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

Jun 25, 2024 – 03:40 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 5W79 |
| Title | : | Crystal Structure of the Group II Chaperonin from Methanococcus Maripaludis, Cysteine-less mutant in the Apo State |
| Authors | : | Dalton, K.M.; Lopez, T.; Liu, C.; Ralston, C.Y.; Pereira, J.H.; Chartron, J.W.; McAndrew, R.P.; Douglas, N.R.; Adams, P.D.; Pande, V.S.; Frydman, J. |
| Deposited on | : | 2017-06-19 |
| Resolution | : | 3.12 Å(reported) |

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

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

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

---

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

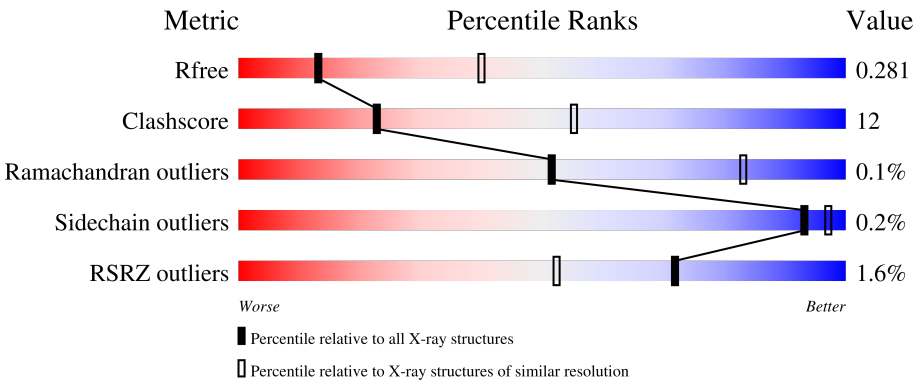
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.37.1 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.37.1 |

# 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 3.12 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 | 1292 (3.14-3.10) |
| Clashscore | 141614 | 1389 (3.14-3.10) |
| Ramachandran outliers | 138981 | 1337 (3.14-3.10) |
| Sidechain outliers | 138945 | 1337 (3.14-3.10) |
| RSRZ outliers | 127900 | 1260 (3.14-3.10) |

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 | 543 | 2% 69% 26% 5% |
| 1 | B | 543 | 2% 73% 21% 5% |
| 1 | C | 543 | . % 69% 26% 5% |
| 1 | D | 543 | . % 70% 24% 5% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | E | 543 | 3% 71% 23% 5% |
| 1 | F | 543 | .% 70% 25% 5% |
| 1 | G | 543 | .% 71% 24% 5% |
| 1 | H | 543 | 2% 70% 25% 5% |

# 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 31143 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 Chaperonin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | B | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | C | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | D | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | E | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | F | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | G | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |
| 1 | H | 515 | 3887 | 2419 | 670 | 778 | 20 | 0 | 0 | 0 |

There are 64 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| A | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| A | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| A | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| A | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| A | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| A | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| A | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| B | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| B | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| B | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| B | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| B | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |

*Continued on next page...*

*Continued from previous page...*

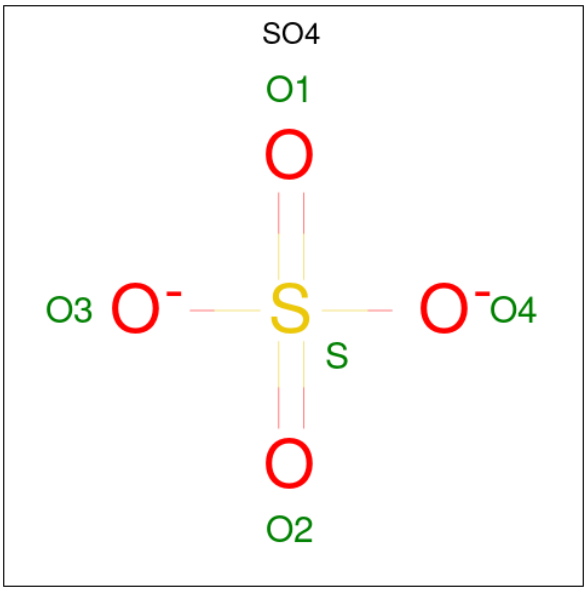
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| B | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| B | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| C | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| C | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| C | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| C | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| C | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| C | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| C | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| C | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| D | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| D | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| D | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| D | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| D | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| D | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| D | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| D | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| E | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| E | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| E | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| E | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| E | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| E | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| E | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| E | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| F | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| F | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| F | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| F | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| F | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| F | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| F | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| F | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| G | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| G | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| G | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| G | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| G | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| G | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| G | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 484 | THR | CYS | engineered mutation | UNP Q877G8 |
| H | 140 | MET | CYS | engineered mutation | UNP Q877G8 |
| H | 237 | GLU | CYS | engineered mutation | UNP Q877G8 |
| H | 286 | VAL | CYS | engineered mutation | UNP Q877G8 |
| H | 304 | MET | VAL | engineered mutation | UNP Q877G8 |
| H | 359 | VAL | CYS | engineered mutation | UNP Q877G8 |
| H | 393 | SER | CYS | engineered mutation | UNP Q877G8 |
| H | 470 | TYR | CYS | engineered mutation | UNP Q877G8 |
| H | 484 | THR | CYS | engineered mutation | UNP Q877G8 |

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: $O_4S$).




| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | O | S | | | |
| 2 | A | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | B | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | C | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | D | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | E | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | F | 1 | 5 | 4 | 1 | | 0 | 0 |
| 2 | G | 1 | 5 | 4 | 1 | | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | O | S | | |
| 2 | H | 1 | 5 | 4 | 1 | 0 | 0 |

- Molecule 3 is water.

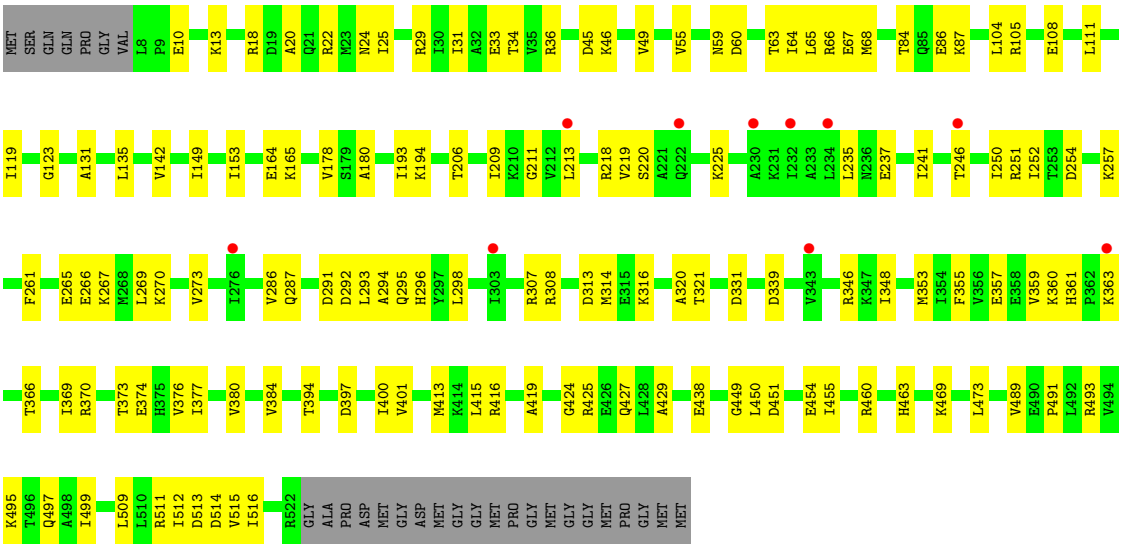
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 3 | A | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | C | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | D | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | E | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | F | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | G | 1 | 1 | 1 | 0 | 0 |
| | | | Total | O | | |
| 3 | H | 1 | 1 | 1 | 0 | 0 |

# 3 Residue-property plots (i)

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

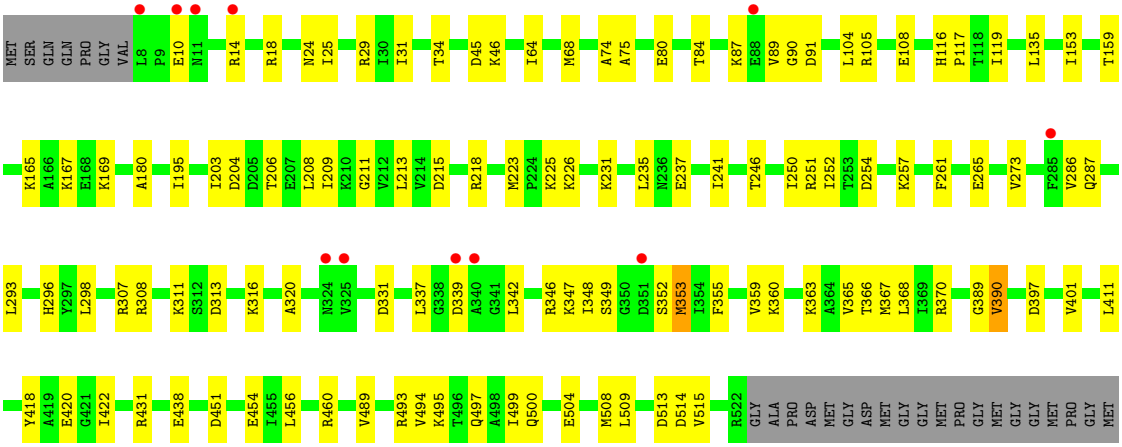
• Molecule 1: Chaperonin

Chain A:




• Molecule 1: Chaperonin

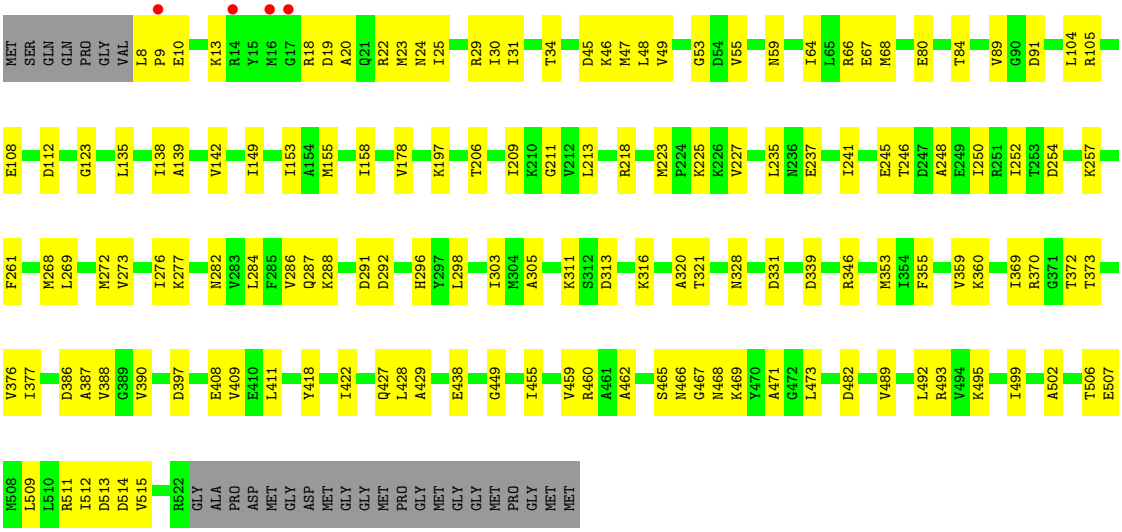
Chain B:



MET

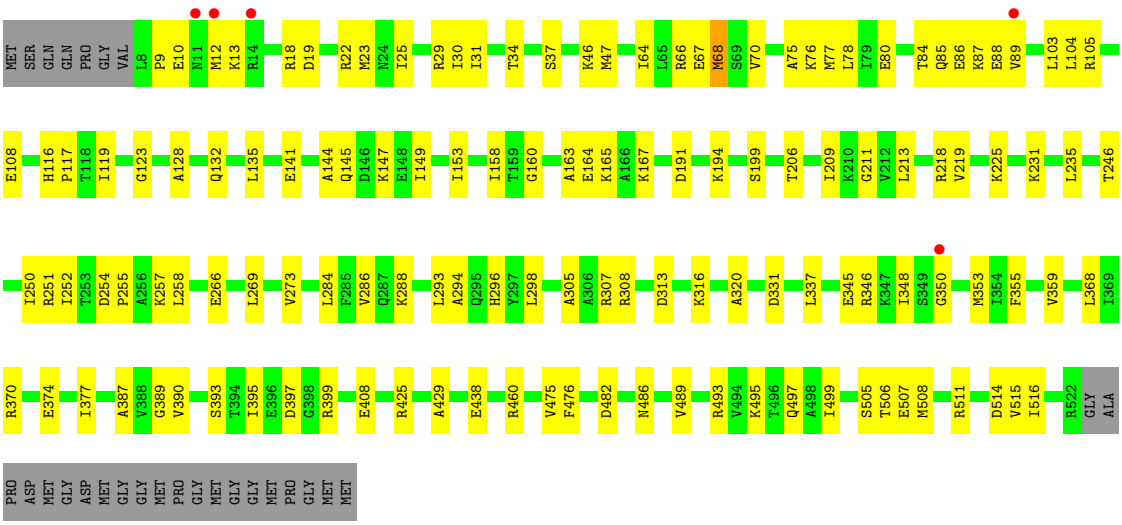
• Molecule 1: Chaperonin

Chain C:



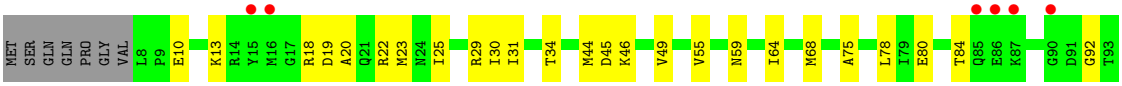

• Molecule 1: Chaperonin

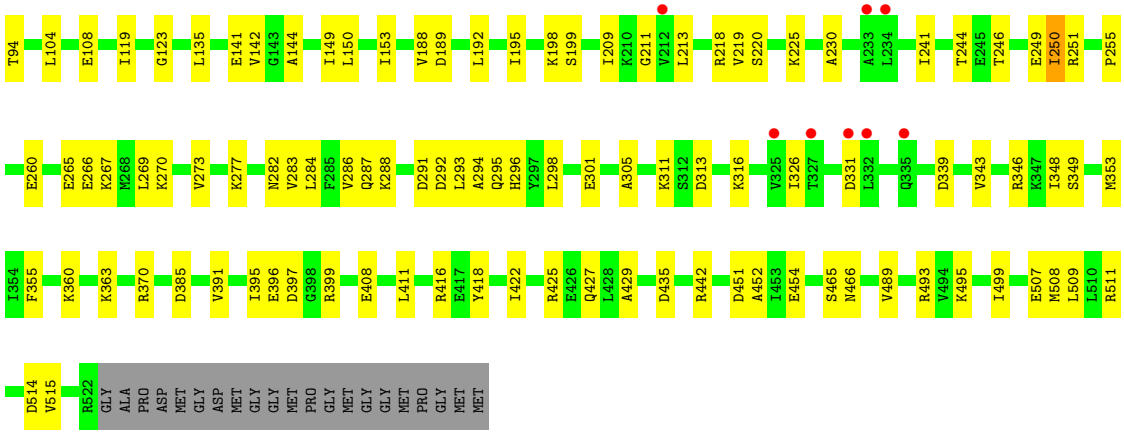
Chain D:




• Molecule 1: Chaperonin

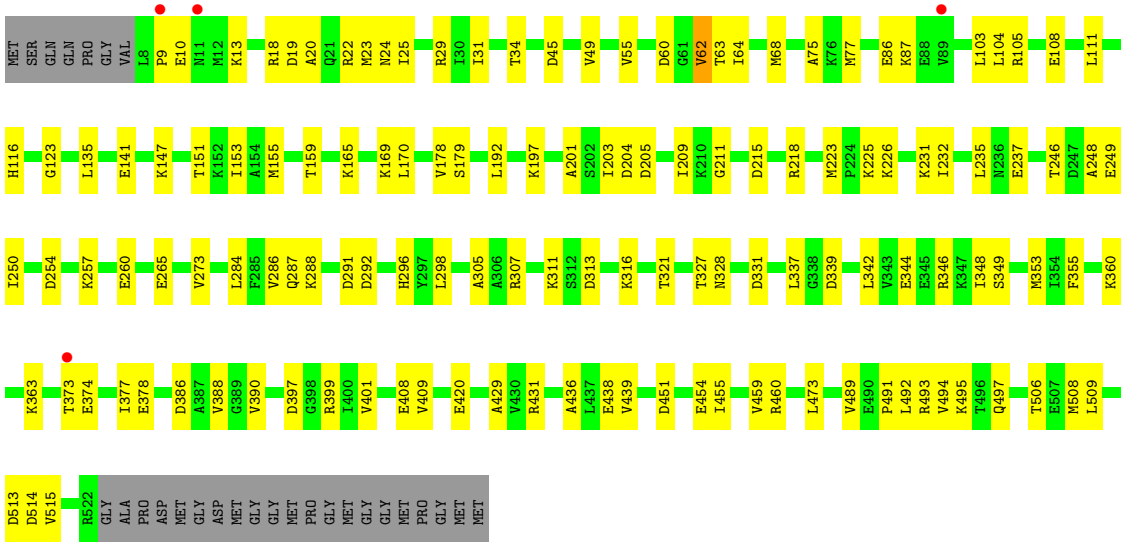
Chain E:





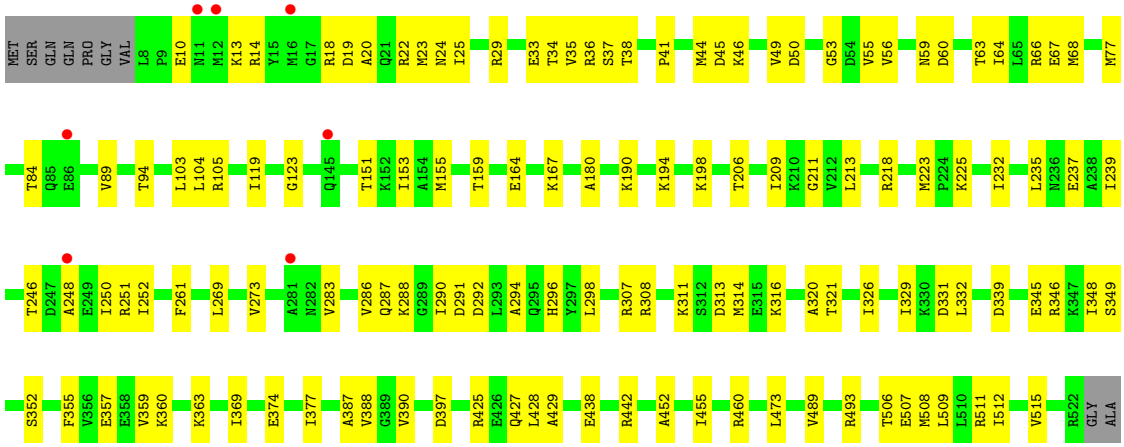

• Molecule 1: Chaperonin

Chain F:




• Molecule 1: Chaperonin

Chain G:



PRO ASP MET GLY ASP MET GLY GLY MET PRO GLY MET GLY GLY MET PRO GLY MET MET

- Molecule 1: Chaperonin

Chain H:

MET SER GLN GLN PRO GLY VAL L8 P9 E10 N11 M12 K13 R14 R18 Q21 R22 M23 N24 I25 R29 I30 T34 D45 K46 V49 V55 N59 I64 L65 R66 E67 M68 K76 E80 T84 Q85 E86 K87 T95 L104 R105 E108 L111

H116 G123 L135 V142 I149 I153 A154 I158 K161 G162 A163 E164 K165 D183 K187 K194 I209 K210 G211 V212 L213 R218 V219 K225 K231 I232 L235 N236 E237 I241 T246 D247 A248 E249 I250 R251 I252 T253 D254 K257 L258

F261 E265 M272 V273 V283 L284 F285 V286 Q287 K288 L293 H296 Y297 L298 M304 R307 R308 V309 K310 K311 S312 D313 M314 E315 K316 A320 T321 N328 D331 L337 E344 E345 R346 K347 I348 S349 M353 I354 F355 V356 E357 E358 V359 K360 H361

T372 T373 I377 V380 A387 V390 D397 V409 E410 L411 I422 S423 G424 Q427 L428 A429 E438 V439 I440 G449 L450 D451 E454 V459 R460 N468 A471 G472 L473 N474 V475 F476 V489 R493 A502 T506 E507 M508 L509 L510 R511 I512

D513 D514 V515 A518 L521 R522 GLY ALA PRO ASP MET GLY ASP MET GLY GLY GLY MET PRO GLY MET GLY GLY MET PRO GLY MET MET

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 32 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 149.98Å 149.98Å 416.48Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 81.24 – 3.12<br>81.24 – 3.12 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 99.0 (81.24-3.12)<br>99.0 (81.24-3.12) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.66 (at 3.13Å) | Xtriage |
| Refinement program | PHENIX | Depositor |
| R, $R_{free}$ | 0.249 , 0.281<br>0.249 , 0.281 | Depositor<br>DCC |
| $R_{free}$ test set | 4942 reflections (5.13%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 73.3 | Xtriage |
| Anisotropy | 0.051 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.33 , 24.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | 0.022 for -h,-k,l | Xtriage |
| $F_o$,$F_c$ correlation | 0.91 | EDS |
| Total number of atoms | 31143 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 64.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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 (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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 | 0.41 | 0/3911 | 0.63 | 0/5262 |
| 1 | B | 0.39 | 0/3911 | 0.61 | 1/5262 (0.0%) |
| 1 | C | 0.40 | 0/3911 | 0.61 | 0/5262 |
| 1 | D | 0.42 | 0/3911 | 0.63 | 1/5262 (0.0%) |
| 1 | E | 0.42 | 1/3911 (0.0%) | 0.61 | 0/5262 |
| 1 | F | 0.40 | 0/3911 | 0.62 | 0/5262 |
| 1 | G | 0.40 | 0/3911 | 0.61 | 1/5262 (0.0%) |
| 1 | H | 0.40 | 0/3911 | 0.62 | 1/5262 (0.0%) |
| All | All | 0.40 | 1/31288 (0.0%) | 0.62 | 4/42096 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | E | 92 | GLY | C-O | 5.98 | 1.33 | 1.23 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 497 | GLN | CA-CB-CG | 6.68 | 128.10 | 113.40 |
| 1 | G | 59 | ASN | CB-CA-C | -6.40 | 97.60 | 110.40 |
| 1 | D | 68 | MET | CB-CA-C | -5.25 | 99.89 | 110.40 |
| 1 | H | 165 | LYS | N-CA-C | -5.16 | 97.08 | 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 | 3887 | 0 | 4039 | 110 | 0 |
| 1 | B | 3887 | 0 | 4040 | 93 | 0 |
| 1 | C | 3887 | 0 | 4040 | 102 | 0 |
| 1 | D | 3887 | 0 | 4040 | 97 | 0 |
| 1 | E | 3887 | 0 | 4040 | 102 | 0 |
| 1 | F | 3887 | 0 | 4040 | 96 | 0 |
| 1 | G | 3887 | 0 | 4040 | 101 | 0 |
| 1 | H | 3887 | 0 | 4040 | 120 | 0 |
| 2 | A | 5 | 0 | 0 | 0 | 0 |
| 2 | B | 5 | 0 | 0 | 1 | 0 |
| 2 | C | 5 | 0 | 0 | 0 | 0 |
| 2 | D | 5 | 0 | 0 | 0 | 0 |
| 2 | E | 5 | 0 | 0 | 1 | 0 |
| 2 | F | 5 | 0 | 0 | 0 | 0 |
| 2 | G | 5 | 0 | 0 | 1 | 0 |
| 2 | H | 5 | 0 | 0 | 0 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |
| 3 | H | 1 | 0 | 0 | 1 | 0 |
| All | All | 31143 | 0 | 32319 | 730 | 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 12.

