# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 09:40 am GMT

| | | |
|---|---|---|
| PDB ID | : | 4AEF |
| Title | : | THE CRYSTAL STRUCTURE OF THERMOSTABLE AMYLASE FROM THE PYROCOCCUS |
| Authors | : | Song, H.-N.; Jung, T.-Y.; Yoon, S.-M.; Yang, S.-J.; Park, K.-H.; Woo, E.-J. |
| Deposited on | : | 2012-01-10 |
| Resolution | : | 2.34 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.

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

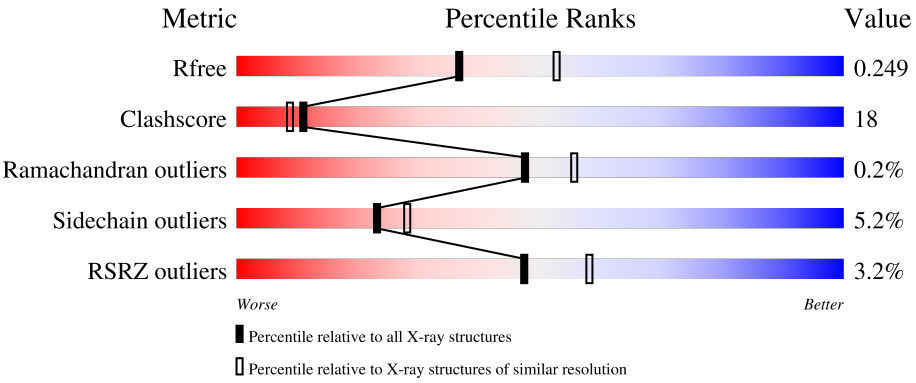
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 2.34 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 | 2096 (2.36-2.32) |
| Clashscore | 141614 | 2193 (2.36-2.32) |
| Ramachandran outliers | 138981 | 2159 (2.36-2.32) |
| Sidechain outliers | 138945 | 2160 (2.36-2.32) |
| RSRZ outliers | 127900 | 2067 (2.36-2.32) |

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 | 645 | 3% 69% 26% |
| 1 | B | 645 | 3% 68% 28% |

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10882 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 NEOPULLULANASE (ALPHA-AMYLASE II).

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 636 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5321 | 3485 | 891 | 929 | 16 | | | |
| 1 | B | 636 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 5321 | 3485 | 891 | 929 | 16 | | | |

- Molecule 2 is water.

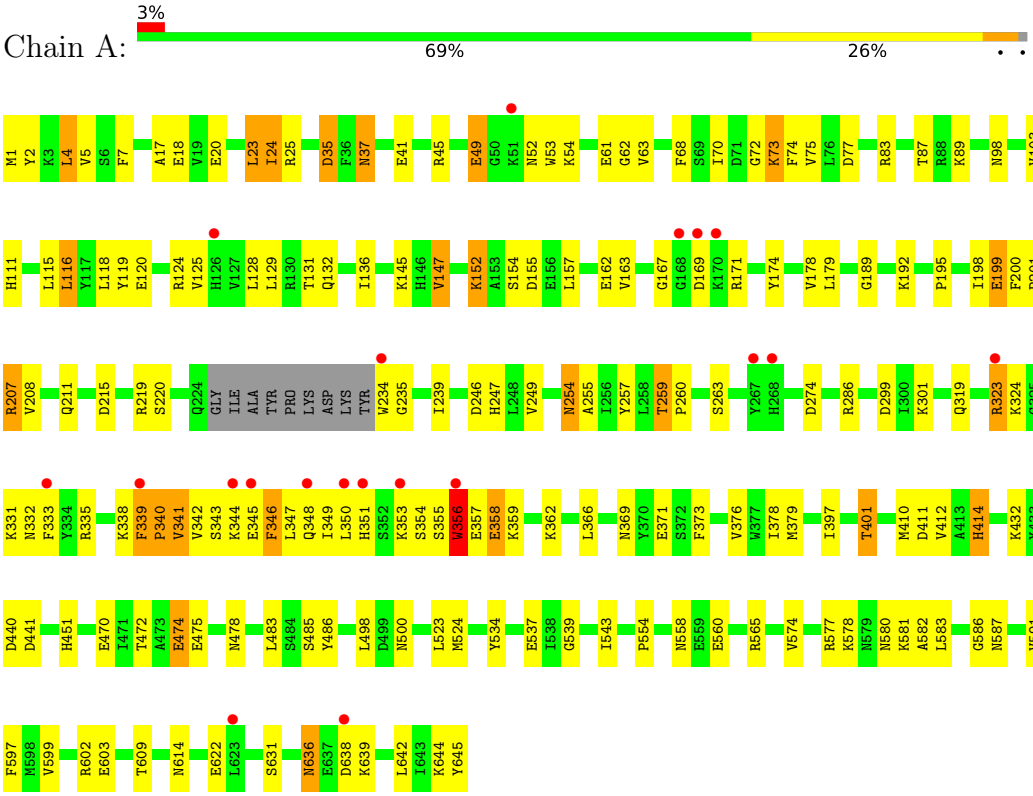
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | A | 124 | Total | O | 0 | 0 |
| | | | 124 | 124 | | |
| 2 | B | 116 | Total | O | 0 | 0 |
| | | | 116 | 116 | | |

# 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.

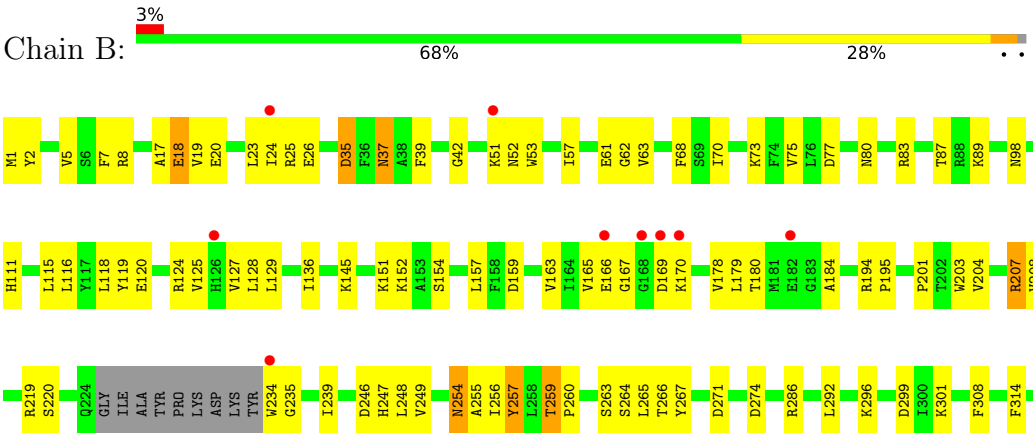
• Molecule 1: NEOPULLULANASE (ALPHA-AMYLASE II)

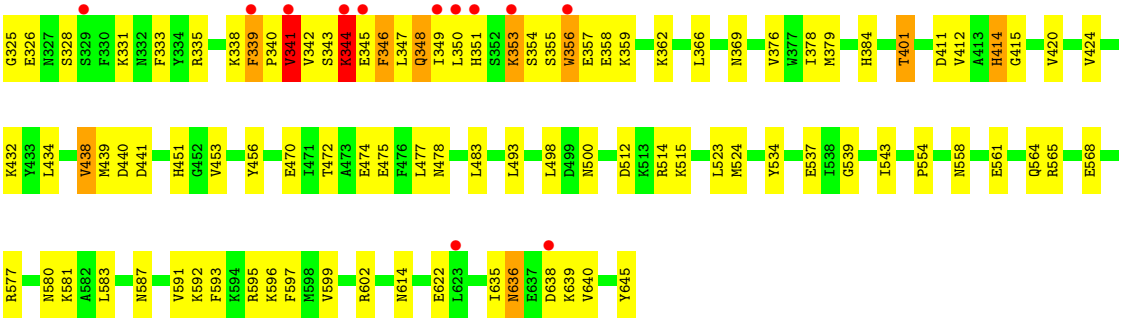
Chain A:




