | 0.47 |
| 1:D:189:PRO:HD2 | 1:D:197:VAL:HG11 | 1.95 | 0.47 |
| 1:D:325:SER:HB3 | 1:D:390:GLN:HG3 | 1.96 | 0.47 |
| 1:A:161:ALA:HB2 | 1:A:193:GLY:O | 2.14 | 0.47 |
| 1:A:208:HIS:CE1 | 3:D:430:HOH:O | 2.66 | 0.47 |
| 1:B:4:GLU:O | 1:B:5:SER:HB2 | 2.13 | 0.47 |
| 1:B:95:HIS:C | 1:B:139:THR:HA | 2.34 | 0.47 |
| 1:C:8:PHE:CZ | 1:C:67:LEU:HD22 | 2.48 | 0.47 |
| 1:C:54:ASN:HD21 | 1:C:56:ASN:HB2 | 1.80 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:150:PRO:HB3 | 1:C:369:ARG:HD2 | 1.95 | 0.47 |
| 1:C:220:ASN:HD22 | 1:C:222:PRO:HD2 | 1.75 | 0.47 |
| 1:D:124:THR:HG22 | 1:D:125:ASN:O | 2.14 | 0.47 |
| 1:A:197:VAL:HG23 | 1:A:217:ALA:O | 2.14 | 0.47 |
| 1:A:292:TYR:HE2 | 1:A:296:LEU:HD11 | 1.79 | 0.47 |
| 1:B:84:ALA:O | 1:B:85:THR:C | 2.52 | 0.47 |
| 1:B:92:GLN:HA | 1:B:92:GLN:OE1 | 2.14 | 0.47 |
| 1:B:179:ASN:HD22 | 1:B:199:HIS:CE1 | 2.32 | 0.47 |
| 1:B:190:LEU:HD13 | 1:B:219:ASN:OD1 | 2.14 | 0.47 |
| 1:C:311:ARG:CB | 1:C:311:ARG:NH1 | 2.77 | 0.47 |
| 1:A:234:ILE:HG13 | 1:A:236:ALA:H | 1.79 | 0.47 |
| 1:C:3:GLN:C | 1:C:4:GLU:HG3 | 2.35 | 0.47 |
| 1:C:99:ILE:HD11 | 1:C:144:ILE:HG23 | 1.96 | 0.47 |
| 1:C:274:ASP:OD1 | 1:C:274:ASP:O | 2.33 | 0.47 |
| 1:D:43:PRO:C | 1:D:45:GLY:H | 2.17 | 0.47 |
| 1:D:294:VAL:HA | 1:D:297:LYS:CG | 2.44 | 0.47 |
| 1:A:278:VAL:HG11 | 1:A:281:VAL:CG2 | 2.44 | 0.47 |
| 1:B:88:GLN:OE1 | 1:B:234:ILE:HD13 | 2.14 | 0.47 |
| 1:B:95:HIS:HB3 | 1:B:139:THR:CA | 2.44 | 0.47 |
| 1:C:37:GLN:NE2 | 1:C:43:PRO:CG | 2.70 | 0.47 |
| 1:C:158:GLN:HA | 1:C:158:GLN:NE2 | 2.29 | 0.47 |
| 1:C:249:GLY:O | 1:C:256:ARG:NH2 | 2.37 | 0.47 |
| 1:C:270:PHE:HB2 | 3:C:412:HOH:O | 2.14 | 0.47 |
| 1:D:121:THR:HG22 | 1:D:123:PHE:CE1 | 2.50 | 0.47 |
| 1:D:146:THR:CB | 1:D:147:PRO:HD3 | 2.45 | 0.47 |
| 1:D:351:GLY:O | 1:D:353:ILE:N | 2.39 | 0.47 |
| 1:B:48:GLU:HG3 | 1:B:49:TYR:N | 2.30 | 0.47 |
| 1:B:111:THR:O | 1:B:114:ALA:HB3 | 2.15 | 0.47 |
| 1:B:141:LEU:HD12 | 1:B:174:ILE:HG13 | 1.97 | 0.47 |
| 1:C:3:GLN:HE21 | 1:C:11:LYS:CG | 2.24 | 0.47 |
| 1:D:131:LEU:N | 1:D:132:PRO:CD | 2.78 | 0.47 |
| 1:A:145:GLU:O | 1:A:146:THR:C | 2.52 | 0.47 |
| 1:A:344:VAL:N | 1:A:348:MET:CE | 2.78 | 0.47 |
| 1:B:95:HIS:O | 1:B:140:LYS:N | 2.48 | 0.47 |
| 1:D:91:PRO:HG2 | 1:D:94:SER:OG | 2.15 | 0.47 |
| 1:C:322:PHE:O | 1:C:326:THR:HG23 | 2.14 | 0.47 |
| 1:C:347:VAL:CG2 | 1:C:348:MET:H | 2.14 | 0.47 |
| 1:D:146:THR:HG21 | 1:D:157:ILE:HD11 | 1.97 | 0.47 |
| 1:D:203:LYS:O | 1:D:336:GLY:O | 2.33 | 0.47 |
| 1:A:113:VAL:C | 1:A:115:ASN:H | 2.18 | 0.46 |
| 1:A:132:PRO:HG2 | 1:A:133:GLN:H | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:344:VAL:HB | 1:B:348:MET:HE3 | 1.97 | 0.46 |
| 1:B:369:ARG:HG2 | 1:B:369:ARG:NH1 | 2.28 | 0.46 |
| 1:C:210:ASP:OD2 | 1:C:210:ASP:N | 2.46 | 0.46 |
| 1:D:202:THR:HG23 | 1:D:211:VAL:O | 2.16 | 0.46 |
| 1:D:358:ARG:NH1 | 1:D:358:ARG:CB | 2.77 | 0.46 |
| 1:B:204:TYR:CZ | 1:B:336:GLY:CA | 2.98 | 0.46 |
| 1:A:347:VAL:CG2 | 1:A:348:MET:H | 2.15 | 0.46 |
| 1:B:135:ILE:HD11 | 1:B:164:ILE:HA | 1.97 | 0.46 |
| 1:B:316:ALA:HB1 | 3:B:410:HOH:O | 2.15 | 0.46 |
| 1:C:131:LEU:N | 1:C:132:PRO:CD | 2.78 | 0.46 |
| 1:C:321:LYS:CG | 1:C:391:ALA:HA | 2.20 | 0.46 |
| 1:D:282:ASN:HB2 | 1:D:309:SER:HB3 | 1.98 | 0.46 |
| 1:B:3:GLN:C | 1:B:4:GLU:HG3 | 2.36 | 0.46 |
| 1:B:42:ASN:HA | 1:B:43:PRO:HD3 | 1.78 | 0.46 |
| 1:C:162:ASP:HA | 1:C:165:LYS:NZ | 2.31 | 0.46 |
| 1:C:306:GLY:O | 1:C:372:VAL:HG23 | 2.16 | 0.46 |
| 1:C:344:VAL:N | 1:C:348:MET:HE1 | 2.29 | 0.46 |
| 1:D:264:ALA:O | 1:D:308:ILE:HD11 | 2.15 | 0.46 |
| 1:D:355:LYS:HB2 | 1:D:358:ARG:NH2 | 2.31 | 0.46 |
| 1:A:196:ILE:HG23 | 1:A:218:THR:HG23 | 1.97 | 0.46 |
| 1:C:46:THR:O | 1:C:46:THR:CG2 | 2.63 | 0.46 |
| 1:C:317:GLU:O | 1:C:318:ALA:C | 2.51 | 0.46 |
| 1:B:267:ILE:O | 1:B:267:ILE:HG22 | 2.15 | 0.46 |
| 1:C:53:GLN:NE2 | 1:C:58:GLU:HB2 | 2.31 | 0.46 |
| 1:C:75:ALA:CA | 1:C:215:VAL:HG12 | 2.42 | 0.46 |
| 1:C:333:GLU:OE1 | 1:C:343:GLU:HG3 | 2.15 | 0.46 |
| 1:D:106:THR:CA | 1:D:110:PHE:CD1 | 2.96 | 0.46 |
| 1:A:33:THR:HG23 | 1:A:49:TYR:CE1 | 2.51 | 0.46 |
| 1:B:268:ALA:O | 1:B:271:LEU:N | 2.49 | 0.46 |
| 1:D:11:LYS:HD3 | 3:D:452:HOH:O | 2.16 | 0.46 |
| 1:D:18:HIS:CB | 1:D:27:GLU:HG3 | 2.46 | 0.46 |
| 1:D:95:HIS:HB2 | 1:D:138:ASN:HB3 | 1.96 | 0.46 |
| 1:D:213:LEU:HD23 | 1:D:213:LEU:C | 2.35 | 0.46 |
| 1:A:42:ASN:HA | 1:A:43:PRO:HD3 | 1.79 | 0.46 |
| 1:A:95:HIS:CE1 | 1:A:139:THR:HG22 | 2.42 | 0.46 |
| 1:A:206:ASN:ND2 | 1:A:246:THR:HA | 2.26 | 0.46 |
| 1:B:144:ILE:O | 1:B:177:VAL:HA | 2.16 | 0.46 |
| 1:D:33:THR:HG22 | 1:D:34:THR:N | 2.31 | 0.46 |
| 1:A:95:HIS:HB3 | 1:A:139:THR:HA | 1.97 | 0.46 |
| 1:C:70:ALA:HB2 | 1:C:190:LEU:CD1 | 2.46 | 0.46 |
| 1:D:87:LEU:HD11 | 1:D:110:PHE:CD1 | 2.51 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:239:SER:HB2 | 1:B:242:ASP:OD1 | 2.16 | 0.46 |
| 1:B:323:ALA:HB1 | 1:B:331:LEU:CD1 | 2.32 | 0.46 |
| 1:D:124:THR:OG1 | 1:D:134:LEU:CD1 | 2.64 | 0.46 |
| 1:A:111:THR:O | 1:A:114:ALA:HB3 | 2.16 | 0.45 |
| 1:A:124:THR:OG1 | 1:A:134:LEU:HD11 | 2.16 | 0.45 |
| 1:A:153:LYS:NZ | 1:A:153:LYS:CB | 2.79 | 0.45 |
| 1:C:316:ALA:HA | 3:C:494:HOH:O | 2.16 | 0.45 |
| 1:D:29:ILE:HG22 | 1:D:31:LEU:HD21 | 1.98 | 0.45 |
| 1:D:42:ASN:HA | 1:D:43:PRO:HD3 | 1.75 | 0.45 |
| 1:A:347:VAL:CG2 | 1:A:348:MET:N | 2.75 | 0.45 |
| 1:B:114:ALA:O | 1:B:115:ASN:C | 2.55 | 0.45 |