All (730) 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:D:408:GLU:OE2 | 1:D:495:LYS:NZ | 1.92 | 1.03 |
| 1:H:34:THR:O | 1:H:46:LYS:NZ | 1.94 | 1.00 |
| 1:H:218:ARG:HH22 | 1:H:225:LYS:HZ3 | 1.02 | 0.97 |
| 1:F:344:GLU:OE1 | 1:F:346:ARG:NH1 | 1.99 | 0.95 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:408:GLU:OE2 | 1:C:495:LYS:NZ | 2.01 | 0.91 |
| 1:D:219:VAL:HG23 | 1:D:307:ARG:HH11 | 1.35 | 0.90 |
| 1:D:145:GLN:OE1 | 1:D:147:LYS:NZ | 2.05 | 0.90 |
| 1:D:438:GLU:OE2 | 1:D:460:ARG:NH2 | 2.03 | 0.90 |
| 1:B:24:ASN:HD22 | 1:B:74:ALA:HB2 | 1.36 | 0.89 |
| 1:A:346:ARG:NH2 | 1:A:357:GLU:OE2 | 2.10 | 0.84 |
| 1:E:198:LYS:HD2 | 1:E:348:ILE:HD11 | 1.59 | 0.84 |
| 1:E:507:GLU:OE2 | 1:E:511:ARG:NH2 | 2.11 | 0.84 |
| 1:E:408:GLU:OE2 | 1:E:495:LYS:NZ | 2.10 | 0.84 |
| 1:F:86:GLU:HG3 | 1:F:497:GLN:HE22 | 1.42 | 0.84 |
| 1:D:85:GLN:HB3 | 1:D:497:GLN:HE21 | 1.44 | 0.81 |
| 1:E:218:ARG:HH22 | 1:E:225:LYS:HZ1 | 1.24 | 0.81 |
| 1:G:37:SER:OG | 1:G:46:LYS:NZ | 2.12 | 0.81 |
| 1:A:86:GLU:HG2 | 1:H:372:THR:HG21 | 1.62 | 0.81 |
| 1:A:296:HIS:ND1 | 1:B:331:ASP:OD1 | 2.12 | 0.81 |
| 1:D:18:ARG:HH11 | 1:D:22:ARG:HH11 | 1.28 | 0.81 |
| 1:D:296:HIS:ND1 | 1:E:331:ASP:OD1 | 2.14 | 0.81 |
| 1:C:372:THR:HG21 | 1:D:86:GLU:HG2 | 1.63 | 0.80 |
| 1:D:218:ARG:NH1 | 1:D:345:GLU:OE1 | 2.13 | 0.80 |
| 1:E:218:ARG:HH12 | 1:E:225:LYS:HZ3 | 1.27 | 0.79 |
| 1:E:34:THR:O | 1:E:46:LYS:NZ | 2.15 | 0.79 |
| 1:A:400:ILE:HD12 | 1:A:489:VAL:HG21 | 1.64 | 0.79 |
| 1:C:47:MET:HB3 | 1:D:515:VAL:HG12 | 1.66 | 0.78 |
| 1:A:416:ARG:NH2 | 1:A:438:GLU:OE2 | 2.17 | 0.78 |
| 1:C:53:GLY:O | 1:D:76:LYS:NZ | 2.15 | 0.78 |
| 1:H:218:ARG:HH22 | 1:H:225:LYS:NZ | 1.81 | 0.77 |
| 1:B:500:GLN:NE2 | 1:B:504:GLU:OE2 | 2.16 | 0.77 |
| 1:H:283:VAL:HG12 | 1:H:304:MET:HB3 | 1.66 | 0.77 |
| 1:G:53:GLY:O | 1:H:76:LYS:NZ | 2.16 | 0.77 |
| 1:B:265:GLU:OE2 | 1:C:245:GLU:HB3 | 1.86 | 0.76 |
| 1:H:158:ILE:HD11 | 1:H:387:ALA:HB2 | 1.67 | 0.76 |
| 1:A:66:ARG:NH1 | 1:A:67:GLU:OE2 | 2.18 | 0.76 |
| 1:F:296:HIS:ND1 | 1:G:331:ASP:OD1 | 2.18 | 0.76 |
| 1:A:331:ASP:OD1 | 1:H:296:HIS:ND1 | 2.17 | 0.75 |
| 1:H:507:GLU:OE2 | 1:H:511:ARG:NH2 | 2.20 | 0.75 |
| 1:D:37:SER:OG | 1:D:46:LYS:NZ | 2.20 | 0.74 |
| 1:H:218:ARG:NH2 | 1:H:225:LYS:HZ3 | 1.83 | 0.74 |
| 1:H:142:VAL:HG11 | 1:H:149:ILE:HG12 | 1.69 | 0.74 |
| 1:E:422:ILE:O | 1:E:427:GLN:NE2 | 2.15 | 0.74 |
| 1:A:65:LEU:HD23 | 1:A:68:MET:HE1 | 1.69 | 0.74 |
| 1:F:408:GLU:OE2 | 1:F:495:LYS:NZ | 2.16 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:191:ASP:O | 1:D:194:LYS:NZ | 2.20 | 0.73 |
| 1:F:86:GLU:O | 1:F:497:GLN:NE2 | 2.21 | 0.73 |
| 1:C:438:GLU:OE2 | 1:C:460:ARG:NH2 | 2.16 | 0.72 |
| 1:E:218:ARG:NH1 | 1:E:225:LYS:HZ3 | 1.86 | 0.72 |
| 1:G:250:ILE:HG23 | 1:H:248:ALA:HA | 1.71 | 0.72 |
| 1:C:397:ASP:OD2 | 1:C:493:ARG:HB2 | 1.89 | 0.71 |
| 1:G:507:GLU:OE2 | 1:G:511:ARG:NH2 | 2.22 | 0.71 |
| 1:B:438:GLU:OE2 | 1:B:460:ARG:NH2 | 2.23 | 0.70 |
| 1:H:218:ARG:HH12 | 1:H:225:LYS:HZ2 | 1.39 | 0.70 |
| 1:B:64:ILE:O | 1:B:68:MET:HG3 | 1.92 | 0.70 |
| 1:H:64:ILE:O | 1:H:68:MET:HG3 | 1.91 | 0.70 |
| 1:G:218:ARG:HH22 | 1:G:225:LYS:NZ | 1.89 | 0.70 |
| 1:H:45:ASP:OD1 | 1:H:59:ASN:HB3 | 1.91 | 0.70 |
| 1:H:468:ASN:HB3 | 1:H:471:ALA:HB2 | 1.74 | 0.69 |
| 1:G:209:ILE:HG22 | 1:G:211:GLY:H | 1.56 | 0.69 |
| 1:F:209:ILE:HG22 | 1:F:211:GLY:H | 1.58 | 0.69 |
| 1:A:451:ASP:HB3 | 1:A:454:GLU:HG2 | 1.75 | 0.69 |
| 1:F:197:LYS:NZ | 1:F:378:GLU:OE1 | 2.25 | 0.69 |
| 1:A:219:VAL:HG23 | 1:A:307:ARG:HE | 1.58 | 0.69 |
| 1:A:246:THR:OG1 | 1:H:265:GLU:OE2 | 2.09 | 0.69 |
| 1:B:397:ASP:OD2 | 1:B:493:ARG:HB2 | 1.92 | 0.68 |
| 1:B:252:ILE:HB | 1:C:250:ILE:HG12 | 1.76 | 0.68 |
| 1:A:87:LYS:H | 1:A:497:GLN:HE22 | 1.40 | 0.68 |
| 1:H:422:ILE:O | 1:H:427:GLN:NE2 | 2.25 | 0.68 |
| 1:H:287:GLN:HE21 | 1:H:314:MET:HG3 | 1.60 | 0.67 |
| 1:A:235:LEU:HB3 | 1:A:286:VAL:HG12 | 1.77 | 0.67 |
| 1:H:346:ARG:NH2 | 1:H:357:GLU:OE2 | 2.28 | 0.67 |
| 1:F:346:ARG:HH21 | 1:F:355:PHE:HD2 | 1.41 | 0.67 |
| 1:B:250:ILE:HG23 | 1:C:248:ALA:HA | 1.76 | 0.67 |
| 1:F:397:ASP:OD2 | 1:F:493:ARG:HB2 | 1.95 | 0.66 |
| 1:D:158:ILE:HD11 | 1:D:387:ALA:HB2 | 1.77 | 0.66 |
| 1:G:438:GLU:OE2 | 1:G:460:ARG:NH2 | 2.29 | 0.66 |
| 1:D:507:GLU:OE2 | 1:D:511:ARG:NH2 | 2.28 | 0.66 |
| 1:D:199:SER:OG | 1:D:374:GLU:OE2 | 2.14 | 0.66 |
| 1:B:320:ALA:HB1 | 1:B:359:VAL:HG21 | 1.77 | 0.66 |
| 1:G:198:LYS:HG2 | 1:G:348:ILE:HD13 | 1.77 | 0.65 |
| 1:A:361:HIS:CE1 | 1:A:363:LYS:HB2 | 2.30 | 0.65 |
| 1:D:219:VAL:CG2 | 1:D:307:ARG:HH11 | 2.09 | 0.65 |
| 1:G:296:HIS:ND1 | 1:H:331:ASP:OD1 | 2.30 | 0.65 |
| 1:C:45:ASP:HB3 | 1:C:59:ASN:HB3 | 1.79 | 0.64 |
| 1:E:29:ARG:NH2 | 1:F:10:GLU:OE2 | 2.31 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:219:VAL:O | 1:E:295:GLN:NE2 | 2.30 | 0.64 |
| 1:D:219:VAL:HG23 | 1:D:307:ARG:NH1 | 2.09 | 0.64 |
| 1:A:135:LEU:HD11 | 1:A:499:ILE:HD12 | 1.79 | 0.64 |
| 1:C:296:HIS:ND1 | 1:D:331:ASP:OD1 | 2.29 | 0.64 |
| 1:H:346:ARG:HH21 | 1:H:355:PHE:HD2 | 1.46 | 0.64 |
| 1:A:361:HIS:HE1 | 1:A:363:LYS:HB2 | 1.64 | 0.63 |
| 1:E:349:SER:HB2 | 1:E:370:ARG:HH22 | 1.61 | 0.63 |