• Molecule 1: NEOPULLULANASE (ALPHA-AMYLASE II)

Chain B:




G325 E326 N327 S328 S329 F330 K331 N332 F333 Y334 R335 K338 F339 P340 V341 V342 S343 K344 E345 F346 L347 Q348 I349 L350 H351 S352 K353 S354 S355 W356 E357 E358 K359 K362 L366 N369 V376 W377 I378 M379 H384 T401 D411 V412 A413 H414 G415 V420 V424
K432 Y433 L434 V438 M439 D440 D441 H451 G452 V453 Y456 E470 I471 T472 A473 E474 E475 F476 L477 N478 L483 L493 L498 D499 N500 D512 K513 R514 K515 L523 M524 Y534 E537 I538 G539 I543 P554 N558 E561 Q564 R565 E568
R577 N580 K581 A582 L583 N587 V591 K592 F593 K594 R595 K596 F597 M598 V599 R602 N614 E622 L623 I635 N636 E637 D638 K639 V640 Y645

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 41 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 150.06Å 150.06Å 67.86Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 29.43 – 2.34<br>47.72 – 2.34 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 95.8 (29.43-2.34)<br>95.8 (47.72-2.34) | Depositor<br>EDS |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 5.99 (at 2.34Å) | Xtriage |
| Refinement program | CNS 1.2 | Depositor |
| R, $R_{free}$ | 0.211 , 0.251<br>0.209 , 0.249 | Depositor<br>DCC |
| $R_{free}$ test set | 3095 reflections (4.86%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 29.1 | Xtriage |
| Anisotropy | 0.294 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.37 , 21.7 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | 0.486 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 10882 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 31.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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

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 | 0.37 | 0/5467 | 0.66 | 5/7365 (0.1%) |
| 1 | B | 0.37 | 0/5467 | 0.63 | 4/7365 (0.1%) |
| All | All | 0.37 | 0/10934 | 0.64 | 9/14730 (0.1%) |

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 49 | GLU | CB-CA-C | 10.52 | 131.44 | 110.40 |
| 1 | A | 340 | PRO | N-CA-C | -9.70 | 86.89 | 112.10 |
| 1 | A | 327 | ASN | CB-CA-C | -6.47 | 97.46 | 110.40 |
| 1 | B | 356 | TRP | N-CA-C | 5.96 | 127.08 | 111.00 |
| 1 | A | 49 | GLU | N-CA-C | -5.79 | 95.37 | 111.00 |
| 1 | A | 356 | TRP | N-CA-C | 5.78 | 126.61 | 111.00 |
| 1 | B | 353 | LYS | N-CA-C | 5.68 | 126.34 | 111.00 |
| 1 | B | 344 | LYS | CB-CA-C | -5.52 | 99.37 | 110.40 |
| 1 | B | 356 | TRP | N-CA-CB | -5.43 | 100.82 | 110.60 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 534 | TYR | Sidechain |
| 1 | B | 534 | TYR | Sidechain |