| 1:C:382:GLU:OE2 | 1:C:385:LYS:HD2 | 2.16 | 0.45 |
| 1:D:39:SER:O | 1:D:40:PRO:C | 2.54 | 0.45 |
| 1:D:295:VAL:O | 1:D:299:HIS:HB2 | 2.16 | 0.45 |
| 1:D:101:ASP:CB | 1:D:148:THR:HB | 2.46 | 0.45 |
| 1:D:247:HIS:HE1 | 3:D:437:HOH:O | 1.99 | 0.45 |
| 1:D:293:ASP:O | 1:D:297:LYS:HG2 | 2.17 | 0.45 |
| 1:A:159:LYS:NZ | 3:A:462:HOH:O | 2.49 | 0.45 |
| 1:B:376:ASP:CB | 1:C:7:LYS:HB2 | 2.45 | 0.45 |
| 1:C:108:ARG:NH1 | 1:D:232:ASN:ND2 | 2.65 | 0.45 |
| 1:C:312:ILE:C | 1:C:314:GLY:H | 2.19 | 0.45 |
| 1:A:149:ASN:HB2 | 1:A:181:PHE:CE2 | 2.51 | 0.45 |
| 1:A:348:MET:HE2 | 1:B:40:PRO:CB | 2.47 | 0.45 |
| 1:B:376:ASP:HB2 | 1:C:7:LYS:HB2 | 1.97 | 0.45 |
| 1:C:136:LYS:CG | 1:C:137:GLU:H | 2.29 | 0.45 |
| 1:A:343:GLU:HG2 | 1:A:344:VAL:H | 1.82 | 0.45 |
| 1:B:91:PRO:HG3 | 1:B:140:LYS:HE2 | 1.98 | 0.45 |
| 1:B:111:THR:O | 1:B:114:ALA:N | 2.49 | 0.45 |
| 1:C:33:THR:HG23 | 1:C:49:TYR:CE1 | 2.52 | 0.45 |
| 1:C:300:ARG:NH1 | 3:C:488:HOH:O | 2.41 | 0.45 |
| 1:D:210:ASP:O | 1:D:211:VAL:HG23 | 2.17 | 0.45 |
| 1:A:23:GLY:C | 1:C:35:PHE:HA | 2.37 | 0.45 |
| 1:B:109:TYR:O | 1:B:110:PHE:C | 2.54 | 0.45 |
| 1:B:358:ARG:CZ | 1:B:358:ARG:HB2 | 2.46 | 0.45 |
| 1:D:329:PHE:CE1 | 1:D:380:LEU:HD22 | 2.51 | 0.45 |
| 1:A:31:LEU:O | 1:A:32:SER:C | 2.55 | 0.45 |
| 1:A:146:THR:HB | 1:A:147:PRO:HD3 | 1.99 | 0.45 |
| 1:B:276:GLU:HB3 | 1:B:277:ASN:HD22 | 1.81 | 0.45 |
| 1:D:279:VAL:HG11 | 1:D:311:ARG:NE | 2.31 | 0.45 |
| 1:A:18:HIS:HB3 | 1:A:27:GLU:HG3 | 1.99 | 0.45 |
| 1:A:46:THR:O | 1:A:46:THR:CG2 | 2.63 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:53:GLN:HA | 1:A:57:ARG:NH2 | 2.31 | 0.45 |
| 1:A:277:ASN:HA | 1:A:313:LYS:CB | 2.47 | 0.45 |
| 1:B:94:SER:HA | 1:B:138:ASN:ND2 | 2.32 | 0.45 |
| 1:C:34:THR:C | 3:C:469:HOH:O | 2.55 | 0.45 |
| 1:D:349:THR:O | 1:D:351:GLY:N | 2.49 | 0.45 |
| 1:A:190:LEU:C | 1:A:192:PHE:N | 2.70 | 0.45 |
| 1:B:385:LYS:O | 1:B:387:ALA:N | 2.50 | 0.45 |
| 1:C:71:GLN:H | 1:C:219:ASN:HD22 | 1.62 | 0.45 |
| 1:C:166:LYS:HE2 | 1:C:167:HIS:CE1 | 2.51 | 0.45 |
| 1:D:321:LYS:O | 1:D:324:SER:N | 2.46 | 0.45 |
| 1:D:355:LYS:HB2 | 1:D:358:ARG:HH21 | 1.82 | 0.45 |
| 1:A:115:ASN:O | 1:A:116:ALA:HB3 | 2.17 | 0.44 |
| 1:B:136:LYS:NZ | 1:B:138:ASN:HA | 2.32 | 0.44 |
| 1:C:132:PRO:HB3 | 1:C:167:HIS:NE2 | 2.32 | 0.44 |
| 1:C:343:GLU:OE1 | 1:C:345:PRO:HD3 | 2.17 | 0.44 |
| 1:D:255:LEU:HD23 | 1:D:255:LEU:HA | 1.75 | 0.44 |
| 1:A:1:THR:HA | 1:D:327:ARG:O | 2.18 | 0.44 |
| 1:A:292:TYR:CE2 | 1:A:296:LEU:HD11 | 2.53 | 0.44 |
| 1:B:335:LEU:O | 1:B:336:GLY:C | 2.51 | 0.44 |
| 1:C:272:ALA:HB3 | 3:C:451:HOH:O | 2.17 | 0.44 |
| 1:D:344:VAL:N | 1:D:348:MET:CE | 2.74 | 0.44 |
| 1:A:135:ILE:O | 1:A:139:THR:HG21 | 2.17 | 0.44 |
| 1:B:248:ARG:HH11 | 1:C:248:ARG:NH1 | 2.16 | 0.44 |
| 1:B:283:TYR:O | 1:B:285:GLY:N | 2.50 | 0.44 |
| 1:B:381:LEU:HG | 1:B:385:LYS:HE3 | 1.99 | 0.44 |
| 1:C:72:TYR:O | 1:C:217:ALA:HA | 2.17 | 0.44 |
| 1:A:20:ASP:OD2 | 1:A:22:HIS:ND1 | 2.51 | 0.44 |
| 1:A:330:THR:HG21 | 1:B:36:LYS:HG2 | 1.98 | 0.44 |
| 1:B:8:PHE:CE1 | 1:B:185:TYR:HA | 2.53 | 0.44 |
| 1:C:124:THR:HG21 | 1:C:130:ASP:HB2 | 2.00 | 0.44 |
| 1:A:58:GLU:CD | 1:A:62:ARG:HH21 | 2.21 | 0.44 |
| 1:A:102:VAL:CG1 | 1:A:103:TYR:H | 2.30 | 0.44 |
| 1:A:183:SER:O | 1:A:184:PRO:C | 2.56 | 0.44 |
| 1:A:190:LEU:O | 1:A:192:PHE:N | 2.50 | 0.44 |
| 1:A:234:ILE:HG13 | 1:A:235:GLY:N | 2.33 | 0.44 |
| 1:B:74:LEU:HD12 | 1:B:216:LEU:HD21 | 1.98 | 0.44 |
| 1:C:277:ASN:H | 1:C:277:ASN:ND2 | 2.09 | 0.44 |
| 1:C:294:VAL:HA | 1:C:297:LYS:HD2 | 1.99 | 0.44 |
| 1:D:144:ILE:HD11 | 1:D:160:VAL:HG11 | 2.00 | 0.44 |
| 1:A:292:TYR:CE2 | 1:A:296:LEU:HG | 2.53 | 0.44 |
| 1:B:3:GLN:HA | 1:B:6:ASP:OD2 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:95:HIS:CA | 1:B:120:GLU:HB2 | 2.46 | 0.44 |
| 1:C:35:PHE:CZ | 1:C:47:TYR:HB3 | 2.52 | 0.44 |
| 1:C:113:VAL:O | 1:C:113:VAL:HG12 | 2.18 | 0.44 |
| 1:C:362:GLY:O | 1:C:364:PHE:N | 2.50 | 0.44 |
| 1:D:334:SER:O | 1:D:335:LEU:HB3 | 2.17 | 0.44 |
| 1:A:8:PHE:C | 1:A:8:PHE:CD2 | 2.91 | 0.44 |
| 1:C:50:SER:O | 1:C:53:GLN:N | 2.50 | 0.44 |
| 1:D:17:GLU:HG2 | 1:D:18:HIS:N | 2.33 | 0.44 |
| 1:C:33:THR:HG22 | 1:C:34:THR:HG23 | 1.99 | 0.44 |
| 1:C:335:LEU:HD22 | 1:C:369:ARG:HH21 | 1.82 | 0.44 |
| 1:D:161:ALA:HB2 | 1:D:193:GLY:O | 2.17 | 0.44 |
| 1:D:322:PHE:C | 1:D:324:SER:N | 2.71 | 0.44 |
| 1:D:358:ARG:NH1 | 1:D:358:ARG:HB2 | 2.32 | 0.44 |
| 1:D:386:GLN:HG2 | 3:D:436:HOH:O | 2.16 | 0.44 |
| 1:A:144:ILE:HD12 | 1:A:175:LEU:HD11 | 2.00 | 0.44 |
| 1:A:287:LYS:HA | 1:A:292:TYR:CD1 | 2.53 | 0.44 |
| 1:C:76:PHE:HA | 1:C:238:PRO:HD3 | 2.00 | 0.44 |
| 1:C:189:PRO:HD2 | 1:C:197:VAL:HG11 | 2.00 | 0.44 |
| 1:D:376:ASP:HB3 | 1:D:379:ASP:HB2 | 2.00 | 0.44 |
| 1:A:114:ALA:CA | 1:A:119:VAL:H | 2.31 | 0.43 |
| 1:A:330:THR:CG2 | 1:B:36:LYS:HG2 | 2.48 | 0.43 |
| 1:B:22:HIS:ND1 | 1:B:22:HIS:N | 2.66 | 0.43 |
| 1:B:76:PHE:HA | 1:B:238:PRO:HD3 | 2.00 | 0.43 |
| 1:B:172:ASP:HB3 | 3:B:448:HOH:O | 2.18 | 0.43 |
| 1:C:55:PRO:O | 1:C:59:ASN:ND2 | 2.51 | 0.43 |
| 1:C:216:LEU:HD23 | 1:C:216:LEU:O | 2.17 | 0.43 |
| 1:A:75:ALA:CB | 1:A:215:VAL:HG12 | 2.48 | 0.43 |
| 1:A:106:THR:HA | 1:A:110:PHE:CE1 | 2.53 | 0.43 |
| 1:B:95:HIS:CE1 | 1:B:122:SER:OG | 2.71 | 0.43 |
| 1:B:124:THR:OG1 | 1:B:134:LEU:HD11 | 2.17 | 0.43 |
| 1:B:136:LYS:CA | 1:B:139:THR:HG23 | 2.46 | 0.43 |
| 1:A:79:GLY:O | 1:A:82:THR:HB | 2.18 | 0.43 |