| 1:F:373:THR:HG22 | 1:G:84:THR:HG21 | 1.80 | 0.63 |
| 1:E:45:ASP:HB3 | 1:E:59:ASN:HB3 | 1.80 | 0.63 |
| 1:B:235:LEU:HB3 | 1:B:286:VAL:HG12 | 1.80 | 0.63 |
| 1:H:344:GLU:OE1 | 1:H:346:ARG:NH1 | 2.32 | 0.63 |
| 1:C:252:ILE:HB | 1:D:250:ILE:HG12 | 1.80 | 0.63 |
| 1:A:142:VAL:HG11 | 1:A:149:ILE:HG21 | 1.80 | 0.63 |
| 1:G:397:ASP:OD1 | 1:G:493:ARG:NH2 | 2.32 | 0.62 |
| 1:A:219:VAL:O | 1:A:295:GLN:NE2 | 2.32 | 0.62 |
| 1:B:347:LYS:HA | 1:B:352:SER:HB3 | 1.81 | 0.62 |
| 1:D:141:GLU:HG2 | 1:D:399:ARG:HG2 | 1.81 | 0.62 |
| 1:H:18:ARG:NH2 | 1:H:21:GLN:OE1 | 2.33 | 0.62 |
| 1:A:313:ASP:HA | 1:A:316:LYS:HE2 | 1.82 | 0.61 |
| 1:C:468:ASN:HB3 | 1:C:471:ALA:HB2 | 1.81 | 0.61 |
| 1:A:45:ASP:HB3 | 1:A:59:ASN:HB3 | 1.82 | 0.61 |
| 1:A:254:ASP:HB3 | 1:A:257:LYS:HG2 | 1.82 | 0.61 |
| 1:C:339:ASP:HB2 | 1:C:360:LYS:HE2 | 1.82 | 0.61 |
| 1:A:18:ARG:O | 1:A:22:ARG:HG2 | 1.99 | 0.61 |
| 1:A:320:ALA:HB1 | 1:A:359:VAL:HG21 | 1.81 | 0.61 |
| 1:G:287:GLN:HG2 | 1:G:314:MET:HG3 | 1.81 | 0.61 |
| 1:G:64:ILE:O | 1:G:68:MET:HG3 | 2.00 | 0.61 |
| 1:B:153:ILE:HD13 | 1:B:489:VAL:HG23 | 1.81 | 0.61 |
| 1:H:163:ALA:HB2 | 1:H:380:VAL:HG22 | 1.82 | 0.61 |
| 1:E:18:ARG:NH1 | 1:E:22:ARG:HH11 | 1.99 | 0.61 |
| 1:E:296:HIS:ND1 | 1:F:331:ASP:OD1 | 2.33 | 0.61 |
| 1:F:64:ILE:O | 1:F:68:MET:HG3 | 2.01 | 0.61 |
| 1:E:64:ILE:O | 1:E:68:MET:HG3 | 2.01 | 0.60 |
| 1:G:105:ARG:HH22 | 1:H:8:LEU:HD23 | 1.67 | 0.60 |
| 1:D:85:GLN:HB3 | 1:D:497:GLN:NE2 | 2.14 | 0.60 |
| 1:D:78:LEU:HD12 | 1:D:505:SER:HB2 | 1.83 | 0.60 |
| 1:A:13:LYS:HE2 | 1:H:34:THR:HG22 | 1.81 | 0.60 |
| 1:A:60:ASP:OD2 | 1:A:63:THR:OG1 | 2.10 | 0.60 |
| 1:G:218:ARG:HH22 | 1:G:225:LYS:HZ1 | 1.49 | 0.60 |
| 1:B:508:MET:HG3 | 1:B:509:LEU:HD22 | 1.84 | 0.60 |
| 1:E:250:ILE:HG23 | 1:F:248:ALA:HA | 1.84 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:451:ASP:HB3 | 1:F:454:GLU:HG2 | 1.82 | 0.60 |
| 1:E:230:ALA:HA | 1:E:282:ASN:HD21 | 1.68 | 0.59 |
| 1:H:209:ILE:HG22 | 1:H:211:GLY:H | 1.67 | 0.59 |
| 1:A:251:ARG:HD2 | 1:B:251:ARG:HG2 | 1.84 | 0.59 |
| 1:B:296:HIS:ND1 | 1:C:331:ASP:OD1 | 2.34 | 0.59 |
| 1:D:438:GLU:CD | 1:D:460:ARG:HH21 | 2.02 | 0.59 |
| 1:E:18:ARG:O | 1:E:22:ARG:HG2 | 2.00 | 0.59 |
| 1:G:206:THR:HG23 | 1:G:369:ILE:HA | 1.84 | 0.59 |
| 1:C:153:ILE:HD13 | 1:C:489:VAL:HG23 | 1.85 | 0.59 |
| 1:B:231:LYS:HB3 | 1:B:337:LEU:HD13 | 1.84 | 0.59 |
| 1:F:170:LEU:HD22 | 1:F:203:ILE:HD11 | 1.83 | 0.59 |
| 1:D:34:THR:O | 1:D:46:LYS:HE2 | 2.03 | 0.59 |
| 1:C:48:LEU:HD23 | 1:D:516:ILE:HG13 | 1.83 | 0.59 |
| 1:A:250:ILE:HD11 | 1:A:261:PHE:CD1 | 2.37 | 0.59 |
| 1:E:218:ARG:HH22 | 1:E:225:LYS:NZ | 1.99 | 0.58 |
| 1:E:230:ALA:HA | 1:E:282:ASN:ND2 | 2.18 | 0.58 |
| 1:C:209:ILE:HG22 | 1:C:211:GLY:H | 1.68 | 0.58 |
| 1:E:34:THR:HG22 | 1:F:13:LYS:HE2 | 1.86 | 0.58 |
| 1:F:169:LYS:NZ | 1:F:204:ASP:O | 2.29 | 0.58 |
| 1:G:218:ARG:NH1 | 1:G:225:LYS:HG2 | 2.18 | 0.58 |
| 1:H:153:ILE:HD13 | 1:H:489:VAL:HG23 | 1.84 | 0.58 |
| 1:A:10:GLU:OE2 | 1:H:29:ARG:NH2 | 2.33 | 0.58 |
| 1:A:455:ILE:HG21 | 1:A:473:LEU:HD22 | 1.85 | 0.58 |
| 1:D:254:ASP:HB3 | 1:D:257:LYS:HG2 | 1.86 | 0.58 |
| 1:A:20:ALA:HB1 | 1:A:515:VAL:HG12 | 1.85 | 0.58 |
| 1:A:250:ILE:HD12 | 1:H:258:LEU:HD21 | 1.84 | 0.58 |
| 1:F:86:GLU:CG | 1:F:497:GLN:HE22 | 2.12 | 0.58 |
| 1:G:29:ARG:NH2 | 1:H:10:GLU:OE2 | 2.37 | 0.58 |
| 1:G:339:ASP:HB2 | 1:G:360:LYS:HE2 | 1.85 | 0.58 |
| 1:F:18:ARG:O | 1:F:22:ARG:HG2 | 2.03 | 0.58 |
| 1:B:46:LYS:NZ | 1:C:513:ASP:OD1 | 2.35 | 0.58 |
| 1:C:64:ILE:O | 1:C:68:MET:HG3 | 2.04 | 0.58 |
| 1:E:192:LEU:HD13 | 1:E:363:LYS:HB3 | 1.85 | 0.58 |
| 1:F:250:ILE:HG23 | 1:G:248:ALA:HA | 1.86 | 0.58 |
| 1:G:348:ILE:HD12 | 1:G:349:SER:O | 2.04 | 0.58 |
| 1:H:18:ARG:HH11 | 1:H:22:ARG:HH11 | 1.52 | 0.58 |
| 1:E:273:VAL:HG13 | 1:E:298:LEU:HD23 | 1.86 | 0.58 |
| 1:G:33:GLU:OE1 | 1:G:36:ARG:HD3 | 2.04 | 0.58 |
| 1:B:346:ARG:HD2 | 1:B:355:PHE:CD2 | 2.39 | 0.57 |
| 1:F:491:PRO:O | 1:F:494:VAL:HG12 | 2.05 | 0.57 |
| 1:B:135:LEU:HD11 | 1:B:499:ILE:HD12 | 1.86 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:E:283:VAL:HG11 | 1:E:343:VAL:HG11 | 1.86 | 0.57 |
| 1:F:22:ARG:HH22 | 1:F:111:LEU:HB2 | 1.70 | 0.57 |
| 1:G:66:ARG:NH1 | 1:G:67:GLU:OE2 | 2.38 | 0.57 |
| 1:E:25:ILE:HG23 | 1:E:104:LEU:HB3 | 1.85 | 0.57 |
| 1:E:209:ILE:HG22 | 1:E:211:GLY:H | 1.70 | 0.57 |
| 1:B:80:GLU:O | 1:B:84:THR:HG23 | 2.04 | 0.57 |
| 1:B:347:LYS:HA | 1:B:352:SER:CB | 2.35 | 0.57 |
| 1:D:153:ILE:HD13 | 1:D:489:VAL:HG23 | 1.87 | 0.57 |
| 1:H:409:VAL:HG11 | 1:H:459:VAL:HG12 | 1.87 | 0.57 |
| 1:A:123:GLY:HA3 | 1:A:429:ALA:HB3 | 1.85 | 0.57 |
| 1:A:307:ARG:HD3 | 1:A:308:ARG:HH11 | 1.70 | 0.57 |
| 1:H:518:ALA:HB3 | 1:H:521:LEU:HD11 | 1.85 | 0.57 |
| 1:D:218:ARG:HH12 | 1:D:225:LYS:HZ3 | 1.51 | 0.57 |
| 1:G:25:ILE:HG23 | 1:G:104:LEU:HB3 | 1.86 | 0.57 |
| 1:C:507:GLU:OE2 | 1:C:511:ARG:NH2 | 2.38 | 0.56 |
| 1:D:46:LYS:HD2 | 1:E:514:ASP:HB3 | 1.87 | 0.56 |
| 1:F:438:GLU:OE2 | 1:F:460:ARG:NH2 | 2.30 | 0.56 |
| 1:A:287:GLN:HG2 | 1:A:314:MET:HG3 | 1.87 | 0.56 |
| 1:A:449:GLY:HA3 | 1:B:119:ILE:HD11 | 1.86 | 0.56 |
| 1:E:277:LYS:HG2 | 1:E:301:GLU:OE2 | 2.05 | 0.56 |
| 1:E:339:ASP:HB2 | 1:E:360:LYS:HE3 | 1.87 | 0.56 |