## 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 | 5321 | 0 | 5297 | 193 | 0 |
| 1 | B | 5321 | 0 | 5297 | 193 | 0 |
| 2 | A | 124 | 0 | 0 | 2 | 0 |
| 2 | B | 116 | 0 | 0 | 3 | 0 |
| All | All | 10882 | 0 | 10594 | 385 | 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 18.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:338:LYS:HB3 | 1:A:369:ASN:HD22 | 1.01 | 1.11 |
| 1:B:340:PRO:O | 1:B:341:VAL:HG23 | 1.58 | 1.02 |
| 1:B:401:THR:HG23 | 1:B:432:LYS:HE3 | 1.42 | 0.99 |
| 1:B:77:ASP:H | 1:B:98:ASN:HD21 | 1.03 | 0.96 |
| 1:A:401:THR:HG23 | 1:A:432:LYS:HE3 | 1.51 | 0.93 |
| 1:A:376:VAL:HG21 | 1:A:379:MET:HE2 | 1.50 | 0.92 |
| 1:B:286:ARG:HH11 | 1:B:286:ARG:HB2 | 1.32 | 0.92 |
| 1:A:77:ASP:H | 1:A:98:ASN:HD21 | 0.98 | 0.92 |
| 1:A:77:ASP:H | 1:A:98:ASN:ND2 | 1.67 | 0.92 |
| 1:B:636:ASN:HD21 | 1:B:639:LYS:HB3 | 1.37 | 0.90 |
| 1:A:338:LYS:HB3 | 1:A:369:ASN:ND2 | 1.86 | 0.88 |
| 1:B:23:LEU:O | 1:B:52:ASN:HB2 | 1.75 | 0.87 |
| 1:B:77:ASP:H | 1:B:98:ASN:ND2 | 1.74 | 0.86 |
| 1:B:342:VAL:HB | 1:B:347:LEU:HD13 | 1.59 | 0.84 |
| 1:A:25:ARG:HB2 | 1:A:52:ASN:HA | 1.58 | 0.84 |
| 1:B:345:GLU:O | 1:B:349:ILE:CG2 | 2.26 | 0.84 |
| 1:A:373:PHE:O | 1:A:376:VAL:HG12 | 1.76 | 0.83 |
| 1:B:434:LEU:H | 1:B:451:HIS:HD2 | 1.27 | 0.82 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:338:LYS:CB | 1:A:369:ASN:HD22 | 1.89 | 0.82 |
| 1:B:286:ARG:HB2 | 1:B:286:ARG:NH1 | 1.95 | 0.81 |
| 1:A:73:LYS:HE2 | 1:A:73:LYS:HA | 1.62 | 0.81 |
| 1:A:319:GLN:O | 1:A:323:ARG:HD2 | 1.81 | 0.81 |
| 1:B:635:ILE:HD12 | 1:B:640:VAL:HG22 | 1.63 | 0.80 |
| 1:B:345:GLU:O | 1:B:349:ILE:HG22 | 1.81 | 0.80 |
| 1:B:564:GLN:O | 1:B:568:GLU:HG3 | 1.81 | 0.79 |
| 1:A:434:LEU:H | 1:A:451:HIS:HD2 | 1.28 | 0.77 |
| 1:A:338:LYS:HG2 | 1:A:340:PRO:HD2 | 1.66 | 0.77 |
| 1:A:580:ASN:HD22 | 1:A:583:LEU:H | 1.32 | 0.77 |
| 1:B:343:SER:HG | 1:B:347:LEU:HB2 | 1.51 | 0.75 |
| 1:A:355:SER:O | 1:A:358:GLU:HG3 | 1.84 | 0.75 |
| 1:B:338:LYS:HG2 | 1:B:340:PRO:HD2 | 1.67 | 0.75 |
| 1:A:259:THR:HG23 | 1:A:260:PRO:HD2 | 1.69 | 0.75 |
| 1:B:580:ASN:HD22 | 1:B:583:LEU:H | 1.34 | 0.75 |
| 1:A:77:ASP:N | 1:A:98:ASN:HD21 | 1.81 | 0.75 |
| 1:A:25:ARG:H | 1:A:52:ASN:HA | 1.53 | 0.73 |
| 1:A:4:LEU:HD13 | 1:A:17:ALA:HB1 | 1.71 | 0.73 |
| 1:B:70:ILE:HG12 | 1:B:75:VAL:HG11 | 1.71 | 0.71 |
| 1:B:259:THR:HG23 | 1:B:260:PRO:HD2 | 1.72 | 0.71 |
| 1:A:286:ARG:HB2 | 1:A:286:ARG:NH1 | 2.05 | 0.71 |
| 1:B:25:ARG:H | 1:B:52:ASN:HA | 1.55 | 0.71 |
| 1:B:350:LEU:O | 1:B:359:LYS:HE3 | 1.90 | 0.71 |
| 1:B:340:PRO:C | 1:B:341:VAL:HG23 | 2.12 | 0.70 |
| 1:B:154:SER:H | 1:B:478:ASN:HD21 | 1.37 | 0.70 |
| 1:A:154:SER:H | 1:A:478:ASN:HD21 | 1.38 | 0.70 |
| 1:A:376:VAL:HG22 | 1:A:378:ILE:HG22 | 1.74 | 0.69 |
| 1:B:219:ARG:NH1 | 1:B:235:GLY:HA3 | 2.07 | 0.69 |
| 1:A:414:HIS:HD2 | 1:A:439:MET:H | 1.41 | 0.68 |
| 1:A:70:ILE:HG12 | 1:A:75:VAL:HG11 | 1.76 | 0.68 |
| 1:B:319:GLN:O | 1:B:323:ARG:HD2 | 1.93 | 0.68 |
| 1:B:68:PHE:HB2 | 1:B:75:VAL:HG13 | 1.75 | 0.68 |
| 1:B:340:PRO:C | 1:B:341:VAL:CG2 | 2.61 | 0.68 |
| 1:B:344:LYS:O | 1:B:344:LYS:HG2 | 1.93 | 0.67 |
| 1:A:5:VAL:HG22 | 1:A:18:GLU:O | 1.94 | 0.67 |
| 1:A:344:LYS:H | 1:A:344:LYS:HD2 | 1.60 | 0.67 |
| 1:B:77:ASP:N | 1:B:98:ASN:HD21 | 1.87 | 0.67 |
| 1:B:636:ASN:ND2 | 1:B:639:LYS:HB3 | 2.07 | 0.67 |
| 1:A:595:ARG:HG2 | 1:A:595:ARG:HH11 | 1.60 | 0.67 |
| 1:B:24:ILE:HA | 1:B:52:ASN:HB3 | 1.78 | 0.66 |
| 1:B:344:LYS:H | 1:B:344:LYS:HD2 | 1.60 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:414:HIS:HD2 | 1:B:439:MET:H | 1.42 | 0.66 |
| 1:A:23:LEU:O | 1:A:52:ASN:HB2 | 1.93 | 0.66 |
| 1:A:376:VAL:CG2 | 1:A:378:ILE:HG22 | 2.25 | 0.66 |
| 1:A:342:VAL:HG21 | 1:A:348:GLN:HE22 | 1.61 | 0.66 |
| 1:A:591:VAL:HB | 1:A:599:VAL:HG13 | 1.77 | 0.66 |
| 1:B:376:VAL:HG12 | 1:B:378:ILE:HG22 | 1.77 | 0.66 |
| 1:A:592:LYS:HB3 | 1:A:599:VAL:CG1 | 2.26 | 0.65 |
| 1:A:68:PHE:HB2 | 1:A:75:VAL:HG13 | 1.79 | 0.65 |
| 1:A:342:VAL:HB | 1:A:347:LEU:HD13 | 1.79 | 0.65 |
| 1:B:376:VAL:CG1 | 1:B:378:ILE:HG22 | 2.28 | 0.64 |
| 1:A:286:ARG:HB2 | 1:A:286:ARG:HH11 | 1.61 | 0.64 |
| 1:A:171:ARG:HH21 | 1:A:192:LYS:HD3 | 1.62 | 0.64 |
| 1:A:340:PRO:O | 1:A:340:PRO:HG2 | 1.96 | 0.64 |
| 1:B:37:ASN:C | 1:B:37:ASN:HD22 | 2.01 | 0.64 |
| 1:B:638:ASP:O | 1:B:639:LYS:HB2 | 1.96 | 0.64 |
| 1:A:592:LYS:HB3 | 1:A:599:VAL:HG12 | 1.79 | 0.63 |
| 1:A:201:PRO:O | 1:A:204:VAL:HG22 | 1.97 | 0.63 |
| 1:B:326:GLU:C | 1:B:328:SER:H | 2.01 | 0.63 |
| 1:A:597:PHE:CE2 | 1:A:622:GLU:HG2 | 2.33 | 0.63 |
| 1:A:63:VAL:HG23 | 1:A:157:LEU:HG | 1.80 | 0.62 |
| 1:B:580:ASN:ND2 | 1:B:583:LEU:HG | 2.13 | 0.62 |
| 1:B:83:ARG:HH11 | 1:B:83:ARG:HG3 | 1.64 | 0.62 |
| 1:A:207:ARG:HG3 | 1:A:255:ALA:HB2 | 1.79 | 0.62 |
| 1:B:343:SER:OG | 1:B:347:LEU:HB2 | 2.00 | 0.62 |
| 1:A:350:LEU:HD23 | 1:A:362:LYS:HG3 | 1.82 | 0.62 |
| 1:A:25:ARG:HB2 | 1:A:52:ASN:CA | 2.30 | 0.61 |
| 1:A:345:GLU:O | 1:A:349:ILE:HG22 | 2.00 | 0.61 |
| 1:A:263:SER:HB2 | 1:A:274:ASP:HB3 | 1.83 | 0.61 |
| 1:B:203:TRP:O | 1:B:207:ARG:HD3 | 1.99 | 0.61 |
| 1:A:324:LYS:O | 1:A:326:GLU:O | 2.19 | 0.61 |
| 1:A:37:ASN:C | 1:A:37:ASN:HD22 | 2.02 | 0.61 |
| 1:A:207:ARG:HA | 1:A:254:ASN:HD21 | 1.66 | 0.61 |
| 1:B:207:ARG:HA | 1:B:254:ASN:HD21 | 1.66 | 0.61 |
| 1:B:340:PRO:O | 1:B:341:VAL:CG2 | 2.42 | 0.60 |