| 1:A:95:HIS:C | 1:A:139:THR:HA | 2.38 | 0.43 |
| 1:A:202:THR:HB | 1:A:203:LYS:HD2 | 1.99 | 0.43 |
| 1:C:114:ALA:HB1 | 1:C:119:VAL:N | 2.34 | 0.43 |
| 1:C:168:ALA:O | 1:C:171:GLN:HG3 | 2.18 | 0.43 |
| 1:C:190:LEU:HD21 | 1:C:197:VAL:HG22 | 1.99 | 0.43 |
| 1:C:283:TYR:O | 1:C:285:GLY:N | 2.52 | 0.43 |
| 1:D:8:PHE:CE1 | 1:D:185:TYR:HA | 2.53 | 0.43 |
| 1:D:95:HIS:CA | 1:D:120:GLU:HB2 | 2.49 | 0.43 |
| 1:D:344:VAL:H | 1:D:348:MET:HE1 | 1.79 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:344:VAL:O | 1:D:345:PRO:C | 2.55 | 0.43 |
| 1:D:358:ARG:HH11 | 1:D:358:ARG:CB | 2.32 | 0.43 |
| 1:A:106:THR:CA | 1:A:110:PHE:CD1 | 3.01 | 0.43 |
| 1:A:116:ALA:HB3 | 1:B:92:GLN:HB2 | 2.00 | 0.43 |
| 1:A:197:VAL:O | 1:A:216:LEU:HA | 2.18 | 0.43 |
| 1:C:73:GLY:HA2 | 1:C:216:LEU:O | 2.18 | 0.43 |
| 1:D:232:ASN:HB3 | 3:D:404:HOH:O | 2.18 | 0.43 |
| 1:D:311:ARG:NH1 | 1:D:366:ASP:OD1 | 2.47 | 0.43 |
| 1:D:338:ILE:CG2 | 1:D:339:GLU:N | 2.80 | 0.43 |
| 1:A:128:LEU:CD1 | 1:A:159:LYS:HD3 | 2.44 | 0.43 |
| 1:A:301:ASP:O | 1:A:302:ALA:HB3 | 2.19 | 0.43 |
| 1:B:74:LEU:O | 1:B:215:VAL:HA | 2.19 | 0.43 |
| 1:B:197:VAL:O | 1:B:216:LEU:HA | 2.19 | 0.43 |
| 1:B:338:ILE:CG1 | 1:B:374:ILE:HD11 | 2.47 | 0.43 |
| 1:C:335:LEU:HD12 | 1:C:336:GLY:N | 2.33 | 0.43 |
| 1:D:37:GLN:HA | 1:D:43:PRO:HA | 2.00 | 0.43 |
| 1:D:125:ASN:OD1 | 1:D:126:ASP:N | 2.51 | 0.43 |
| 1:A:37:GLN:CA | 1:A:43:PRO:HA | 2.44 | 0.43 |
| 1:A:71:GLN:HB2 | 1:A:219:ASN:HA | 2.01 | 0.43 |
| 1:A:144:ILE:CD1 | 1:A:175:LEU:HD11 | 2.47 | 0.43 |
| 1:A:220:ASN:ND2 | 1:A:220:ASN:C | 2.71 | 0.43 |
| 1:B:57:ARG:HD3 | 3:B:433:HOH:O | 2.17 | 0.43 |
| 1:C:112:LYS:O | 1:C:115:ASN:N | 2.51 | 0.43 |
| 1:C:301:ASP:O | 1:C:302:ALA:HB3 | 2.19 | 0.43 |
| 1:C:323:ALA:HA | 1:C:342:LEU:HD11 | 2.00 | 0.43 |
| 1:D:343:GLU:OE1 | 1:D:345:PRO:HD3 | 2.17 | 0.43 |
| 1:D:347:VAL:O | 1:D:348:MET:C | 2.57 | 0.43 |
| 1:B:37:GLN:NE2 | 1:B:43:PRO:HG3 | 2.34 | 0.43 |
| 1:B:204:TYR:CZ | 1:B:336:GLY:HA3 | 2.54 | 0.43 |
| 1:C:3:GLN:NE2 | 1:C:11:LYS:HA | 2.33 | 0.43 |
| 1:C:124:THR:OG1 | 1:C:134:LEU:CD1 | 2.67 | 0.43 |
| 1:C:146:THR:HG1 | 1:C:147:PRO:HD3 | 1.81 | 0.43 |
| 1:C:196:ILE:HD11 | 1:C:223:LEU:HD21 | 2.00 | 0.43 |
| 1:D:332:ALA:O | 1:D:343:GLU:HB2 | 2.19 | 0.43 |
| 1:A:195:ASP:O | 1:A:218:THR:HG22 | 2.18 | 0.43 |
| 1:A:274:ASP:O | 1:A:276:GLU:N | 2.52 | 0.43 |
| 1:A:344:VAL:H | 1:A:348:MET:HE1 | 1.81 | 0.43 |
| 1:B:32:SER:HB3 | 1:D:26:ILE:HB | 1.99 | 0.43 |
| 1:C:48:GLU:HG3 | 1:C:49:TYR:N | 2.34 | 0.43 |
| 1:C:53:GLN:NE2 | 1:C:58:GLU:OE2 | 2.52 | 0.43 |
| 1:C:65:ALA:HB3 | 3:C:432:HOH:O | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:271:LEU:O | 1:C:278:VAL:HG11 | 2.19 | 0.43 |
| 1:D:311:ARG:HB3 | 1:D:311:ARG:HH11 | 1.83 | 0.43 |
| 1:B:190:LEU:C | 1:B:192:PHE:H | 2.20 | 0.43 |
| 1:C:348:MET:CG | 1:D:40:PRO:O | 2.66 | 0.43 |
| 1:A:108:ARG:HB3 | 1:B:233:ALA:HB1 | 2.01 | 0.43 |
| 1:A:120:GLU:OE1 | 1:A:137:GLU:HG2 | 2.19 | 0.43 |
| 1:B:7:LYS:HB3 | 3:B:449:HOH:O | 2.19 | 0.43 |
| 1:B:317:GLU:O | 1:B:320:SER:N | 2.52 | 0.43 |
| 1:C:190:LEU:CD2 | 1:C:197:VAL:HG22 | 2.49 | 0.43 |
| 1:C:348:MET:HE2 | 1:D:40:PRO:CB | 2.44 | 0.43 |
| 1:D:323:ALA:O | 1:D:331:LEU:HB2 | 2.19 | 0.43 |
| 1:A:348:MET:CG | 1:B:40:PRO:O | 2.46 | 0.42 |
| 1:B:74:LEU:HB2 | 1:B:216:LEU:CD2 | 2.46 | 0.42 |
| 1:B:115:ASN:O | 1:B:117:HIS:N | 2.50 | 0.42 |
| 1:D:136:LYS:CD | 1:D:138:ASN:H | 2.32 | 0.42 |
| 1:A:23:GLY:CA | 1:C:36:LYS:HB2 | 2.48 | 0.42 |
| 1:A:329:PHE:CD2 | 1:A:340:SER:HB3 | 2.54 | 0.42 |
| 1:B:136:LYS:O | 1:B:137:GLU:CB | 2.68 | 0.42 |
| 1:C:195:ASP:O | 1:C:218:THR:HG22 | 2.18 | 0.42 |
| 1:C:283:TYR:C | 1:C:285:GLY:H | 2.23 | 0.42 |
| 1:C:331:LEU:HD11 | 1:C:348:MET:CE | 2.49 | 0.42 |
| 1:D:99:ILE:O | 1:D:102:VAL:CG2 | 2.64 | 0.42 |
| 1:D:359:GLU:OE1 | 1:D:364:PHE:CD2 | 2.72 | 0.42 |
| 1:A:72:TYR:HD1 | 1:A:218:THR:O | 2.02 | 0.42 |
| 1:A:106:THR:O | 1:A:107:HIS:C | 2.58 | 0.42 |
| 1:A:294:VAL:HA | 1:A:297:LYS:CG | 2.49 | 0.42 |
| 1:A:323:ALA:HA | 1:A:342:LEU:HD11 | 2.01 | 0.42 |
| 1:B:12:ALA:CA | 1:B:67:LEU:HD21 | 2.50 | 0.42 |
| 1:B:75:ALA:CA | 1:B:215:VAL:HG12 | 2.49 | 0.42 |
| 1:B:106:THR:O | 1:B:107:HIS:C | 2.57 | 0.42 |
| 1:B:294:VAL:HA | 1:B:297:LYS:HG3 | 2.01 | 0.42 |
| 1:C:145:GLU:O | 1:C:146:THR:C | 2.56 | 0.42 |
| 1:C:173:VAL:O | 1:C:173:VAL:HG12 | 2.20 | 0.42 |
| 1:C:271:LEU:HD21 | 1:C:384:ILE:HG21 | 2.01 | 0.42 |
| 1:D:51:ARG:HG3 | 1:D:237:ILE:CD1 | 2.44 | 0.42 |
| 1:A:95:HIS:HB3 | 1:A:139:THR:CA | 2.49 | 0.42 |
| 1:B:123:PHE:CD1 | 1:B:123:PHE:N | 2.88 | 0.42 |
| 1:B:190:LEU:CD2 | 1:B:197:VAL:HG22 | 2.49 | 0.42 |
| 2:B:400:PLP:H6 | 3:B:409:HOH:O | 2.20 | 0.42 |
| 1:C:121:THR:HB | 3:C:426:HOH:O | 2.19 | 0.42 |
| 1:D:364:PHE:HD2 | 1:D:364:PHE:HA | 1.75 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:334:SER:HB2 | 1:B:34:THR:HG23 | 2.01 | 0.42 |
| 1:A:338:ILE:HD13 | 1:A:338:ILE:HG21 | 1.86 | 0.42 |
| 1:B:17:GLU:OE1 | 1:D:36:LYS:NZ | 2.50 | 0.42 |
| 1:B:96:ALA:HB1 | 1:B:141:LEU:HB3 | 2.01 | 0.42 |
| 1:C:287:LYS:HA | 1:C:292:TYR:CD1 | 2.55 | 0.42 |
| 1:D:91:PRO:O | 1:D:94:SER:OG | 2.33 | 0.42 |
| 1:D:160:VAL:O | 1:D:164:ILE:HG13 | 2.19 | 0.42 |
| 1:A:136:LYS:CG | 1:A:137:GLU:N | 2.73 | 0.42 |
| 1:A:312:ILE:HD12 | 1:A:318:ALA:HB1 | 2.01 | 0.42 |
| 1:B:134:LEU:C | 1:B:136:LYS:N | 2.72 | 0.42 |