| 1:G:50:ASP:HB3 | 1:H:521:LEU:HD13 | 1.86 | 0.56 |
| 1:B:29:ARG:NH2 | 1:B:105:ARG:HH11 | 2.03 | 0.56 |
| 1:C:31:ILE:O | 1:C:34:THR:OG1 | 2.22 | 0.56 |
| 1:D:34:THR:HG22 | 1:E:13:LYS:HE2 | 1.87 | 0.56 |
| 1:D:160:GLY:N | 1:D:164:GLU:OE2 | 2.36 | 0.56 |
| 1:G:153:ILE:HD13 | 1:G:489:VAL:HG23 | 1.85 | 0.56 |
| 1:G:198:LYS:NZ | 1:G:348:ILE:HD11 | 2.20 | 0.56 |
| 1:G:442:ARG:HG3 | 1:G:452:ALA:HB1 | 1.88 | 0.56 |
| 1:D:30:ILE:O | 1:D:34:THR:HG23 | 2.06 | 0.56 |
| 1:G:320:ALA:HB1 | 1:G:359:VAL:HG21 | 1.87 | 0.56 |
| 1:G:374:GLU:HA | 1:G:377:ILE:HG22 | 1.87 | 0.56 |
| 1:A:10:GLU:OE2 | 1:H:105:ARG:HD3 | 2.06 | 0.56 |
| 1:A:119:ILE:HD11 | 1:H:449:GLY:HA3 | 1.87 | 0.56 |
| 1:C:197:LYS:HB2 | 1:C:377:ILE:HG23 | 1.88 | 0.56 |
| 1:B:273:VAL:HG13 | 1:B:298:LEU:HD23 | 1.87 | 0.56 |
| 1:D:64:ILE:O | 1:D:68:MET:HG3 | 2.05 | 0.56 |
| 1:D:209:ILE:HG22 | 1:D:211:GLY:H | 1.70 | 0.56 |
| 1:E:218:ARG:HH12 | 1:E:225:LYS:NZ | 2.02 | 0.56 |
| 1:E:255:PRO:HG3 | 1:F:260:GLU:HG2 | 1.87 | 0.56 |
| 1:F:218:ARG:NH1 | 1:F:225:LYS:HG2 | 2.21 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:34:THR:HG22 | 1:G:13:LYS:HE2 | 1.87 | 0.56 |
| 1:A:24:ASN:HB3 | 1:A:509:LEU:HD22 | 1.88 | 0.55 |
| 1:E:397:ASP:OD2 | 1:E:493:ARG:HB2 | 2.06 | 0.55 |
| 1:H:320:ALA:HB1 | 1:H:359:VAL:HG21 | 1.89 | 0.55 |
| 1:A:220:SER:HB2 | 1:A:295:GLN:HG2 | 1.89 | 0.55 |
| 1:A:287:GLN:HE21 | 1:A:314:MET:HG3 | 1.71 | 0.55 |
| 1:B:209:ILE:HD12 | 1:B:213:LEU:HD11 | 1.88 | 0.55 |
| 1:A:194:LYS:HE3 | 1:A:316:LYS:HB3 | 1.88 | 0.55 |
| 1:B:235:LEU:O | 1:B:286:VAL:HA | 2.07 | 0.55 |
| 1:D:119:ILE:HD11 | 1:D:425:ARG:HH21 | 1.71 | 0.55 |
| 1:E:153:ILE:HD13 | 1:E:489:VAL:HG23 | 1.89 | 0.55 |
| 1:H:29:ARG:NH1 | 1:H:108:GLU:OE1 | 2.39 | 0.55 |
| 1:A:514:ASP:HB3 | 1:H:46:LYS:HD2 | 1.89 | 0.55 |
| 1:E:451:ASP:HB3 | 1:E:454:GLU:HG2 | 1.88 | 0.55 |
| 1:G:151:THR:O | 1:G:155:MET:HG2 | 2.07 | 0.55 |
| 1:C:320:ALA:HB1 | 1:C:359:VAL:HG21 | 1.88 | 0.55 |
| 1:F:24:ASN:HB3 | 1:F:509:LEU:HD12 | 1.89 | 0.55 |
| 1:B:420:GLU:OE2 | 1:B:431:ARG:NH2 | 2.38 | 0.55 |
| 1:E:144:ALA:HB1 | 1:E:395:ILE:HG23 | 1.89 | 0.55 |
| 1:E:218:ARG:NH2 | 1:E:225:LYS:HZ1 | 2.00 | 0.55 |
| 1:E:141:GLU:HG2 | 1:E:399:ARG:HG2 | 1.89 | 0.54 |
| 1:A:194:LYS:HG3 | 1:A:316:LYS:HD2 | 1.89 | 0.54 |
| 1:B:105:ARG:HH22 | 1:C:8:LEU:HD23 | 1.71 | 0.54 |
| 1:D:286:VAL:HG22 | 1:D:288:LYS:H | 1.73 | 0.54 |
| 1:F:153:ILE:HD13 | 1:F:489:VAL:HG23 | 1.90 | 0.54 |
| 1:G:218:ARG:NH1 | 1:G:345:GLU:OE1 | 2.38 | 0.54 |
| 1:H:86:GLU:HG2 | 1:H:87:LYS:HG2 | 1.89 | 0.54 |
| 1:H:287:GLN:HG2 | 1:H:314:MET:HG3 | 1.90 | 0.54 |
| 1:A:250:ILE:HD11 | 1:A:261:PHE:CE1 | 2.43 | 0.54 |
| 1:C:22:ARG:NH2 | 1:C:112:ASP:OD1 | 2.37 | 0.54 |
| 1:H:194:LYS:HE3 | 1:H:316:LYS:HB3 | 1.88 | 0.54 |
| 1:A:348:ILE:HD11 | 1:A:370:ARG:NH1 | 2.22 | 0.54 |
| 1:B:397:ASP:OD1 | 1:B:493:ARG:NH2 | 2.38 | 0.54 |
| 1:D:307:ARG:HE | 1:D:308:ARG:NH2 | 2.06 | 0.54 |
| 1:F:19:ASP:O | 1:F:23:MET:HG2 | 2.08 | 0.54 |
| 1:A:273:VAL:HG13 | 1:A:298:LEU:HD23 | 1.90 | 0.54 |
| 1:C:24:ASN:HB3 | 1:C:509:LEU:HD12 | 1.89 | 0.54 |
| 1:G:164:GLU:HA | 1:G:167:LYS:HE3 | 1.90 | 0.54 |
| 1:B:135:LEU:HD21 | 1:B:411:LEU:HD11 | 1.90 | 0.53 |
| 1:F:25:ILE:HG23 | 1:F:104:LEU:HB3 | 1.90 | 0.53 |
| 1:C:273:VAL:HG13 | 1:C:298:LEU:HD23 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:465:SER:OG | 1:C:466:ASN:N | 2.40 | 0.53 |
| 1:F:29:ARG:NH2 | 1:G:10:GLU:OE2 | 2.40 | 0.53 |
| 1:A:287:GLN:CG | 1:A:314:MET:HG3 | 2.37 | 0.53 |
| 1:D:252:ILE:HD13 | 1:D:258:LEU:HD23 | 1.91 | 0.53 |
| 1:E:49:VAL:HG22 | 1:E:55:VAL:HG12 | 1.90 | 0.53 |
| 1:E:189:ASP:HB3 | 1:E:192:LEU:HD12 | 1.91 | 0.53 |
| 1:E:346:ARG:HD2 | 1:E:355:PHE:CE2 | 2.43 | 0.53 |
| 1:A:209:ILE:HG22 | 1:A:211:GLY:H | 1.73 | 0.53 |
| 1:F:60:ASP:OD2 | 1:F:62:VAL:HG12 | 2.09 | 0.53 |
| 1:G:287:GLN:HE22 | 1:G:311:LYS:HG3 | 1.74 | 0.53 |
| 1:G:374:GLU:O | 1:G:377:ILE:HG22 | 2.08 | 0.53 |
| 1:H:346:ARG:NH2 | 1:H:355:PHE:HD2 | 2.07 | 0.53 |
| 1:G:307:ARG:NH1 | 1:G:308:ARG:NH2 | 2.57 | 0.53 |
| 1:B:29:ARG:NH2 | 1:C:10:GLU:OE2 | 2.38 | 0.53 |
| 1:H:213:LEU:HD13 | 1:H:355:PHE:CD1 | 2.44 | 0.53 |
| 1:B:24:ASN:ND2 | 1:B:74:ALA:HB2 | 2.16 | 0.52 |
| 1:C:235:LEU:HG | 1:C:237:GLU:H | 1.74 | 0.52 |
| 1:D:266:GLU:HG2 | 1:D:293:LEU:HD21 | 1.91 | 0.52 |
| 1:G:20:ALA:HB1 | 1:G:515:VAL:HG12 | 1.91 | 0.52 |
| 1:A:213:LEU:HD21 | 1:A:353:MET:HE1 | 1.90 | 0.52 |
| 1:B:105:ARG:HD2 | 1:C:10:GLU:OE2 | 2.08 | 0.52 |
| 1:D:206:THR:HG23 | 1:D:368:LEU:O | 2.10 | 0.52 |
| 1:E:80:GLU:O | 1:E:84:THR:HG23 | 2.09 | 0.52 |
| 1:G:29:ARG:NH2 | 1:G:105:ARG:HH11 | 2.07 | 0.52 |
| 1:A:64:ILE:O | 1:A:68:MET:HG3 | 2.09 | 0.52 |
| 1:A:416:ARG:HH12 | 1:A:460:ARG:CZ | 2.22 | 0.52 |
| 1:B:514:ASP:OD1 | 1:B:515:VAL:N | 2.41 | 0.52 |
| 1:E:135:LEU:HD21 | 1:E:411:LEU:HD11 | 1.91 | 0.52 |
| 1:A:413:MET:HE1 | 1:A:463:HIS:HB3 | 1.92 | 0.52 |
| 1:B:29:ARG:NH1 | 1:B:108:GLU:OE1 | 2.43 | 0.52 |
| 1:C:313:ASP:HA | 1:C:316:LYS:HE2 | 1.90 | 0.52 |
| 1:F:29:ARG:NH1 | 1:F:108:GLU:OE1 | 2.42 | 0.52 |
| 1:F:123:GLY:HA3 | 1:F:429:ALA:HB3 | 1.90 | 0.52 |
| 1:A:401:VAL:HG21 | 1:A:495:LYS:HG3 | 1.92 | 0.52 |