| 1:A:331:LYS:HG3 | 1:A:332:ASN:OD1 | 2.00 | 0.60 |
| 1:B:5:VAL:HG22 | 1:B:18:GLU:O | 2.01 | 0.60 |
| 1:A:356:TRP:O | 1:A:357:GLU:HB2 | 2.00 | 0.60 |
| 1:B:80:ASN:O | 1:B:83:ARG:NH1 | 2.33 | 0.60 |
| 1:B:635:ILE:CD1 | 1:B:640:VAL:HG13 | 2.31 | 0.60 |
| 1:A:25:ARG:N | 1:A:52:ASN:HA | 2.16 | 0.60 |
| 1:B:170:LYS:HB3 | 1:B:194:ARG:HD3 | 1.82 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:286:ARG:HH11 | 1:B:286:ARG:CB | 2.09 | 0.60 |
| 1:B:342:VAL:CB | 1:B:347:LEU:HD13 | 2.31 | 0.60 |
| 1:B:207:ARG:HG3 | 1:B:255:ALA:HB2 | 1.82 | 0.60 |
| 1:B:63:VAL:HG23 | 1:B:157:LEU:HG | 1.83 | 0.59 |
| 1:A:331:LYS:HB2 | 1:A:339:PHE:HZ | 1.67 | 0.59 |
| 1:A:118:LEU:CD1 | 1:A:195:PRO:HA | 2.32 | 0.59 |
| 1:A:580:ASN:ND2 | 1:A:583:LEU:HG | 2.18 | 0.59 |
| 1:B:266:THR:HG22 | 1:B:267:TYR:H | 1.68 | 0.59 |
| 1:A:115:LEU:HD12 | 1:A:116:LEU:HD13 | 1.84 | 0.59 |
| 1:A:326:GLU:O | 1:A:327:ASN:HB2 | 2.03 | 0.58 |
| 1:B:215:ASP:OD1 | 1:B:234:TRP:O | 2.21 | 0.58 |
| 1:A:24:ILE:HA | 1:A:52:ASN:HB3 | 1.85 | 0.58 |
| 1:B:111:HIS:HD2 | 1:B:128:LEU:O | 1.86 | 0.58 |
| 1:A:341:VAL:HG23 | 1:A:342:VAL:H | 1.67 | 0.58 |
| 1:B:338:LYS:HB2 | 1:B:338:LYS:NZ | 2.18 | 0.58 |
| 1:A:111:HIS:HD2 | 1:A:128:LEU:O | 1.87 | 0.58 |
| 1:B:595:ARG:HG2 | 1:B:595:ARG:HH11 | 1.68 | 0.58 |
| 1:B:266:THR:HG22 | 1:B:267:TYR:N | 2.19 | 0.58 |
| 1:A:208:VAL:H | 1:A:254:ASN:HD21 | 1.52 | 0.57 |
| 1:A:414:HIS:CD2 | 1:A:438:VAL:HA | 2.39 | 0.57 |
| 1:B:344:LYS:H | 1:B:344:LYS:CD | 2.17 | 0.57 |
| 1:B:2:TYR:HA | 1:B:20:GLU:O | 2.04 | 0.57 |
| 1:A:353:LYS:HB3 | 1:A:353:LYS:NZ | 2.20 | 0.57 |
| 1:B:346:PHE:O | 1:B:350:LEU:HD13 | 2.03 | 0.57 |
| 1:A:324:LYS:HB2 | 1:A:328:SER:HB2 | 1.87 | 0.57 |
| 1:A:642:LEU:HD21 | 1:A:644:LYS:HD2 | 1.87 | 0.57 |
| 1:A:132:GLN:HG3 | 2:A:2033:HOH:O | 2.05 | 0.57 |
| 1:B:376:VAL:HG11 | 1:B:379:MET:HE2 | 1.86 | 0.57 |
| 1:A:152:LYS:HE3 | 1:A:162:GLU:CD | 2.25 | 0.57 |
| 1:B:89:LYS:HE2 | 1:B:470:GLU:OE2 | 2.04 | 0.57 |
| 1:A:220:SER:HB2 | 1:A:239:ILE:HB | 1.87 | 0.57 |
| 1:B:597:PHE:CE2 | 1:B:622:GLU:HG2 | 2.39 | 0.57 |
| 1:B:170:LYS:O | 1:B:194:ARG:HA | 2.05 | 0.57 |
| 1:B:591:VAL:HB | 1:B:599:VAL:HG13 | 1.86 | 0.57 |
| 1:A:211:GLN:HE22 | 1:A:500:ASN:HB2 | 1.69 | 0.56 |
| 1:A:349:ILE:HG23 | 1:A:350:LEU:HD13 | 1.88 | 0.56 |
| 1:B:118:LEU:HD12 | 1:B:195:PRO:HA | 1.87 | 0.56 |
| 1:A:349:ILE:HG23 | 1:A:350:LEU:CD1 | 2.36 | 0.56 |
| 1:B:354:SER:O | 1:B:359:LYS:HD2 | 2.05 | 0.55 |
| 1:A:215:ASP:OD1 | 1:A:234:TRP:O | 2.25 | 0.55 |
| 1:A:338:LYS:HB2 | 1:A:338:LYS:NZ | 2.21 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:342:VAL:CB | 1:A:347:LEU:HD13 | 2.36 | 0.55 |
| 1:B:259:THR:HG23 | 1:B:260:PRO:CD | 2.36 | 0.55 |
| 1:B:248:LEU:HD13 | 1:B:256:ILE:HD11 | 1.88 | 0.55 |
| 1:A:219:ARG:NH1 | 1:A:235:GLY:HA3 | 2.21 | 0.55 |
| 1:A:73:LYS:HE2 | 1:A:74:PHE:H | 1.70 | 0.55 |
| 1:A:355:SER:O | 1:A:358:GLU:CG | 2.54 | 0.55 |
| 1:B:263:SER:HB2 | 1:B:274:ASP:HB3 | 1.89 | 0.55 |
| 1:A:350:LEU:O | 1:A:359:LYS:HD2 | 2.07 | 0.54 |
| 1:B:136:ILE:HD12 | 1:B:178:VAL:CG1 | 2.37 | 0.54 |
| 1:A:125:VAL:HG23 | 1:A:167:GLY:HA2 | 1.88 | 0.54 |
| 1:B:335:ARG:HG3 | 1:B:335:ARG:HH11 | 1.73 | 0.54 |
| 1:A:4:LEU:HD21 | 1:A:7:PHE:CZ | 2.43 | 0.54 |
| 1:A:204:VAL:O | 1:A:207:ARG:HB2 | 2.08 | 0.54 |
| 1:B:211:GLN:HE22 | 1:B:500:ASN:HB2 | 1.72 | 0.54 |
| 1:A:434:LEU:H | 1:A:451:HIS:CD2 | 2.18 | 0.54 |
| 1:A:354:SER:O | 1:A:359:LYS:HD3 | 2.08 | 0.53 |
| 1:B:208:VAL:H | 1:B:254:ASN:HD21 | 1.56 | 0.53 |
| 1:B:524:MET:O | 1:B:577:ARG:HD3 | 2.08 | 0.53 |
| 1:A:203:TRP:O | 1:A:207:ARG:HD3 | 2.08 | 0.53 |
| 1:A:136:ILE:HD12 | 1:A:178:VAL:CG1 | 2.38 | 0.53 |
| 1:A:259:THR:HG23 | 1:A:260:PRO:CD | 2.38 | 0.53 |
| 1:A:208:VAL:H | 1:A:254:ASN:ND2 | 2.06 | 0.53 |
| 1:A:343:SER:HG | 1:A:347:LEU:H | 1.57 | 0.53 |
| 1:B:384:HIS:HD2 | 2:B:2009:HOH:O | 1.92 | 0.53 |
| 1:A:595:ARG:NH1 | 1:A:596:LYS:HG3 | 2.23 | 0.53 |
| 1:A:343:SER:OG | 1:A:347:LEU:N | 2.42 | 0.53 |
| 1:B:203:TRP:CE3 | 1:B:301:LYS:HG3 | 2.44 | 0.53 |
| 1:A:340:PRO:O | 1:A:340:PRO:CG | 2.57 | 0.52 |
| 1:A:346:PHE:O | 1:A:350:LEU:HD13 | 2.10 | 0.52 |
| 1:A:319:GLN:HB3 | 1:A:323:ARG:HH11 | 1.74 | 0.52 |
| 1:B:414:HIS:CD2 | 1:B:438:VAL:HA | 2.44 | 0.52 |
| 1:B:326:GLU:O | 1:B:328:SER:N | 2.42 | 0.52 |
| 1:B:115:LEU:HD12 | 1:B:116:LEU:CD1 | 2.39 | 0.52 |
| 1:B:118:LEU:CD1 | 1:B:195:PRO:HA | 2.40 | 0.52 |
| 1:A:376:VAL:O | 1:A:376:VAL:HG13 | 2.09 | 0.52 |
| 1:B:37:ASN:C | 1:B:37:ASN:ND2 | 2.63 | 0.52 |
| 1:B:167:GLY:C | 1:B:169:ASP:H | 2.13 | 0.52 |
| 1:B:565:ARG:HD3 | 1:B:645:TYR:O | 2.10 | 0.52 |
| 1:A:524:MET:O | 1:A:577:ARG:HD3 | 2.10 | 0.52 |
| 1:B:1:MET:N | 1:B:77:ASP:OD2 | 2.43 | 0.52 |
| 1:B:292:LEU:HD22 | 1:B:296:LYS:HE2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:25:ARG:HA | 1:A:53:TRP:CD1 | 2.45 | 0.51 |
| 1:B:339:PHE:C | 1:B:341:VAL:H | 2.12 | 0.51 |
| 1:A:565:ARG:HD3 | 1:A:645:TYR:O | 2.10 | 0.51 |
| 1:A:73:LYS:CE | 1:A:74:PHE:H | 2.24 | 0.51 |
| 1:A:470:GLU:OE2 | 1:B:470:GLU:OE2 | 2.29 | 0.51 |
| 1:B:24:ILE:HD12 | 1:B:51:LYS:O | 2.11 | 0.51 |
| 1:A:376:VAL:HG11 | 1:A:379:MET:HE3 | 1.92 | 0.51 |
| 1:A:343:SER:HG | 1:A:347:LEU:HB2 | 1.75 | 0.51 |
| 1:B:341:VAL:O | 1:B:369:ASN:HB2 | 2.11 | 0.51 |
| 1:A:558:ASN:OD1 | 1:A:560:GLU:HG2 | 2.10 | 0.51 |