| 1:D:104:GLY:O | 1:D:107:HIS:HB3 | 2.20 | 0.42 |
| 1:D:136:LYS:HZ1 | 1:D:138:ASN:HA | 1.84 | 0.42 |
| 1:D:204:TYR:CZ | 1:D:336:GLY:CA | 3.03 | 0.42 |
| 1:A:18:HIS:CB | 1:A:27:GLU:HG3 | 2.50 | 0.42 |
| 1:A:88:GLN:HG3 | 1:A:230:LEU:HD22 | 2.01 | 0.42 |
| 1:A:146:THR:CB | 1:A:147:PRO:CD | 2.98 | 0.42 |
| 1:A:182:LEU:HD22 | 1:A:186:ILE:HG21 | 2.01 | 0.42 |
| 1:C:54:ASN:ND2 | 1:C:56:ASN:H | 2.17 | 0.42 |
| 1:C:331:LEU:O | 1:C:332:ALA:HB2 | 2.20 | 0.42 |
| 1:C:375:GLU:HB2 | 1:C:380:LEU:HD11 | 2.01 | 0.42 |
| 1:C:389:LYS:O | 1:C:390:GLN:C | 2.57 | 0.42 |
| 1:D:105:GLY:O | 1:D:106:THR:C | 2.57 | 0.42 |
| 1:A:18:HIS:CG | 1:A:27:GLU:HG3 | 2.54 | 0.42 |
| 1:A:21:VAL:O | 1:C:44:ILE:O | 2.38 | 0.42 |
| 1:A:354:PRO:C | 1:A:356:GLU:N | 2.73 | 0.42 |
| 1:B:47:TYR:HE1 | 1:D:22:HIS:HD2 | 1.67 | 0.42 |
| 1:B:113:VAL:C | 1:B:115:ASN:H | 2.23 | 0.42 |
| 1:B:203:LYS:HD2 | 1:B:203:LYS:N | 2.34 | 0.42 |
| 1:B:310:PHE:HE1 | 1:B:312:ILE:HG23 | 1.85 | 0.42 |
| 1:B:344:VAL:HB | 1:B:347:VAL:HG22 | 2.02 | 0.42 |
| 1:C:150:PRO:HB3 | 1:C:369:ARG:CD | 2.50 | 0.42 |
| 1:D:21:VAL:O | 1:D:21:VAL:CG1 | 2.67 | 0.42 |
| 1:A:274:ASP:O | 1:A:275:LYS:C | 2.58 | 0.42 |
| 1:C:26:ILE:HD13 | 1:C:26:ILE:HA | 1.81 | 0.42 |
| 1:C:72:TYR:HD1 | 1:C:218:THR:O | 2.03 | 0.42 |
| 1:C:331:LEU:HD21 | 1:D:40:PRO:CA | 2.49 | 0.42 |
| 1:D:289:HIS:CD2 | 1:D:291:ASN:H | 2.38 | 0.42 |
| 1:A:98:SER:HA | 1:A:143:TRP:O | 2.20 | 0.42 |
| 1:A:137:GLU:O | 1:A:137:GLU:CG | 2.68 | 0.42 |
| 1:A:228:GLN:O | 1:A:231:GLN:HB3 | 2.20 | 0.42 |
| 1:B:135:ILE:HG21 | 1:B:168:ALA:HB2 | 2.02 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:135:ILE:CG2 | 1:B:168:ALA:HB2 | 2.50 | 0.42 |
| 1:C:333:GLU:O | 1:C:334:SER:HB3 | 2.20 | 0.42 |
| 1:D:311:ARG:NH1 | 1:D:364:PHE:CD1 | 2.88 | 0.42 |
| 1:B:248:ARG:NH1 | 1:C:248:ARG:HH11 | 2.18 | 0.41 |
| 1:C:88:GLN:HG3 | 1:C:230:LEU:HD13 | 2.02 | 0.41 |
| 1:D:168:ALA:O | 1:D:171:GLN:HG2 | 2.19 | 0.41 |
| 1:A:114:ALA:O | 1:A:115:ASN:C | 2.59 | 0.41 |
| 1:A:311:ARG:HH11 | 1:A:311:ARG:CB | 2.32 | 0.41 |
| 1:B:334:SER:C | 1:B:335:LEU:HD23 | 2.41 | 0.41 |
| 1:C:42:ASN:HA | 1:C:43:PRO:HD3 | 1.71 | 0.41 |
| 1:D:340:SER:C | 1:D:341:LEU:HD23 | 2.40 | 0.41 |
| 1:A:70:ALA:HB2 | 1:A:190:LEU:HD12 | 2.02 | 0.41 |
| 1:A:286:LEU:O | 1:A:289:HIS:N | 2.49 | 0.41 |
| 1:B:91:PRO:O | 1:B:92:GLN:C | 2.59 | 0.41 |
| 1:B:385:LYS:C | 1:B:387:ALA:N | 2.72 | 0.41 |
| 1:C:226:ARG:O | 1:C:229:PHE:HB3 | 2.20 | 0.41 |
| 1:D:343:GLU:HG2 | 1:D:344:VAL:N | 2.36 | 0.41 |
| 1:A:37:GLN:CB | 1:A:43:PRO:HA | 2.51 | 0.41 |
| 1:A:154:VAL:HB | 1:A:291:ASN:HB2 | 2.02 | 0.41 |
| 1:A:293:ASP:O | 1:A:297:LYS:HG2 | 2.20 | 0.41 |
| 1:A:317:GLU:O | 1:A:318:ALA:C | 2.58 | 0.41 |
| 1:B:8:PHE:CD2 | 1:B:8:PHE:C | 2.94 | 0.41 |
| 1:C:250:LEU:C | 1:C:250:LEU:HD23 | 2.41 | 0.41 |
| 1:A:30:SER:HB2 | 1:A:55:PRO:HG2 | 2.02 | 0.41 |
| 1:A:53:GLN:OE1 | 1:A:58:GLU:HB2 | 2.20 | 0.41 |
| 1:A:264:ALA:CA | 1:A:308:ILE:HD11 | 2.50 | 0.41 |
| 1:A:274:ASP:OD1 | 1:A:277:ASN:N | 2.53 | 0.41 |
| 1:B:101:ASP:CB | 1:B:148:THR:HB | 2.51 | 0.41 |
| 1:B:203:LYS:HG2 | 1:B:335:LEU:HG | 2.01 | 0.41 |
| 1:C:1:THR:CG2 | 1:C:2:LEU:N | 2.83 | 0.41 |
| 1:C:114:ALA:CB | 1:C:119:VAL:N | 2.78 | 0.41 |
| 1:C:156:ASP:HB3 | 1:C:159:LYS:HB2 | 2.01 | 0.41 |
| 1:C:331:LEU:HD21 | 1:D:40:PRO:CD | 2.51 | 0.41 |
| 1:C:386:GLN:N | 3:C:472:HOH:O | 2.53 | 0.41 |
| 1:D:120:GLU:HA | 3:D:424:HOH:O | 2.21 | 0.41 |
| 1:D:121:THR:CG2 | 1:D:123:PHE:CE1 | 3.04 | 0.41 |
| 1:A:33:THR:HG23 | 1:A:49:TYR:HE1 | 1.85 | 0.41 |
| 1:B:144:ILE:HB | 1:B:177:VAL:HG22 | 2.02 | 0.41 |
| 1:C:182:LEU:HD23 | 1:C:182:LEU:HA | 1.90 | 0.41 |
| 1:D:130:ASP:O | 1:D:134:LEU:HG | 2.20 | 0.41 |
| 1:A:157:ILE:HD13 | 1:A:189:PRO:HB3 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:181:PHE:N | 1:A:181:PHE:CD1 | 2.89 | 0.41 |
| 1:A:344:VAL:N | 1:A:348:MET:HE1 | 2.34 | 0.41 |
| 1:A:380:LEU:O | 1:A:384:ILE:HG12 | 2.20 | 0.41 |
| 1:B:94:SER:O | 1:B:120:GLU:N | 2.45 | 0.41 |
| 1:B:149:ASN:HA | 1:B:150:PRO:HA | 1.81 | 0.41 |
| 1:B:172:ASP:CB | 3:B:448:HOH:O | 2.67 | 0.41 |
| 1:B:175:LEU:HD23 | 1:B:193:GLY:O | 2.21 | 0.41 |
| 1:B:189:PRO:HB2 | 1:B:197:VAL:HG13 | 2.01 | 0.41 |
| 1:B:242:ASP:O | 1:B:246:THR:OG1 | 2.25 | 0.41 |
| 1:B:358:ARG:NH1 | 1:B:358:ARG:HB2 | 2.35 | 0.41 |
| 1:C:33:THR:HG22 | 1:C:34:THR:N | 2.35 | 0.41 |
| 1:C:115:ASN:OD1 | 1:D:88:GLN:HA | 2.20 | 0.41 |
| 1:C:294:VAL:HA | 1:C:297:LYS:HG3 | 2.02 | 0.41 |
| 1:D:134:LEU:O | 1:D:136:LYS:O | 2.39 | 0.41 |
| 1:A:6:ASP:OD1 | 1:D:327:ARG:NH2 | 2.43 | 0.41 |
| 1:A:95:HIS:O | 1:A:140:LYS:N | 2.47 | 0.41 |
| 1:A:258:ARG:O | 1:A:262:LEU:HG | 2.21 | 0.41 |
| 1:A:348:MET:SD | 1:B:40:PRO:HA | 2.60 | 0.41 |
| 1:B:143:TRP:CE3 | 1:B:176:VAL:HG11 | 2.56 | 0.41 |
| 1:B:358:ARG:O | 1:B:359:GLU:HG2 | 2.21 | 0.41 |
| 1:C:135:ILE:C | 1:C:139:THR:HG21 | 2.40 | 0.41 |
| 1:C:280:ALA:CB | 1:C:311:ARG:HD3 | 2.48 | 0.41 |
| 1:D:100:GLY:O | 1:D:102:VAL:N | 2.54 | 0.41 |
| 1:D:221:LYS:HE2 | 1:D:225:GLU:OE2 | 2.20 | 0.41 |
| 1:A:35:PHE:CD2 | 1:C:22:HIS:HB3 | 2.56 | 0.41 |
| 1:A:357:ALA:C | 1:A:359:GLU:H | 2.22 | 0.41 |
| 1:B:72:TYR:CD2 | 1:B:224:TYR:CD2 | 3.08 | 0.41 |
| 1:B:345:PRO:O | 1:B:350:HIS:N | 2.54 | 0.41 |
| 1:C:220:ASN:ND2 | 1:C:223:LEU:H | 2.19 | 0.41 |
| 1:C:332:ALA:HA | 1:D:37:GLN:HG3 | 2.02 | 0.41 |
| 1:C:386:GLN:O | 1:C:386:GLN:CD | 2.59 | 0.41 |