| 1:B:209:ILE:HG22 | 1:B:211:GLY:H | 1.74 | 0.52 |
| 1:H:30:ILE:O | 1:H:34:THR:HG23 | 2.10 | 0.52 |
| 1:F:218:ARG:HD2 | 1:F:223:MET:HB2 | 1.90 | 0.52 |
| 1:H:348:ILE:HG22 | 1:H:349:SER:H | 1.73 | 0.52 |
| 1:A:424:GLY:O | 1:A:427:GLN:HG3 | 2.10 | 0.52 |
| 1:C:135:LEU:HA | 1:C:138:ILE:HG22 | 1.91 | 0.52 |
| 1:F:265:GLU:OE2 | 1:G:246:THR:HB | 2.10 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:451:ASP:HB3 | 1:H:454:GLU:HG2 | 1.91 | 0.52 |
| 1:B:169:LYS:NZ | 1:B:204:ASP:O | 2.32 | 0.52 |
| 1:F:339:ASP:HB2 | 1:F:360:LYS:HE2 | 1.91 | 0.52 |
| 1:H:25:ILE:HG23 | 1:H:104:LEU:HB3 | 1.92 | 0.52 |
| 1:F:273:VAL:HG13 | 1:F:298:LEU:HD23 | 1.91 | 0.52 |
| 1:G:250:ILE:HD11 | 1:G:261:PHE:CD1 | 2.44 | 0.52 |
| 1:C:135:LEU:HD11 | 1:C:499:ILE:HD12 | 1.92 | 0.52 |
| 1:E:286:VAL:HG22 | 1:E:288:LYS:H | 1.75 | 0.51 |
| 1:H:123:GLY:HA3 | 1:H:429:ALA:HB3 | 1.93 | 0.51 |
| 1:H:286:VAL:HG12 | 1:H:288:LYS:H | 1.75 | 0.51 |
| 1:C:155:MET:HA | 1:C:158:ILE:HG22 | 1.93 | 0.51 |
| 1:E:220:SER:HB2 | 1:E:295:GLN:HG2 | 1.91 | 0.51 |
| 1:F:29:ARG:NH2 | 1:F:105:ARG:HH11 | 2.08 | 0.51 |
| 1:B:307:ARG:HD2 | 1:B:308:ARG:NH1 | 2.25 | 0.51 |
| 1:D:144:ALA:HB1 | 1:D:395:ILE:HG23 | 1.92 | 0.51 |
| 1:H:287:GLN:CG | 1:H:314:MET:HG3 | 2.40 | 0.51 |
| 1:H:321:THR:HG22 | 1:H:359:VAL:HG23 | 1.93 | 0.51 |
| 1:A:105:ARG:HD2 | 1:B:10:GLU:OE2 | 2.10 | 0.51 |
| 1:C:20:ALA:HB1 | 1:C:515:VAL:HG12 | 1.92 | 0.51 |
| 1:H:237:GLU:OE1 | 1:H:328:ASN:HA | 2.11 | 0.51 |
| 1:E:241:ILE:HD13 | 1:E:265:GLU:OE1 | 2.11 | 0.51 |
| 1:H:235:LEU:HG | 1:H:237:GLU:H | 1.76 | 0.51 |
| 1:E:250:ILE:HG21 | 1:F:246:THR:HG23 | 1.91 | 0.51 |
| 1:H:66:ARG:NH1 | 1:H:67:GLU:OE2 | 2.44 | 0.51 |
| 1:A:449:GLY:HA3 | 1:B:119:ILE:CD1 | 2.40 | 0.51 |
| 1:E:292:ASP:O | 1:E:295:GLN:HB3 | 2.10 | 0.51 |
| 1:F:60:ASP:O | 1:F:64:ILE:HD12 | 2.10 | 0.51 |
| 1:F:192:LEU:HD13 | 1:F:363:LYS:HB3 | 1.93 | 0.51 |
| 1:E:465:SER:OG | 1:E:466:ASN:N | 2.44 | 0.51 |
| 1:G:123:GLY:HA3 | 1:G:429:ALA:HB3 | 1.93 | 0.51 |
| 1:C:29:ARG:NH1 | 1:C:108:GLU:OE1 | 2.44 | 0.50 |
| 1:D:66:ARG:NH1 | 1:D:67:GLU:OE2 | 2.44 | 0.50 |
| 1:G:346:ARG:HD2 | 1:G:355:PHE:CD2 | 2.46 | 0.50 |
| 1:F:286:VAL:HG13 | 1:F:307:ARG:HA | 1.93 | 0.50 |
| 1:H:24:ASN:HB3 | 1:H:509:LEU:HD12 | 1.94 | 0.50 |
| 1:C:287:GLN:HE22 | 1:C:311:LYS:HD2 | 1.77 | 0.50 |
| 1:G:56:VAL:HG23 | 1:H:521:LEU:HD23 | 1.94 | 0.50 |
| 1:G:252:ILE:HG12 | 1:G:261:PHE:CE2 | 2.46 | 0.50 |
| 1:H:18:ARG:NH1 | 1:H:111:LEU:HB3 | 2.26 | 0.50 |
| 1:A:373:THR:OG1 | 1:A:376:VAL:HG22 | 2.12 | 0.50 |
| 1:F:254:ASP:HB3 | 1:F:257:LYS:HG3 | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:291:ASP:OD1 | 1:G:292:ASP:N | 2.44 | 0.50 |
| 1:H:232:ILE:HG12 | 1:H:283:VAL:CG2 | 2.41 | 0.50 |
| 1:A:213:LEU:HB3 | 1:A:366:THR:HG21 | 1.93 | 0.50 |
| 1:B:209:ILE:HD13 | 1:B:213:LEU:HD21 | 1.93 | 0.50 |
| 1:C:468:ASN:HD21 | 1:C:482:ASP:HB2 | 1.75 | 0.50 |
| 1:E:119:ILE:HD13 | 1:E:425:ARG:HE | 1.76 | 0.50 |
| 1:F:235:LEU:HG | 1:F:237:GLU:H | 1.77 | 0.50 |
| 1:F:237:GLU:HB2 | 1:F:327:THR:O | 2.11 | 0.50 |
| 1:H:218:ARG:NH1 | 1:H:225:LYS:HZ2 | 2.08 | 0.50 |
| 1:A:397:ASP:OD2 | 1:A:493:ARG:HB2 | 2.11 | 0.50 |
| 1:B:215:ASP:HA | 1:B:353:MET:HB2 | 1.94 | 0.50 |
| 1:B:451:ASP:HB3 | 1:B:454:GLU:HG2 | 1.94 | 0.50 |
| 1:C:19:ASP:O | 1:C:23:MET:HG2 | 2.11 | 0.50 |
| 1:D:29:ARG:NH1 | 1:D:108:GLU:OE1 | 2.45 | 0.49 |
| 1:D:346:ARG:HD2 | 1:D:355:PHE:CE2 | 2.47 | 0.49 |
| 1:F:313:ASP:OD1 | 1:F:316:LYS:HE2 | 2.12 | 0.49 |
| 1:H:273:VAL:HG13 | 1:H:298:LEU:HD23 | 1.93 | 0.49 |
| 1:A:463:HIS:HE1 | 1:A:469:LYS:O | 1.94 | 0.49 |
| 1:E:442:ARG:HG3 | 1:E:452:ALA:HB1 | 1.94 | 0.49 |
| 1:G:239:ILE:HD12 | 1:G:290:ILE:HG12 | 1.94 | 0.49 |
| 1:G:287:GLN:NE2 | 1:G:311:LYS:HG3 | 2.26 | 0.49 |
| 1:B:339:ASP:HB2 | 1:B:360:LYS:HE3 | 1.95 | 0.49 |
| 1:E:30:ILE:O | 1:E:34:THR:HG23 | 2.13 | 0.49 |
| 1:H:231:LYS:HB3 | 1:H:337:LEU:HD13 | 1.94 | 0.49 |
| 1:H:348:ILE:HG22 | 1:H:349:SER:N | 2.28 | 0.49 |
| 1:H:397:ASP:OD2 | 1:H:493:ARG:HB2 | 2.12 | 0.49 |
| 1:E:346:ARG:HD2 | 1:E:355:PHE:CD2 | 2.47 | 0.49 |
| 1:E:326:ILE:HG23 | 1:E:331:ASP:HB2 | 1.94 | 0.49 |
| 1:F:284:LEU:O | 1:F:305:ALA:HA | 2.12 | 0.49 |
| 1:C:218:ARG:HH12 | 1:C:225:LYS:HZ3 | 1.60 | 0.49 |
| 1:C:291:ASP:OD1 | 1:C:292:ASP:N | 2.45 | 0.49 |
| 1:F:105:ARG:HD2 | 1:G:10:GLU:OE2 | 2.12 | 0.49 |
| 1:C:47:MET:HE1 | 1:D:77:MET:HG3 | 1.94 | 0.49 |
| 1:E:416:ARG:NH1 | 1:E:435:ASP:OD1 | 2.45 | 0.49 |
| 1:G:34:THR:O | 1:G:46:LYS:HE2 | 2.12 | 0.49 |
| 1:E:267:LYS:HD2 | 1:E:270:LYS:HE3 | 1.95 | 0.49 |
| 1:F:409:VAL:HG11 | 1:F:459:VAL:HG12 | 1.95 | 0.49 |
| 1:H:502:ALA:O | 1:H:506:THR:HG22 | 2.13 | 0.49 |
| 1:A:33:GLU:OE1 | 1:A:36:ARG:HD3 | 2.13 | 0.48 |
| 1:C:237:GLU:OE1 | 1:C:328:ASN:HA | 2.12 | 0.48 |
| 1:C:427:GLN:HG3 | 1:C:428:LEU:HD12 | 1.94 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:20:ALA:HB1 | 1:F:515:VAL:HG12 | 1.94 | 0.48 |
| 1:G:24:ASN:HB3 | 1:G:509:LEU:HD12 | 1.95 | 0.48 |
| 1:G:29:ARG:NH2 | 1:G:105:ARG:NH1 | 2.61 | 0.48 |
| 1:H:213:LEU:HD21 | 1:H:353:MET:HE1 | 1.95 | 0.48 |
| 1:D:163:ALA:O | 1:D:165:LYS:N | 2.45 | 0.48 |
| 1:F:49:VAL:HG22 | 1:F:55:VAL:HG12 | 1.95 | 0.48 |