| 1:A:109:VAL:HG22 | 1:A:131:THR:HG22 | 1.92 | 0.51 |
| 1:B:247:HIS:HE1 | 1:B:537:GLU:OE2 | 1.94 | 0.50 |
| 1:A:25:ARG:CB | 1:A:52:ASN:HA | 2.36 | 0.50 |
| 1:A:347:LEU:O | 1:A:351:HIS:HB2 | 2.12 | 0.50 |
| 1:B:434:LEU:H | 1:B:451:HIS:CD2 | 2.18 | 0.50 |
| 1:A:319:GLN:HB3 | 1:A:323:ARG:NH1 | 2.27 | 0.50 |
| 1:A:595:ARG:HH11 | 1:A:596:LYS:HG3 | 1.75 | 0.50 |
| 1:A:350:LEU:HD21 | 1:A:362:LYS:NZ | 2.27 | 0.50 |
| 1:A:120:GLU:HA | 1:A:124:ARG:O | 2.12 | 0.50 |
| 1:B:635:ILE:HD11 | 1:B:640:VAL:HG13 | 1.93 | 0.49 |
| 1:A:49:GLU:OE1 | 1:A:54:LYS:HD2 | 2.12 | 0.49 |
| 1:A:4:LEU:HD21 | 1:A:7:PHE:CE2 | 2.47 | 0.49 |
| 1:A:125:VAL:HG23 | 1:A:167:GLY:CA | 2.42 | 0.49 |
| 1:B:344:LYS:O | 1:B:345:GLU:HB2 | 2.13 | 0.49 |
| 1:A:24:ILE:HD13 | 1:A:24:ILE:C | 2.33 | 0.49 |
| 1:B:438:VAL:HG11 | 1:B:453:VAL:HG11 | 1.95 | 0.49 |
| 1:B:201:PRO:O | 1:B:204:VAL:HG22 | 2.13 | 0.49 |
| 1:A:118:LEU:HD12 | 1:A:195:PRO:HA | 1.94 | 0.48 |
| 1:A:167:GLY:C | 1:A:169:ASP:H | 2.16 | 0.48 |
| 1:A:344:LYS:O | 1:A:346:PHE:N | 2.45 | 0.48 |
| 1:A:595:ARG:HG2 | 1:A:595:ARG:NH1 | 2.28 | 0.48 |
| 1:A:89:LYS:HE2 | 1:A:470:GLU:OE2 | 2.13 | 0.48 |
| 1:A:2:TYR:HA | 1:A:20:GLU:O | 2.14 | 0.48 |
| 1:A:37:ASN:C | 1:A:37:ASN:ND2 | 2.67 | 0.48 |
| 1:A:498:LEU:HG | 1:A:523:LEU:HD22 | 1.95 | 0.48 |
| 1:B:339:PHE:C | 1:B:341:VAL:N | 2.66 | 0.48 |
| 1:B:348:GLN:HG3 | 1:B:349:ILE:N | 2.28 | 0.48 |
| 1:A:62:GLY:HA2 | 1:A:157:LEU:HD12 | 1.95 | 0.48 |
| 1:B:472:THR:OG1 | 1:B:475:GLU:HG3 | 2.13 | 0.48 |
| 1:A:24:ILE:O | 1:A:24:ILE:HG23 | 2.13 | 0.48 |
| 1:B:266:THR:HG22 | 1:B:267:TYR:CD1 | 2.48 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:45:ARG:NH1 | 1:A:335:ARG:NH1 | 2.61 | 0.48 |
| 1:B:539:GLY:HA2 | 2:B:2102:HOH:O | 2.14 | 0.48 |
| 1:B:23:LEU:HD11 | 1:B:70:ILE:HD11 | 1.95 | 0.47 |
| 1:B:83:ARG:HH11 | 1:B:83:ARG:CG | 2.27 | 0.47 |
| 1:A:73:LYS:HA | 1:A:73:LYS:CE | 2.39 | 0.47 |
| 1:B:208:VAL:H | 1:B:254:ASN:ND2 | 2.12 | 0.47 |
| 1:B:70:ILE:HG12 | 1:B:75:VAL:CG1 | 2.43 | 0.47 |
| 1:B:341:VAL:HB | 1:B:342:VAL:H | 1.47 | 0.47 |
| 1:B:349:ILE:HG23 | 1:B:350:LEU:HD13 | 1.95 | 0.47 |
| 1:B:592:LYS:HB3 | 1:B:599:VAL:HG12 | 1.96 | 0.47 |
| 1:B:70:ILE:CG1 | 1:B:75:VAL:HG11 | 2.43 | 0.47 |
| 1:A:350:LEU:CD2 | 1:A:362:LYS:HG3 | 2.45 | 0.47 |
| 1:A:286:ARG:HH11 | 1:A:286:ARG:CB | 2.26 | 0.47 |
| 1:A:247:HIS:HE1 | 1:A:537:GLU:OE2 | 1.98 | 0.47 |
| 1:A:355:SER:HB2 | 1:A:359:LYS:HD3 | 1.97 | 0.47 |
| 1:A:474:GLU:H | 1:A:474:GLU:CD | 2.18 | 0.47 |
| 1:A:638:ASP:O | 1:A:639:LYS:HB2 | 2.15 | 0.47 |
| 1:B:543:ILE:HD13 | 1:B:554:PRO:HD3 | 1.97 | 0.47 |
| 1:A:344:LYS:C | 1:A:346:PHE:H | 2.17 | 0.47 |
| 1:B:350:LEU:HD23 | 1:B:362:LYS:HG3 | 1.97 | 0.47 |
| 1:A:147:VAL:HG22 | 1:A:163:VAL:HG21 | 1.97 | 0.47 |
| 1:A:155:ASP:OD1 | 1:A:486:TYR:OH | 2.33 | 0.47 |
| 1:B:125:VAL:HG23 | 1:B:167:GLY:CA | 2.45 | 0.47 |
| 1:B:498:LEU:HG | 1:B:523:LEU:HD22 | 1.96 | 0.47 |
| 1:B:220:SER:HB2 | 1:B:239:ILE:HB | 1.96 | 0.46 |
| 1:B:344:LYS:HD2 | 1:B:344:LYS:N | 2.27 | 0.46 |
| 1:B:636:ASN:HD22 | 1:B:636:ASN:N | 2.13 | 0.46 |
| 1:A:1:MET:N | 1:A:77:ASP:OD2 | 2.49 | 0.46 |
| 1:B:109:VAL:HG13 | 1:B:129:LEU:HD11 | 1.98 | 0.46 |
| 1:B:25:ARG:N | 1:B:52:ASN:HA | 2.27 | 0.46 |
| 1:A:152:LYS:HD2 | 1:A:485:SER:OG | 2.15 | 0.46 |
| 1:A:580:ASN:HD21 | 1:A:582:ALA:HB3 | 1.81 | 0.46 |
| 1:B:314:PHE:HE2 | 1:B:378:ILE:HD11 | 1.80 | 0.46 |
| 1:A:343:SER:OG | 1:A:347:LEU:HB2 | 2.16 | 0.46 |
| 1:A:472:THR:OG1 | 1:A:475:GLU:HG3 | 2.16 | 0.46 |
| 1:A:631:SER:HB2 | 1:A:644:LYS:HB3 | 1.98 | 0.46 |
| 1:B:347:LEU:O | 1:B:351:HIS:HB2 | 2.15 | 0.46 |
| 1:A:344:LYS:H | 1:A:344:LYS:CD | 2.27 | 0.45 |
| 1:A:354:SER:O | 1:A:355:SER:HB2 | 2.15 | 0.45 |
| 1:B:8:ARG:NH1 | 1:B:18:GLU:OE2 | 2.49 | 0.45 |
| 1:B:326:GLU:C | 1:B:328:SER:N | 2.67 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:349:ILE:HG23 | 1:B:350:LEU:CD1 | 2.47 | 0.45 |
| 1:B:24:ILE:HG23 | 1:B:24:ILE:O | 2.16 | 0.45 |
| 1:A:25:ARG:HG2 | 1:A:53:TRP:CE2 | 2.52 | 0.45 |
| 1:A:539:GLY:HA2 | 2:A:2107:HOH:O | 2.16 | 0.45 |
| 1:B:331:LYS:HB2 | 1:B:339:PHE:HZ | 1.82 | 0.45 |
| 1:B:349:ILE:HG23 | 1:B:350:LEU:N | 2.32 | 0.45 |
| 1:B:265:LEU:O | 1:B:265:LEU:HD13 | 2.17 | 0.45 |
| 1:A:203:TRP:CE3 | 1:A:301:LYS:HG3 | 2.52 | 0.45 |
| 1:B:203:TRP:CZ3 | 1:B:301:LYS:HG3 | 2.52 | 0.45 |
| 1:A:136:ILE:HG23 | 1:A:178:VAL:HG13 | 1.97 | 0.45 |
| 1:A:83:ARG:NH1 | 1:A:98:ASN:OD1 | 2.50 | 0.45 |
| 1:B:512:ASP:HB2 | 1:B:515:LYS:HG3 | 1.99 | 0.45 |
| 1:A:343:SER:OG | 1:A:346:PHE:HB3 | 2.16 | 0.45 |
| 1:A:109:VAL:HG13 | 1:A:129:LEU:HD11 | 1.99 | 0.44 |
| 1:B:136:ILE:HD12 | 1:B:178:VAL:HG11 | 1.98 | 0.44 |
| 1:A:350:LEU:HD21 | 1:A:362:LYS:HZ1 | 1.82 | 0.44 |
| 1:B:154:SER:N | 1:B:478:ASN:HD21 | 2.09 | 0.44 |
| 1:A:171:ARG:HG3 | 1:A:171:ARG:HH11 | 1.82 | 0.44 |
| 1:B:580:ASN:ND2 | 1:B:583:LEU:H | 2.10 | 0.44 |
| 1:A:338:LYS:HG2 | 1:A:340:PRO:CD | 2.42 | 0.44 |
| 1:A:344:LYS:HD2 | 1:A:344:LYS:N | 2.28 | 0.44 |
| 1:A:349:ILE:HG23 | 1:A:350:LEU:N | 2.33 | 0.44 |
| 1:A:411:ASP:OD2 | 1:A:412:VAL:HG23 | 2.17 | 0.44 |
| 1:A:586:GLY:HA2 | 1:A:603:GLU:O | 2.17 | 0.44 |
| 1:A:412:VAL:HG12 | 1:A:412:VAL:O | 2.18 | 0.44 |
| 1:A:136:ILE:HD12 | 1:A:178:VAL:HG11 | 1.99 | 0.44 |
| 1:A:335:ARG:HB2 | 1:A:371:GLU:HB2 | 1.99 | 0.44 |