| 1:D:228:GLN:O | 1:D:231:GLN:HB3 | 2.21 | 0.41 |
| 1:D:265:ASN:HA | 1:D:283:TYR:CE2 | 2.56 | 0.41 |
| 1:D:335:LEU:CG | 1:D:336:GLY:N | 2.83 | 0.41 |
| 1:A:211:VAL:CG2 | 1:A:245:LEU:HD23 | 2.51 | 0.41 |
| 1:A:355:LYS:O | 1:A:356:GLU:C | 2.60 | 0.41 |
| 1:B:146:THR:CB | 1:B:147:PRO:CD | 2.99 | 0.41 |
| 1:B:208:HIS:CE1 | 1:B:338:ILE:CD1 | 3.03 | 0.41 |
| 1:D:106:THR:OG1 | 1:D:107:HIS:N | 2.53 | 0.41 |
| 1:D:123:PHE:HD1 | 1:D:123:PHE:H | 1.68 | 0.41 |
| 1:A:57:ARG:O | 1:A:60:LEU:HB3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:99:ILE:HG22 | 1:A:100:GLY:N | 2.36 | 0.40 |
| 1:A:131:LEU:O | 1:A:135:ILE:N | 2.49 | 0.40 |
| 1:B:187:SER:C | 1:B:188:ASN:ND2 | 2.74 | 0.40 |
| 1:B:330:THR:HB | 1:B:341:LEU:CD2 | 2.50 | 0.40 |
| 1:B:343:GLU:CG | 1:B:344:VAL:N | 2.84 | 0.40 |
| 1:C:208:HIS:CE1 | 1:C:338:ILE:HD12 | 2.57 | 0.40 |
| 1:C:355:LYS:HA | 1:C:358:ARG:CZ | 2.52 | 0.40 |
| 1:D:301:ASP:O | 1:D:302:ALA:HB3 | 2.20 | 0.40 |
| 1:D:329:PHE:CZ | 1:D:384:ILE:HD11 | 2.56 | 0.40 |
| 1:A:53:GLN:NE2 | 1:A:58:GLU:HG3 | 2.36 | 0.40 |
| 1:A:360:ALA:C | 1:A:362:GLY:N | 2.74 | 0.40 |
| 1:A:369:ARG:HG2 | 1:A:369:ARG:NH1 | 2.36 | 0.40 |
| 1:B:53:GLN:HA | 1:B:57:ARG:NH2 | 2.36 | 0.40 |
| 1:B:95:HIS:NE2 | 1:B:122:SER:OG | 2.55 | 0.40 |
| 1:B:208:HIS:CD2 | 1:B:208:HIS:N | 2.90 | 0.40 |
| 1:C:83:THR:O | 1:C:86:ILE:HB | 2.20 | 0.40 |
| 1:C:125:ASN:OD1 | 1:C:126:ASP:N | 2.55 | 0.40 |
| 1:C:190:LEU:C | 1:C:192:PHE:H | 2.24 | 0.40 |
| 1:A:89:SER:HA | 1:A:230:LEU:HD11 | 2.03 | 0.40 |
| 1:B:139:THR:C | 1:B:140:LYS:HG2 | 2.42 | 0.40 |
| 1:C:260:ALA:CB | 3:C:470:HOH:O | 2.68 | 0.40 |
| 1:D:137:GLU:O | 1:D:137:GLU:CG | 2.68 | 0.40 |
| 1:A:300:ARG:C | 1:A:302:ALA:H | 2.23 | 0.40 |
| 1:B:136:LYS:HA | 1:B:136:LYS:HD2 | 1.90 | 0.40 |
| 1:C:72:TYR:HB3 | 1:C:224:TYR:CD1 | 2.57 | 0.40 |
| 1:C:349:THR:CG2 | 1:C:350:HIS:N | 2.76 | 0.40 |
| 1:D:184:PRO:HD3 | 1:D:199:HIS:CE1 | 2.55 | 0.40 |
| 1:A:81:ALA:CA | 1:B:234:ILE:O | 2.69 | 0.40 |
| 1:A:101:ASP:HB2 | 1:A:148:THR:HB | 2.01 | 0.40 |
| 1:A:229:PHE:O | 1:A:230:LEU:C | 2.60 | 0.40 |
| 1:B:254:HIS:CD2 | 1:B:254:HIS:H | 2.39 | 0.40 |
| 1:C:112:LYS:C | 1:C:114:ALA:N | 2.75 | 0.40 |
| 1:D:52:SER:O | 1:D:53:GLN:HB2 | 2.21 | 0.40 |
| 1:D:99:ILE:HA | 1:D:124:THR:O | 2.21 | 0.40 |
| 1:D:101:ASP:HB2 | 1:D:148:THR:HB | 2.04 | 0.40 |
| 1:D:154:VAL:HG12 | 1:D:294:VAL:CG1 | 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 | 391/393 (100%) | 304 (78%) | 63 (16%) | 24 (6%) | 1 | 1 |
| 1 | B | 391/393 (100%) | 294 (75%) | 63 (16%) | 34 (9%) | 1 | 0 |
| 1 | C | 391/393 (100%) | 310 (79%) | 51 (13%) | 30 (8%) | 1 | 1 |
| 1 | D | 391/393 (100%) | 302 (77%) | 57 (15%) | 32 (8%) | 1 | 1 |
| All | All | 1564/1572 (100%) | 1210 (77%) | 234 (15%) | 120 (8%) | 1 | 1 |

All (120) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 43 | PRO |
| 1 | A | 46 | THR |
| 1 | A | 135 | ILE |
| 1 | A | 137 | GLU |
| 1 | A | 138 | ASN |
| 1 | A | 316 | ALA |
| 1 | B | 46 | THR |
| 1 | B | 101 | ASP |
| 1 | B | 137 | GLU |
| 1 | B | 168 | ALA |
| 1 | B | 316 | ALA |
| 1 | B | 336 | GLY |
| 1 | B | 350 | HIS |
| 1 | C | 43 | PRO |
| 1 | C | 46 | THR |
| 1 | C | 101 | ASP |
| 1 | C | 135 | ILE |
| 1 | C | 137 | GLU |
| 1 | C | 276 | GLU |
| 1 | C | 279 | VAL |
| 1 | C | 316 | ALA |
| 1 | C | 350 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 363 | VAL |
| 1 | D | 46 | THR |
| 1 | D | 108 | ARG |
| 1 | D | 137 | GLU |
| 1 | D | 138 | ASN |
| 1 | D | 168 | ALA |
| 1 | D | 316 | ALA |
| 1 | D | 347 | VAL |
| 1 | D | 350 | HIS |
| 1 | D | 363 | VAL |
| 1 | A | 53 | GLN |
| 1 | A | 101 | ASP |
| 1 | A | 118 | GLY |
| 1 | A | 191 | ASN |
| 1 | A | 279 | VAL |
| 1 | A | 313 | LYS |
| 1 | A | 363 | VAL |
| 1 | B | 108 | ARG |
| 1 | B | 135 | ILE |
| 1 | B | 138 | ASN |
| 1 | B | 209 | SER |
| 1 | B | 279 | VAL |
| 1 | B | 335 | LEU |
| 1 | B | 347 | VAL |
| 1 | B | 352 | GLY |
| 1 | B | 358 | ARG |
| 1 | B | 363 | VAL |
| 1 | C | 53 | GLN |
| 1 | C | 108 | ARG |
| 1 | C | 138 | ASN |
| 1 | C | 146 | THR |
| 1 | C | 203 | LYS |
| 1 | C | 332 | ALA |
| 1 | C | 352 | GLY |
| 1 | D | 101 | ASP |
| 1 | D | 117 | HIS |
| 1 | D | 135 | ILE |
| 1 | D | 323 | ALA |
| 1 | D | 335 | LEU |
| 1 | D | 336 | GLY |
| 1 | D | 355 | LYS |
| 1 | D | 359 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 386 | GLN |
| 1 | A | 146 | THR |
| 1 | A | 168 | ALA |
| 1 | A | 287 | LYS |
| 1 | A | 358 | ARG |
| 1 | B | 43 | PRO |
| 1 | B | 92 | GLN |
| 1 | B | 172 | ASP |
| 1 | B | 332 | ALA |
| 1 | B | 386 | GLN |
| 1 | C | 349 | THR |
| 1 | C | 386 | GLN |
| 1 | D | 334 | SER |
| 1 | D | 352 | GLY |
| 1 | A | 107 | HIS |
| 1 | A | 108 | ARG |
| 1 | A | 203 | LYS |
| 1 | A | 276 | GLU |
| 1 | A | 301 | ASP |
| 1 | A | 359 | GLU |
| 1 | B | 107 | HIS |
| 1 | B | 115 | ASN |
| 1 | B | 276 | GLU |
| 1 | C | 126 | ASP |
| 1 | C | 163 | LEU |
| 1 | C | 168 | ALA |
| 1 | C | 313 | LYS |
| 1 | D | 115 | ASN |
| 1 | D | 128 | LEU |
| 1 | D | 301 | ASP |
| 1 | D | 332 | ALA |
| 1 | A | 275 | LYS |
| 1 | B | 146 | THR |
| 1 | B | 167 | HIS |
| 1 | B | 301 | ASP |
| 1 | B | 355 | LYS |
| 1 | B | 359 | GLU |
| 1 | C | 50 | SER |
| 1 | C | 183 | SER |
| 1 | D | 50 | SER |
| 1 | D | 276 | GLU |
| 1 | D | 349 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 358 | ARG |