| 1:B:5:VAL:CG2 | 1:B:18:GLU:HB3 | 2.48 | 0.44 |
| 1:B:420:VAL:O | 1:B:424:VAL:HG23 | 2.16 | 0.44 |
| 1:B:477:LEU:HB2 | 1:B:593:PHE:CD2 | 2.53 | 0.44 |
| 1:B:558:ASN:ND2 | 1:B:561:GLU:HG3 | 2.33 | 0.44 |
| 1:A:326:GLU:O | 1:A:327:ASN:CB | 2.66 | 0.44 |
| 1:B:61:GLU:HG2 | 1:B:103:VAL:HA | 2.00 | 0.44 |
| 1:B:345:GLU:O | 1:B:349:ILE:HG21 | 2.17 | 0.44 |
| 1:A:349:ILE:O | 1:A:353:LYS:HG2 | 2.17 | 0.44 |
| 1:B:580:ASN:HD22 | 1:B:583:LEU:HG | 1.83 | 0.44 |
| 1:B:125:VAL:HG23 | 1:B:167:GLY:HA3 | 2.00 | 0.43 |
| 1:B:165:VAL:HG12 | 1:B:166:GLU:N | 2.33 | 0.43 |
| 1:B:299:ASP:CG | 1:B:299:ASP:O | 2.57 | 0.43 |
| 1:A:23:LEU:C | 1:A:23:LEU:HD22 | 2.37 | 0.43 |
| 1:B:19:VAL:HG13 | 1:B:57:ILE:HG23 | 2.01 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:115:LEU:O | 1:B:119:TYR:HB3 | 2.18 | 0.43 |
| 1:B:326:GLU:HG3 | 1:B:339:PHE:CD2 | 2.54 | 0.43 |
| 1:A:35:ASP:O | 1:A:440:ASP:HB3 | 2.19 | 0.43 |
| 1:A:376:VAL:HG11 | 1:A:379:MET:CE | 2.48 | 0.43 |
| 1:B:587:ASN:O | 1:B:602:ARG:HA | 2.19 | 0.43 |
| 1:A:246:ASP:O | 1:A:249:VAL:HG22 | 2.19 | 0.43 |
| 1:B:219:ARG:HH12 | 1:B:235:GLY:HA3 | 1.80 | 0.43 |
| 1:A:115:LEU:O | 1:A:119:TYR:HB3 | 2.19 | 0.43 |
| 1:A:583:LEU:HD21 | 1:A:609:THR:HG21 | 2.00 | 0.42 |
| 1:A:636:ASN:N | 1:A:636:ASN:HD22 | 2.16 | 0.42 |
| 1:B:35:ASP:OD1 | 1:B:35:ASP:N | 2.52 | 0.42 |
| 1:A:343:SER:OG | 1:A:366:LEU:HD21 | 2.19 | 0.42 |
| 1:B:35:ASP:O | 1:B:440:ASP:HB3 | 2.20 | 0.42 |
| 1:A:199:GLU:CD | 1:A:200:PHE:N | 2.73 | 0.42 |
| 1:B:145:LYS:HE3 | 1:B:145:LYS:HB2 | 1.84 | 0.42 |
| 1:B:357:GLU:C | 1:B:359:LYS:N | 2.70 | 0.42 |
| 1:B:592:LYS:HB3 | 1:B:599:VAL:CG1 | 2.49 | 0.42 |
| 1:A:171:ARG:HG3 | 1:A:171:ARG:NH1 | 2.35 | 0.42 |
| 1:A:376:VAL:CG2 | 1:A:379:MET:HE2 | 2.36 | 0.42 |
| 1:B:264:SER:HB2 | 1:B:271:ASP:OD1 | 2.20 | 0.42 |
| 1:B:440:ASP:O | 1:B:441:ASP:C | 2.57 | 0.42 |
| 1:A:335:ARG:HG3 | 1:A:335:ARG:HH11 | 1.85 | 0.42 |
| 1:A:440:ASP:O | 1:A:441:ASP:C | 2.56 | 0.42 |
| 1:A:636:ASN:HD22 | 1:A:636:ASN:H | 1.67 | 0.42 |
| 1:B:325:GLY:O | 1:B:328:SER:HB3 | 2.20 | 0.42 |
| 1:B:338:LYS:HG2 | 1:B:340:PRO:CD | 2.43 | 0.42 |
| 1:B:438:VAL:HG12 | 1:B:453:VAL:HB | 2.01 | 0.42 |
| 1:B:635:ILE:HD13 | 1:B:640:VAL:HA | 2.01 | 0.42 |
| 1:B:118:LEU:HD13 | 1:B:195:PRO:HB3 | 2.01 | 0.41 |
| 1:B:204:VAL:HG21 | 1:B:493:LEU:CD1 | 2.50 | 0.41 |
| 1:B:376:VAL:HG11 | 1:B:379:MET:CE | 2.50 | 0.41 |
| 1:A:543:ILE:HD13 | 1:A:554:PRO:HD3 | 2.02 | 0.41 |
| 1:A:580:ASN:HD22 | 1:A:583:LEU:HG | 1.85 | 0.41 |
| 1:B:42:GLY:HA3 | 1:B:415:GLY:O | 2.20 | 0.41 |
| 1:B:151:LYS:HE2 | 1:B:159:ASP:CG | 2.41 | 0.41 |
| 1:B:246:ASP:O | 1:B:249:VAL:HG22 | 2.21 | 0.41 |
| 1:A:339:PHE:C | 1:A:341:VAL:N | 2.74 | 0.41 |
| 1:A:397:ILE:CD1 | 1:A:410:MET:HE1 | 2.50 | 0.41 |
| 1:B:211:GLN:NE2 | 2:B:2043:HOH:O | 2.52 | 0.41 |
| 1:B:438:VAL:CG1 | 1:B:453:VAL:HB | 2.50 | 0.41 |
| 1:B:326:GLU:N | 1:B:339:PHE:HE2 | 2.19 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:411:ASP:OD2 | 1:B:412:VAL:HG23 | 2.19 | 0.41 |
| 1:A:111:HIS:HE1 | 1:A:174:TYR:OH | 2.04 | 0.41 |
| 1:A:145:LYS:HB2 | 1:A:145:LYS:HE3 | 1.79 | 0.41 |
| 1:A:342:VAL:HG21 | 1:A:348:GLN:NE2 | 2.33 | 0.41 |
| 1:B:25:ARG:HA | 1:B:53:TRP:CD1 | 2.55 | 0.41 |
| 1:B:62:GLY:HA2 | 1:B:157:LEU:HD12 | 2.02 | 0.41 |
| 1:B:204:VAL:O | 1:B:207:ARG:HB2 | 2.20 | 0.41 |
| 1:B:595:ARG:HH12 | 1:B:596:LYS:NZ | 2.18 | 0.41 |
| 1:A:61:GLU:HG2 | 1:A:103:VAL:HA | 2.02 | 0.41 |
| 1:B:26:GLU:O | 1:B:26:GLU:HG2 | 2.20 | 0.41 |
| 1:B:354:SER:O | 1:B:355:SER:HB2 | 2.20 | 0.41 |
| 1:A:115:LEU:HD21 | 1:A:198:ILE:HG23 | 2.02 | 0.41 |
| 1:A:353:LYS:HB3 | 1:A:353:LYS:HZ3 | 1.85 | 0.41 |
| 1:A:574:VAL:O | 1:A:578:LYS:HG3 | 2.21 | 0.41 |
| 1:B:7:PHE:CE1 | 1:B:17:ALA:HB2 | 2.56 | 0.41 |
| 1:B:37:ASN:ND2 | 1:B:39:PHE:H | 2.19 | 0.41 |
| 1:B:127:VAL:HB | 1:B:163:VAL:HG12 | 2.03 | 0.41 |
| 1:B:254:ASN:HD22 | 1:B:254:ASN:H | 1.68 | 0.41 |
| 1:B:325:GLY:C | 1:B:326:GLU:O | 2.59 | 0.41 |
| 1:B:338:LYS:HB3 | 1:B:369:ASN:CG | 2.41 | 0.41 |
| 1:B:343:SER:OG | 1:B:366:LEU:HD21 | 2.21 | 0.41 |
| 1:A:24:ILE:HD13 | 1:A:25:ARG:N | 2.37 | 0.40 |
| 1:A:587:ASN:O | 1:A:602:ARG:HA | 2.21 | 0.40 |
| 1:B:51:LYS:O | 1:B:51:LYS:HG3 | 2.20 | 0.40 |
| 1:B:512:ASP:HB3 | 1:B:514:ARG:HG2 | 2.03 | 0.40 |
| 1:A:199:GLU:CD | 1:A:200:PHE:H | 2.25 | 0.40 |
| 1:A:299:ASP:O | 1:A:299:ASP:CG | 2.60 | 0.40 |
| 1:B:120:GLU:HA | 1:B:124:ARG:O | 2.21 | 0.40 |
| 1:B:257:TYR:CD1 | 1:B:257:TYR:C | 2.95 | 0.40 |
| 1:B:180:THR:OG1 | 1:B:184:ALA:HB3 | 2.22 | 0.40 |
| 1:B:354:SER:OG | 1:B:355:SER:N | 2.53 | 0.40 |
| 1:B:439:MET:HA | 1:B:456:TYR:HB2 | 2.03 | 0.40 |
| 1:A:41:GLU:OE2 | 1:A:72:GLY:HA2 | 2.21 | 0.40 |
| 1:A:73:LYS:HE2 | 1:A:73:LYS:CA | 2.42 | 0.40 |
| 1:A:472:THR:HB | 1:A:474:GLU:OE1 | 2.21 | 0.40 |
| 1:B:25:ARG:HB2 | 1:B:52:ASN:HA | 2.03 | 0.40 |
| 1:B:308:PHE:O | 1:B:384:HIS:HE1 | 2.04 | 0.40 |
| 1:B:326:GLU:HG3 | 1:B:339:PHE:CE2 | 2.56 | 0.40 |
| 1:B:353:LYS:HE3 | 1:B:353:LYS:HB3 | 1.98 | 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 | 632/645 (98%) | 577 (91%) | 54 (8%) | 1 (0%) | 47 55 |
| 1 | B | 632/645 (98%) | 588 (93%) | 43 (7%) | 1 (0%) | 47 55 |
| All | All | 1264/1290 (98%) | 1165 (92%) | 97 (8%) | 2 (0%) | 47 55 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 189 | GLY |
| 1 | B | 341 | VAL |

### 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 | 569/576 (99%) | 538 (95%) | 31 (5%) | 22 26 |
| 1 | B | 569/576 (99%) | 541 (95%) | 28 (5%) | 25 31 |
| All | All | 1138/1152 (99%) | 1079 (95%) | 59 (5%) | 23 28 |

All (59) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 4 | LEU |
| 1 | A | 23 | LEU |
| 1 | A | 24 | ILE |
| 1 | A | 35 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 37 | ASN |
| 1 | A | 73 | LYS |
| 1 | A | 87 | THR |
| 1 | A | 108 | LEU |
| 1 | A | 116 | LEU |
| 1 | A | 147 | VAL |
| 1 | A | 152 | LYS |
| 1 | A | 179 | LEU |
| 1 | A | 199 | GLU |
| 1 | A | 207 | ARG |
| 1 | A | 254 | ASN |
| 1 | A | 257 | TYR |
| 1 | A | 259 | THR |
| 1 | A | 323 | ARG |
| 1 | A | 333 | PHE |
| 1 | A | 339 | PHE |
| 1 | A | 341 | VAL |
| 1 | A | 346 | PHE |
| 1 | A | 356 | TRP |
| 1 | A | 358 | GLU |
| 1 | A | 401 | THR |
| 1 | A | 414 | HIS |
| 1 | A | 474 | GLU |
| 1 | A | 483 | LEU |
| 1 | A | 581 | LYS |
| 1 | A | 614 | ASN |
| 1 | A | 636 | ASN |
| 1 | B | 18 | GLU |
| 1 | B | 35 | ASP |
| 1 | B | 37 | ASN |
| 1 | B | 73 | LYS |
| 1 | B | 87 | THR |
| 1 | B | 152 | LYS |
| 1 | B | 179 | LEU |
| 1 | B | 207 | ARG |
| 1 | B | 254 | ASN |
| 1 | B | 257 | TYR |
| 1 | B | 259 | THR |
| 1 | B | 323 | ARG |
| 1 | B | 333 | PHE |
| 1 | B | 339 | PHE |
| 1 | B | 341 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 344 | LYS |
| 1 | B | 346 | PHE |
| 1 | B | 348 | GLN |
| 1 | B | 356 | TRP |
| 1 | B | 358 | GLU |
| 1 | B | 401 | THR |
| 1 | B | 414 | HIS |
| 1 | B | 438 | VAL |
| 1 | B | 474 | GLU |
| 1 | B | 483 | LEU |
| 1 | B | 581 | LYS |
| 1 | B | 614 | ASN |
| 1 | B | 636 | ASN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 37 | ASN |
| 1 | A | 40 | ASN |
| 1 | A | 48 | GLN |
| 1 | A | 98 | ASN |
| 1 | A | 111 | HIS |
| 1 | A | 211 | GLN |
| 1 | A | 247 | HIS |
| 1 | A | 254 | ASN |
| 1 | A | 268 | HIS |
| 1 | A | 327 | ASN |
| 1 | A | 369 | ASN |
| 1 | A | 384 | HIS |
| 1 | A | 451 | HIS |
| 1 | A | 478 | ASN |
| 1 | A | 580 | ASN |
| 1 | A | 614 | ASN |
| 1 | A | 617 | ASN |
| 1 | A | 636 | ASN |
| 1 | B | 37 | ASN |
| 1 | B | 48 | GLN |
| 1 | B | 98 | ASN |
| 1 | B | 111 | HIS |
| 1 | B | 126 | HIS |
| 1 | B | 211 | GLN |
| 1 | B | 247 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 254 | ASN |
| 1 | B | 327 | ASN |
| 1 | B | 369 | ASN |
| 1 | B | 384 | HIS |
| 1 | B | 451 | HIS |
| 1 | B | 478 | ASN |
| 1 | B | 580 | ASN |
| 1 | B | 614 | ASN |
| 1 | B | 636 | ASN |