| 1 | B | 53 | GLN |
| 1 | B | 334 | SER |
| 1 | C | 193 | GLY |
| 1 | C | 205 | ILE |
| 1 | C | 284 | PRO |
| 1 | C | 347 | VAL |
| 1 | D | 348 | MET |
| 1 | B | 284 | PRO |
| 1 | C | 118 | GLY |
| 1 | D | 118 | GLY |
| 1 | D | 93 | GLY |
| 1 | D | 279 | VAL |
| 1 | B | 193 | GLY |

### 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 | 318/324 (98%) | 295 (93%) | 23 (7%) | 14 29 |
| 1 | B | 318/324 (98%) | 288 (91%) | 30 (9%) | 8 17 |
| 1 | C | 318/324 (98%) | 297 (93%) | 21 (7%) | 16 33 |
| 1 | D | 318/324 (98%) | 299 (94%) | 19 (6%) | 19 39 |
| All | All | 1272/1296 (98%) | 1179 (93%) | 93 (7%) | 14 28 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1 | THR |
| 1 | A | 40 | PRO |
| 1 | A | 54 | ASN |
| 1 | A | 103 | TYR |
| 1 | A | 117 | HIS |
| 1 | A | 135 | ILE |
| 1 | A | 139 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 150 | PRO |
| 1 | A | 197 | VAL |
| 1 | A | 216 | LEU |
| 1 | A | 220 | ASN |
| 1 | A | 227 | LEU |
| 1 | A | 239 | SER |
| 1 | A | 247 | HIS |
| 1 | A | 250 | LEU |
| 1 | A | 277 | ASN |
| 1 | A | 290 | PRO |
| 1 | A | 311 | ARG |
| 1 | A | 312 | ILE |
| 1 | A | 335 | LEU |
| 1 | A | 339 | GLU |
| 1 | A | 342 | LEU |
| 1 | A | 343 | GLU |
| 1 | B | 21 | VAL |
| 1 | B | 33 | THR |
| 1 | B | 34 | THR |
| 1 | B | 60 | LEU |
| 1 | B | 77 | SER |
| 1 | B | 103 | TYR |
| 1 | B | 117 | HIS |
| 1 | B | 123 | PHE |
| 1 | B | 130 | ASP |
| 1 | B | 134 | LEU |
| 1 | B | 135 | ILE |
| 1 | B | 139 | THR |
| 1 | B | 146 | THR |
| 1 | B | 150 | PRO |
| 1 | B | 171 | GLN |
| 1 | B | 197 | VAL |
| 1 | B | 216 | LEU |
| 1 | B | 220 | ASN |
| 1 | B | 227 | LEU |
| 1 | B | 239 | SER |
| 1 | B | 247 | HIS |
| 1 | B | 250 | LEU |
| 1 | B | 277 | ASN |
| 1 | B | 290 | PRO |
| 1 | B | 312 | ILE |
| 1 | B | 320 | SER |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 335 | LEU |
| 1 | B | 339 | GLU |
| 1 | B | 342 | LEU |
| 1 | B | 343 | GLU |
| 1 | C | 34 | THR |
| 1 | C | 103 | TYR |
| 1 | C | 117 | HIS |
| 1 | C | 135 | ILE |
| 1 | C | 139 | THR |
| 1 | C | 197 | VAL |
| 1 | C | 216 | LEU |
| 1 | C | 220 | ASN |
| 1 | C | 227 | LEU |
| 1 | C | 247 | HIS |
| 1 | C | 250 | LEU |
| 1 | C | 277 | ASN |
| 1 | C | 290 | PRO |
| 1 | C | 311 | ARG |
| 1 | C | 312 | ILE |
| 1 | C | 320 | SER |
| 1 | C | 339 | GLU |
| 1 | C | 342 | LEU |
| 1 | C | 343 | GLU |
| 1 | C | 354 | PRO |
| 1 | C | 369 | ARG |
| 1 | D | 33 | THR |
| 1 | D | 34 | THR |
| 1 | D | 103 | TYR |
| 1 | D | 117 | HIS |
| 1 | D | 135 | ILE |
| 1 | D | 139 | THR |
| 1 | D | 150 | PRO |
| 1 | D | 197 | VAL |
| 1 | D | 216 | LEU |
| 1 | D | 220 | ASN |
| 1 | D | 227 | LEU |
| 1 | D | 252 | THR |
| 1 | D | 277 | ASN |
| 1 | D | 312 | ILE |
| 1 | D | 335 | LEU |
| 1 | D | 342 | LEU |
| 1 | D | 343 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 354 | PRO |
| 1 | D | 364 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 3 | GLN |
| 1 | A | 37 | GLN |
| 1 | A | 54 | ASN |
| 1 | A | 158 | GLN |
| 1 | A | 179 | ASN |
| 1 | A | 188 | ASN |
| 1 | A | 208 | HIS |
| 1 | A | 219 | ASN |
| 1 | A | 220 | ASN |
| 1 | A | 231 | GLN |
| 1 | A | 254 | HIS |
| 1 | A | 277 | ASN |
| 1 | A | 289 | HIS |
| 1 | A | 350 | HIS |
| 1 | B | 3 | GLN |
| 1 | B | 37 | GLN |
| 1 | B | 179 | ASN |
| 1 | B | 188 | ASN |
| 1 | B | 206 | ASN |
| 1 | B | 208 | HIS |
| 1 | B | 219 | ASN |
| 1 | B | 220 | ASN |
| 1 | B | 231 | GLN |
| 1 | B | 254 | HIS |
| 1 | B | 277 | ASN |
| 1 | B | 350 | HIS |
| 1 | C | 3 | GLN |
| 1 | C | 37 | GLN |
| 1 | C | 53 | GLN |
| 1 | C | 54 | ASN |
| 1 | C | 69 | ASN |
| 1 | C | 115 | ASN |
| 1 | C | 129 | ASN |
| 1 | C | 158 | GLN |
| 1 | C | 188 | ASN |
| 1 | C | 191 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 206 | ASN |
| 1 | C | 208 | HIS |
| 1 | C | 219 | ASN |
| 1 | C | 220 | ASN |
| 1 | C | 231 | GLN |
| 1 | C | 277 | ASN |
| 1 | C | 282 | ASN |
| 1 | C | 350 | HIS |
| 1 | D | 3 | GLN |
| 1 | D | 22 | HIS |
| 1 | D | 37 | GLN |
| 1 | D | 179 | ASN |
| 1 | D | 188 | ASN |
| 1 | D | 208 | HIS |
| 1 | D | 219 | ASN |
| 1 | D | 220 | ASN |
| 1 | D | 231 | GLN |
| 1 | D | 247 | HIS |
| 1 | D | 254 | HIS |
| 1 | D | 277 | ASN |
| 1 | D | 282 | ASN |
| 1 | D | 289 | HIS |
| 1 | D | 291 | ASN |
| 1 | D | 350 | HIS |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 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 | PLP | B | 400 | 1 | 15,15,16 | 3.71 | 6 (40%) | 20,22,23 | 2.59 | 7 (35%) |
| 2 | PLP | A | 400 | 1 | 15,15,16 | 3.37 | 4 (26%) | 20,22,23 | 2.45 | 8 (40%) |
| 2 | PLP | C | 400 | 1 | 15,15,16 | 3.46 | 4 (26%) | 20,22,23 | 2.63 | 9 (45%) |
| 2 | PLP | D | 400 | 1 | 15,15,16 | 3.74 | 7 (46%) | 20,22,23 | 2.51 | 9 (45%) |

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 | PLP | B | 400 | 1 | - | 1/6/6/8 | 0/1/1/1 |
| 2 | PLP | A | 400 | 1 | - | 2/6/6/8 | 0/1/1/1 |
| 2 | PLP | C | 400 | 1 | - | 1/6/6/8 | 0/1/1/1 |
| 2 | PLP | D | 400 | 1 | - | 0/6/6/8 | 0/1/1/1 |

All (21) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | D | 400 | PLP | C5-C4 | 10.95 | 1.52 | 1.40 |
| 2 | B | 400 | PLP | C5-C4 | 10.19 | 1.51 | 1.40 |
| 2 | C | 400 | PLP | C3-C2 | 9.05 | 1.50 | 1.40 |
| 2 | A | 400 | PLP | C3-C2 | 8.76 | 1.49 | 1.40 |
| 2 | B | 400 | PLP | C3-C2 | 8.30 | 1.49 | 1.40 |
| 2 | C | 400 | PLP | C5-C4 | 8.29 | 1.49 | 1.40 |
| 2 | A | 400 | PLP | C5-C4 | 8.15 | 1.49 | 1.40 |
| 2 | D | 400 | PLP | C3-C2 | 6.87 | 1.47 | 1.40 |
| 2 | D | 400 | PLP | C2-N1 | 3.76 | 1.40 | 1.33 |
| 2 | C | 400 | PLP | C2-N1 | 2.93 | 1.39 | 1.33 |
| 2 | B | 400 | PLP | C2-N1 | 2.86 | 1.39 | 1.33 |
| 2 | D | 400 | PLP | P-O3P | -2.74 | 1.44 | 1.54 |
| 2 | C | 400 | PLP | P-O4P | -2.58 | 1.51 | 1.60 |
| 2 | D | 400 | PLP | C6-N1 | 2.47 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 400 | PLP | C5A-C5 | 2.46 | 1.57 | 1.50 |
| 2 | B | 400 | PLP | C4A-C4 | -2.42 | 1.46 | 1.51 |
| 2 | A | 400 | PLP | C2-N1 | 2.39 | 1.38 | 1.33 |
| 2 | A | 400 | PLP | P-O3P | -2.31 | 1.45 | 1.54 |
| 2 | B | 400 | PLP | P-O3P | -2.20 | 1.46 | 1.54 |
| 2 | D | 400 | PLP | C3-C4 | 2.11 | 1.44 | 1.40 |
| 2 | D | 400 | PLP | C5A-C5 | 2.04 | 1.56 | 1.50 |

All (33) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 400 | PLP | C2A-C2-C3 | 7.84 | 130.57 | 120.89 |
| 2 | C | 400 | PLP | C2A-C2-C3 | 6.58 | 129.01 | 120.89 |
| 2 | A | 400 | PLP | C2A-C2-C3 | 6.23 | 128.59 | 120.89 |
| 2 | D | 400 | PLP | C2A-C2-C3 | 6.08 | 128.40 | 120.89 |
| 2 | B | 400 | PLP | C6-N1-C2 | 4.04 | 126.65 | 119.17 |
| 2 | D | 400 | PLP | O3-C3-C4 | 3.81 | 128.13 | 118.10 |
| 2 | C | 400 | PLP | O2P-P-O4P | -3.80 | 96.63 | 106.73 |
| 2 | D | 400 | PLP | C6-N1-C2 | 3.69 | 126.01 | 119.17 |
| 2 | B | 400 | PLP | C3-C2-N1 | -3.68 | 116.01 | 120.77 |
| 2 | A | 400 | PLP | O3-C3-C4 | 3.54 | 127.43 | 118.10 |
| 2 | C | 400 | PLP | C6-C5-C4 | 3.53 | 120.94 | 118.16 |
| 2 | C | 400 | PLP | C6-N1-C2 | 3.44 | 125.55 | 119.17 |
| 2 | A | 400 | PLP | C6-C5-C4 | 3.41 | 120.84 | 118.16 |
| 2 | A | 400 | PLP | C3-C2-N1 | -3.40 | 116.38 | 120.77 |
| 2 | A | 400 | PLP | C6-N1-C2 | 3.38 | 125.42 | 119.17 |
| 2 | C | 400 | PLP | C3-C2-N1 | -3.29 | 116.51 | 120.77 |
| 2 | C | 400 | PLP | O3-C3-C4 | 3.23 | 126.60 | 118.10 |
| 2 | D | 400 | PLP | C3-C2-N1 | -3.16 | 116.68 | 120.77 |
| 2 | B | 400 | PLP | O3-C3-C4 | 2.98 | 125.96 | 118.10 |
| 2 | B | 400 | PLP | C5-C6-N1 | -2.95 | 118.91 | 123.82 |
| 2 | C | 400 | PLP | C5-C6-N1 | -2.87 | 119.04 | 123.82 |
| 2 | D | 400 | PLP | C5-C6-N1 | -2.86 | 119.06 | 123.82 |
| 2 | D | 400 | PLP | O3-C3-C2 | -2.82 | 111.35 | 117.49 |
| 2 | D | 400 | PLP | O4P-C5A-C5 | 2.82 | 114.72 | 109.35 |
| 2 | C | 400 | PLP | O3P-P-O2P | 2.76 | 118.20 | 107.64 |
| 2 | A | 400 | PLP | O3-C3-C2 | -2.56 | 111.92 | 117.49 |
| 2 | D | 400 | PLP | C6-C5-C4 | 2.54 | 120.15 | 118.16 |
| 2 | A | 400 | PLP | C5-C6-N1 | -2.47 | 119.70 | 123.82 |
| 2 | D | 400 | PLP | O3P-P-O2P | 2.30 | 116.41 | 107.64 |
| 2 | A | 400 | PLP | O4P-C5A-C5 | 2.27 | 113.68 | 109.35 |
| 2 | B | 400 | PLP | C2A-C2-N1 | -2.20 | 113.37 | 117.67 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | B | 400 | PLP | C6-C5-C4 | 2.08 | 119.79 | 118.16 |
| 2 | C | 400 | PLP | O3P-P-O1P | 2.03 | 118.62 | 110.68 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | B | 400 | PLP | C4-C5-C5A-O4P |
| 2 | A | 400 | PLP | C6-C5-C5A-O4P |
| 2 | A | 400 | PLP | C4-C5-C5A-O4P |
| 2 | C | 400 | PLP | C4-C5-C5A-O4P |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 400 | PLP | 1 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | OWAB(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|
| 1 | A | 393/393 (100%) | 0.61 | 47 (11%) | 4 2 | 19, 51, 70, 70 | 0 |
| 1 | B | 393/393 (100%) | 0.83 | 58 (14%) | 2 1 | 20, 54, 70, 70 | 0 |
| 1 | C | 393/393 (100%) | 0.88 | 66 (16%) | 1 1 | 24, 56, 70, 70 | 0 |
| 1 | D | 393/393 (100%) | 0.75 | 53 (13%) | 3 1 | 18, 51, 70, 70 | 0 |
| All | All | 1572/1572 (100%) | 0.77 | 224 (14%) | 2 1 | 18, 53, 70, 70 | 0 |

All (224) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 21 | VAL | 13.1 |
| 1 | C | 39 | SER | 13.0 |
| 1 | D | 103 | TYR | 10.9 |
| 1 | B | 117 | HIS | 10.7 |
| 1 | D | 362 | GLY | 10.5 |
| 1 | D | 115 | ASN | 9.7 |
| 1 | C | 38 | SER | 9.6 |
| 1 | C | 116 | ALA | 9.5 |
| 1 | C | 103 | TYR | 9.4 |
| 1 | A | 46 | THR | 9.2 |
| 1 | A | 33 | THR | 9.0 |
| 1 | B | 118 | GLY | 9.0 |
| 1 | D | 118 | GLY | 8.8 |
| 1 | D | 393 | ASN | 8.8 |
| 1 | A | 352 | GLY | 8.8 |
| 1 | D | 116 | ALA | 8.7 |
| 1 | B | 346 | ALA | 8.5 |
| 1 | D | 364 | PHE | 8.3 |
| 1 | B | 391 | ALA | 8.2 |
| 1 | B | 324 | SER | 8.1 |
| 1 | A | 45 | GLY | 7.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 353 | ILE | 7.7 |
| 1 | B | 323 | ALA | 7.7 |
| 1 | B | 354 | PRO | 7.6 |
| 1 | C | 41 | ALA | 7.6 |
| 1 | C | 110 | PHE | 7.6 |
| 1 | B | 320 | SER | 7.4 |
| 1 | A | 313 | LYS | 7.2 |
| 1 | D | 349 | THR | 7.2 |
| 1 | B | 351 | GLY | 7.2 |
| 1 | A | 116 | ALA | 7.1 |
| 1 | B | 316 | ALA | 7.1 |
| 1 | A | 25 | VAL | 7.0 |
| 1 | C | 115 | ASN | 7.0 |
| 1 | A | 42 | ASN | 6.9 |
| 1 | A | 103 | TYR | 6.9 |
| 1 | D | 350 | HIS | 6.9 |
| 1 | D | 356 | GLU | 6.8 |
| 1 | C | 40 | PRO | 6.7 |
| 1 | C | 101 | ASP | 6.6 |
| 1 | D | 101 | ASP | 6.6 |
| 1 | B | 110 | PHE | 6.6 |
| 1 | B | 349 | THR | 6.6 |
| 1 | B | 101 | ASP | 6.5 |
| 1 | C | 49 | TYR | 6.5 |
| 1 | D | 360 | ALA | 6.4 |
| 1 | A | 43 | PRO | 6.4 |
| 1 | D | 41 | ALA | 6.4 |
| 1 | B | 170 | GLY | 6.4 |
| 1 | B | 115 | ASN | 6.2 |
| 1 | D | 353 | ILE | 6.2 |
| 1 | C | 102 | VAL | 6.1 |
| 1 | D | 114 | ALA | 6.1 |