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

### 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 | 636/645 (98%) | -0.04 | 20 (3%) | 49 | 59 | 15, 29, 62, 84 | 1 (0%) |
| 1 | B | 636/645 (98%) | -0.03 | 21 (3%) | 46 | 57 | 13, 28, 64, 84 | 1 (0%) |
| All | All | 1272/1290 (98%) | -0.04 | 41 (3%) | 47 | 58 | 13, 28, 63, 84 | 2 (0%) |

All (41) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 356 | TRP | 10.8 |
| 1 | B | 356 | TRP | 7.8 |
| 1 | B | 169 | ASP | 5.7 |
| 1 | A | 169 | ASP | 5.1 |
| 1 | A | 344 | LYS | 4.7 |
| 1 | B | 350 | LEU | 4.5 |
| 1 | A | 168 | GLY | 4.4 |
| 1 | A | 170 | LYS | 4.2 |
| 1 | A | 339 | PHE | 4.0 |
| 1 | B | 168 | GLY | 4.0 |
| 1 | B | 339 | PHE | 4.0 |
| 1 | A | 623 | LEU | 3.9 |
| 1 | A | 638 | ASP | 3.8 |
| 1 | B | 51 | LYS | 3.7 |
| 1 | B | 170 | LYS | 3.6 |
| 1 | A | 350 | LEU | 3.6 |
| 1 | A | 234 | TRP | 3.6 |
| 1 | B | 234 | TRP | 3.4 |
| 1 | B | 24 | ILE | 3.3 |
| 1 | B | 638 | ASP | 3.3 |
| 1 | A | 353 | LYS | 3.2 |
| 1 | B | 329 | SER | 3.0 |
| 1 | B | 345 | GLU | 2.9 |
| 1 | B | 351 | HIS | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 623 | LEU | 2.8 |
| 1 | B | 182 | GLU | 2.8 |
| 1 | B | 349 | ILE | 2.8 |
| 1 | A | 345 | GLU | 2.8 |
| 1 | B | 353 | LYS | 2.7 |
| 1 | A | 348 | GLN | 2.7 |
| 1 | B | 344 | LYS | 2.5 |
| 1 | B | 126 | HIS | 2.5 |
| 1 | A | 267 | TYR | 2.4 |
| 1 | A | 351 | HIS | 2.4 |
| 1 | A | 51 | LYS | 2.3 |
| 1 | A | 268 | HIS | 2.3 |
| 1 | B | 166 | GLU | 2.3 |
| 1 | A | 126 | HIS | 2.2 |
| 1 | A | 323 | ARG | 2.2 |
| 1 | A | 333 | PHE | 2.1 |
| 1 | B | 341 | VAL | 2.1 |

## 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)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.