| 1 | A | 41 | ALA | 6.1 |
| 1 | C | 44 | ILE | 6.1 |
| 1 | D | 117 | HIS | 5.9 |
| 1 | A | 117 | HIS | 5.9 |
| 1 | B | 352 | GLY | 5.9 |
| 1 | B | 393 | ASN | 5.9 |
| 1 | C | 19 | VAL | 5.8 |
| 1 | C | 118 | GLY | 5.8 |
| 1 | D | 336 | GLY | 5.7 |
| 1 | A | 105 | GLY | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 392 | THR | 5.7 |
| 1 | C | 393 | ASN | 5.6 |
| 1 | C | 36 | LYS | 5.6 |
| 1 | D | 317 | GLU | 5.6 |
| 1 | B | 357 | ALA | 5.5 |
| 1 | C | 50 | SER | 5.4 |
| 1 | C | 43 | PRO | 5.4 |
| 1 | D | 391 | ALA | 5.4 |
| 1 | B | 103 | TYR | 5.4 |
| 1 | D | 319 | ALA | 5.4 |
| 1 | C | 124 | THR | 5.2 |
| 1 | C | 37 | GLN | 5.2 |
| 1 | D | 354 | PRO | 5.2 |
| 1 | D | 352 | GLY | 5.2 |
| 1 | D | 102 | VAL | 5.2 |
| 1 | D | 344 | VAL | 5.2 |
| 1 | B | 345 | PRO | 5.2 |
| 1 | B | 350 | HIS | 5.2 |
| 1 | B | 361 | SER | 5.1 |
| 1 | A | 102 | VAL | 5.1 |
| 1 | B | 161 | ALA | 5.1 |
| 1 | D | 320 | SER | 5.0 |
| 1 | B | 116 | ALA | 5.0 |
| 1 | C | 117 | HIS | 5.0 |
| 1 | C | 23 | GLY | 5.0 |
| 1 | C | 46 | THR | 5.0 |
| 1 | B | 319 | ALA | 4.8 |
| 1 | D | 42 | ASN | 4.8 |
| 1 | C | 32 | SER | 4.8 |
| 1 | C | 42 | ASN | 4.7 |
| 1 | B | 102 | VAL | 4.7 |
| 1 | C | 33 | THR | 4.7 |
| 1 | C | 353 | ILE | 4.6 |
| 1 | C | 123 | PHE | 4.6 |
| 1 | D | 361 | SER | 4.6 |
| 1 | C | 352 | GLY | 4.5 |
| 1 | C | 45 | GLY | 4.5 |
| 1 | A | 19 | VAL | 4.4 |
| 1 | A | 38 | SER | 4.4 |
| 1 | A | 44 | ILE | 4.2 |
| 1 | B | 355 | LYS | 4.2 |
| 1 | C | 21 | VAL | 4.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 35 | PHE | 4.1 |
| 1 | A | 118 | GLY | 4.1 |
| 1 | A | 35 | PHE | 4.1 |
| 1 | D | 1 | THR | 4.1 |
| 1 | C | 133 | GLN | 4.0 |
| 1 | D | 100 | GLY | 4.0 |
| 1 | A | 26 | ILE | 4.0 |
| 1 | A | 115 | ASN | 4.0 |
| 1 | A | 37 | GLN | 3.9 |
| 1 | A | 39 | SER | 3.9 |
| 1 | C | 52 | SER | 3.9 |
| 1 | B | 358 | ARG | 3.8 |
| 1 | B | 124 | THR | 3.8 |
| 1 | D | 48 | GLU | 3.8 |
| 1 | B | 390 | GLN | 3.8 |
| 1 | B | 43 | PRO | 3.8 |
| 1 | D | 357 | ALA | 3.8 |
| 1 | B | 344 | VAL | 3.8 |
| 1 | B | 276 | GLU | 3.8 |
| 1 | C | 20 | ASP | 3.7 |
| 1 | C | 22 | HIS | 3.6 |
| 1 | D | 363 | VAL | 3.6 |
| 1 | C | 25 | VAL | 3.6 |
| 1 | D | 345 | PRO | 3.6 |
| 1 | D | 390 | GLN | 3.6 |
| 1 | C | 24 | SER | 3.5 |
| 1 | A | 36 | LYS | 3.5 |
| 1 | C | 275 | LYS | 3.5 |
| 1 | C | 47 | TYR | 3.5 |
| 1 | D | 359 | GLU | 3.5 |
| 1 | C | 170 | GLY | 3.5 |
| 1 | B | 317 | GLU | 3.4 |
| 1 | C | 18 | HIS | 3.4 |
| 1 | C | 2 | LEU | 3.4 |
| 1 | C | 391 | ALA | 3.4 |
| 1 | A | 101 | ASP | 3.4 |
| 1 | B | 280 | ALA | 3.4 |
| 1 | C | 114 | ALA | 3.4 |
| 1 | D | 365 | ASP | 3.4 |
| 1 | A | 18 | HIS | 3.3 |
| 1 | A | 110 | PHE | 3.3 |
| 1 | B | 348 | MET | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 53 | GLN | 3.3 |
| 1 | A | 393 | ASN | 3.3 |
| 1 | B | 107 | HIS | 3.3 |
| 1 | B | 1 | THR | 3.3 |
| 1 | A | 137 | GLU | 3.3 |
| 1 | A | 34 | THR | 3.3 |
| 1 | C | 318 | ALA | 3.2 |
| 1 | A | 58 | GLU | 3.2 |
| 1 | C | 3 | GLN | 3.2 |
| 1 | B | 360 | ALA | 3.2 |
| 1 | A | 3 | GLN | 3.2 |
| 1 | D | 110 | PHE | 3.1 |
| 1 | A | 52 | SER | 3.1 |
| 1 | C | 1 | THR | 3.1 |
| 1 | D | 323 | ALA | 3.1 |
| 1 | B | 171 | GLN | 3.0 |
| 1 | B | 392 | THR | 3.0 |
| 1 | D | 316 | ALA | 3.0 |
| 1 | B | 362 | GLY | 3.0 |
| 1 | C | 319 | ALA | 3.0 |
| 1 | C | 107 | HIS | 3.0 |
| 1 | B | 168 | ALA | 2.9 |
| 1 | D | 123 | PHE | 2.9 |
| 1 | A | 20 | ASP | 2.9 |
| 1 | A | 47 | TYR | 2.9 |
| 1 | A | 123 | PHE | 2.9 |
| 1 | A | 2 | LEU | 2.9 |
| 1 | C | 356 | GLU | 2.9 |
| 1 | C | 392 | THR | 2.9 |
| 1 | D | 124 | THR | 2.9 |
| 1 | A | 32 | SER | 2.9 |
| 1 | A | 1 | THR | 2.9 |
| 1 | D | 351 | GLY | 2.8 |
| 1 | D | 387 | ALA | 2.8 |
| 1 | B | 131 | LEU | 2.8 |
| 1 | C | 105 | GLY | 2.7 |
| 1 | A | 120 | GLU | 2.7 |
| 1 | B | 100 | GLY | 2.7 |
| 1 | B | 266 | LYS | 2.7 |
| 1 | D | 107 | HIS | 2.6 |
| 1 | D | 277 | ASN | 2.5 |
| 1 | D | 132 | PRO | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 22 | HIS | 2.5 |
| 1 | B | 169 | ALA | 2.5 |
| 1 | D | 347 | VAL | 2.5 |
| 1 | B | 343 | GLU | 2.5 |
| 1 | A | 51 | ARG | 2.5 |
| 1 | A | 107 | HIS | 2.5 |
| 1 | C | 88 | GLN | 2.5 |
| 1 | B | 2 | LEU | 2.4 |
| 1 | C | 4 | GLU | 2.4 |
| 1 | D | 3 | GLN | 2.4 |
| 1 | D | 369 | ARG | 2.4 |
| 1 | C | 344 | VAL | 2.4 |
| 1 | B | 99 | ILE | 2.3 |
| 1 | C | 363 | VAL | 2.3 |
| 1 | B | 135 | ILE | 2.3 |
| 1 | B | 3 | GLN | 2.3 |
| 1 | B | 4 | GLU | 2.3 |
| 1 | B | 368 | VAL | 2.3 |
| 1 | D | 22 | HIS | 2.2 |
| 1 | A | 106 | THR | 2.2 |
| 1 | C | 106 | THR | 2.2 |
| 1 | C | 113 | VAL | 2.2 |
| 1 | A | 312 | ILE | 2.2 |
| 1 | A | 370 | ILE | 2.2 |
| 1 | D | 197 | VAL | 2.2 |
| 1 | C | 138 | ASN | 2.2 |
| 1 | C | 313 | LYS | 2.2 |
| 1 | B | 363 | VAL | 2.1 |
| 1 | B | 120 | GLU | 2.1 |
| 1 | D | 146 | THR | 2.1 |
| 1 | C | 108 | ARG | 2.1 |
| 1 | B | 109 | TYR | 2.1 |
| 1 | C | 272 | ALA | 2.0 |
| 1 | C | 360 | ALA | 2.0 |
| 1 | C | 28 | PRO | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 2 | PLP | D | 400 | 15/16 | 0.82 | 0.40 | 47,62,68,70 | 0 |
| 2 | PLP | B | 400 | 15/16 | 0.86 | 0.34 | 51,64,70,70 | 0 |
| 2 | PLP | C | 400 | 15/16 | 0.88 | 0.28 | 35,59,70,70 | 0 |
| 2 | PLP | A | 400 | 15/16 | 0.89 | 0.23 | 38,56,66,70 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.