| 1:G:250:ILE:HG21 | 1:H:246:THR:HG23 | 1.95 | 0.48 |
| 1:H:313:ASP:HA | 1:H:316:LYS:HE2 | 1.95 | 0.48 |
| 1:A:265:GLU:OE2 | 1:B:246:THR:HB | 2.13 | 0.48 |
| 1:C:286:VAL:HG22 | 1:C:288:LYS:H | 1.77 | 0.48 |
| 1:F:286:VAL:HG22 | 1:F:288:LYS:H | 1.78 | 0.48 |
| 1:H:135:LEU:HD21 | 1:H:411:LEU:HD11 | 1.95 | 0.48 |
| 1:H:287:GLN:HE22 | 1:H:311:LYS:HG3 | 1.78 | 0.48 |
| 1:H:320:ALA:O | 1:H:361:HIS:ND1 | 2.37 | 0.48 |
| 1:B:508:MET:HG3 | 1:B:509:LEU:N | 2.28 | 0.48 |
| 1:E:241:ILE:HG13 | 1:E:269:LEU:HD11 | 1.94 | 0.48 |
| 1:C:213:LEU:HD21 | 1:C:353:MET:HE1 | 1.96 | 0.48 |
| 1:C:514:ASP:OD1 | 1:C:515:VAL:N | 2.47 | 0.48 |
| 1:F:514:ASP:OD1 | 1:F:515:VAL:N | 2.47 | 0.48 |
| 1:G:18:ARG:O | 1:G:22:ARG:HG2 | 2.13 | 0.48 |
| 1:E:29:ARG:NH1 | 1:E:108:GLU:OE1 | 2.47 | 0.48 |
| 1:F:165:LYS:HE3 | 1:F:203:ILE:HG22 | 1.95 | 0.48 |
| 1:B:14:ARG:O | 1:B:18:ARG:HG3 | 2.13 | 0.48 |
| 1:B:213:LEU:HD22 | 1:B:355:PHE:CD1 | 2.49 | 0.48 |
| 1:F:135:LEU:HB3 | 1:F:492:LEU:HD11 | 1.95 | 0.48 |
| 1:H:450:LEU:HD12 | 1:H:473:LEU:HD21 | 1.96 | 0.48 |
| 1:H:518:ALA:CB | 1:H:521:LEU:HD11 | 2.44 | 0.48 |
| 1:A:153:ILE:HD13 | 1:A:489:VAL:HG13 | 1.96 | 0.48 |
| 1:A:180:ALA:O | 1:A:363:LYS:HD2 | 2.14 | 0.48 |
| 1:B:159:THR:OG1 | 1:B:167:LYS:NZ | 2.40 | 0.48 |
| 1:A:269:LEU:HD23 | 1:A:294:ALA:N | 2.28 | 0.48 |
| 1:B:87:LYS:HB3 | 1:B:89:VAL:HG22 | 1.96 | 0.48 |
| 1:C:80:GLU:O | 1:C:84:THR:HG23 | 2.14 | 0.48 |
| 1:F:226:LYS:HE3 | 1:F:342:LEU:HD11 | 1.96 | 0.48 |
| 1:B:29:ARG:NH2 | 1:B:105:ARG:NH1 | 2.62 | 0.48 |
| 1:C:254:ASP:HB3 | 1:C:257:LYS:HG2 | 1.95 | 0.48 |
| 1:C:272:MET:O | 1:C:276:ILE:HD12 | 2.14 | 0.48 |
| 1:E:199:SER:O | 1:E:370:ARG:NH2 | 2.42 | 0.48 |
| 1:F:374:GLU:HA | 1:F:377:ILE:HB | 1.96 | 0.48 |
| 1:A:31:ILE:O | 1:A:34:THR:HG22 | 2.14 | 0.47 |
| 1:B:438:GLU:HB3 | 1:B:456:LEU:HD11 | 1.96 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:424:GLY:O | 1:H:427:GLN:HG3 | 2.14 | 0.47 |
| 1:A:251:ARG:HD2 | 1:B:251:ARG:CG | 2.44 | 0.47 |
| 1:B:346:ARG:O | 1:B:352:SER:HB2 | 2.12 | 0.47 |
| 1:G:60:ASP:OD2 | 1:G:63:THR:OG1 | 2.15 | 0.47 |
| 1:G:346:ARG:NH2 | 1:G:357:GLU:OE1 | 2.47 | 0.47 |
| 1:C:34:THR:O | 1:C:46:LYS:HE3 | 2.14 | 0.47 |
| 1:F:215:ASP:HB2 | 1:F:353:MET:HE3 | 1.96 | 0.47 |
| 1:H:49:VAL:HG22 | 1:H:55:VAL:HG12 | 1.97 | 0.47 |
| 1:A:250:ILE:HG13 | 1:H:252:ILE:HB | 1.96 | 0.47 |
| 1:A:374:GLU:HA | 1:A:377:ILE:HB | 1.95 | 0.47 |
| 1:C:197:LYS:HB2 | 1:C:377:ILE:CG2 | 2.44 | 0.47 |
| 1:D:10:GLU:H | 1:D:10:GLU:HG2 | 1.50 | 0.47 |
| 1:D:273:VAL:HG13 | 1:D:298:LEU:HD23 | 1.97 | 0.47 |
| 1:F:231:LYS:HB3 | 1:F:337:LEU:HD13 | 1.96 | 0.47 |
| 1:G:103:LEU:HB2 | 1:G:506:THR:HG21 | 1.95 | 0.47 |
| 1:G:105:ARG:HD2 | 1:H:10:GLU:OE2 | 2.14 | 0.47 |
| 1:G:232:ILE:HD13 | 1:G:283:VAL:HB | 1.95 | 0.47 |
| 1:A:513:ASP:OD1 | 1:A:514:ASP:N | 2.48 | 0.47 |
| 1:D:218:ARG:NH1 | 1:D:225:LYS:HZ3 | 2.12 | 0.47 |
| 1:D:251:ARG:HA | 1:E:249:GLU:O | 2.15 | 0.47 |
| 1:D:482:ASP:O | 1:D:486:ASN:ND2 | 2.46 | 0.47 |
| 1:G:194:LYS:HE3 | 1:G:316:LYS:HB3 | 1.96 | 0.47 |
| 1:H:211:GLY:HA3 | 1:H:357:GLU:HA | 1.97 | 0.47 |
| 1:D:103:LEU:HB2 | 1:D:506:THR:HG21 | 1.96 | 0.47 |
| 1:E:44:MET:CE | 1:F:116:HIS:HE1 | 2.28 | 0.47 |
| 1:A:252:ILE:HG12 | 1:A:261:PHE:CE2 | 2.50 | 0.47 |
| 1:B:287:GLN:HE22 | 1:B:311:LYS:HE2 | 1.79 | 0.47 |
| 1:B:349:SER:OG | 1:B:370:ARG:NH2 | 2.47 | 0.47 |
| 1:D:25:ILE:HG23 | 1:D:104:LEU:HB3 | 1.97 | 0.47 |
| 1:E:218:ARG:NH2 | 1:E:225:LYS:NZ | 2.61 | 0.47 |
| 1:G:313:ASP:OD1 | 1:G:316:LYS:HE2 | 2.14 | 0.47 |
| 1:H:252:ILE:HD13 | 1:H:258:LEU:HD23 | 1.97 | 0.47 |
| 1:H:284:LEU:HD21 | 1:H:286:VAL:HG23 | 1.96 | 0.47 |
| 1:F:10:GLU:H | 1:F:10:GLU:HG2 | 1.51 | 0.47 |
| 1:A:346:ARG:HD2 | 1:A:355:PHE:CE2 | 2.50 | 0.46 |
| 1:B:34:THR:O | 1:B:46:LYS:HE3 | 2.15 | 0.46 |
| 1:C:502:ALA:O | 1:C:506:THR:HG22 | 2.14 | 0.46 |
| 1:D:231:LYS:HB3 | 1:D:337:LEU:HD13 | 1.97 | 0.46 |
| 1:E:244:THR:HB | 1:E:246:THR:HG22 | 1.97 | 0.46 |
| 1:F:287:GLN:NE2 | 1:F:311:LYS:HB2 | 2.30 | 0.46 |
| 1:H:438:GLU:OE2 | 1:H:460:ARG:NH2 | 2.29 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:178:VAL:HG22 | 1:C:388:VAL:HG13 | 1.97 | 0.46 |
| 1:D:80:GLU:O | 1:D:84:THR:HG23 | 2.16 | 0.46 |
| 1:E:287:GLN:NE2 | 1:E:311:LYS:HB2 | 2.30 | 0.46 |
| 1:F:386:ASP:O | 1:F:390:VAL:HG23 | 2.15 | 0.46 |
| 1:G:49:VAL:HG22 | 1:G:55:VAL:HG12 | 1.97 | 0.46 |
| 1:G:190:LYS:NZ | 1:G:388:VAL:HG12 | 2.29 | 0.46 |
| 1:D:514:ASP:OD1 | 1:D:515:VAL:N | 2.47 | 0.46 |
| 1:B:250:ILE:HG23 | 1:C:248:ALA:CA | 2.45 | 0.46 |
| 1:E:251:ARG:NH1 | 1:F:249:GLU:HB2 | 2.30 | 0.46 |
| 1:E:363:LYS:H | 1:E:363:LYS:HD2 | 1.79 | 0.46 |
| 1:G:46:LYS:HD2 | 1:H:514:ASP:HB3 | 1.97 | 0.46 |
| 1:G:251:ARG:HD2 | 1:H:251:ARG:HG2 | 1.97 | 0.46 |
| 1:A:266:GLU:HG2 | 1:A:293:LEU:CD2 | 2.46 | 0.46 |
| 1:B:165:LYS:HB2 | 1:B:203:ILE:HD11 | 1.97 | 0.46 |
| 1:B:213:LEU:HB3 | 1:B:353:MET:HE1 | 1.97 | 0.46 |
| 1:G:326:ILE:HD13 | 1:G:332:LEU:HA | 1.96 | 0.46 |
| 1:G:455:ILE:HG21 | 1:G:473:LEU:HD22 | 1.97 | 0.46 |
| 1:A:25:ILE:HG23 | 1:A:104:LEU:HB3 | 1.97 | 0.46 |
| 1:C:250:ILE:HD12 | 1:D:246:THR:HG21 | 1.97 | 0.46 |
| 1:F:87:LYS:HD3 | 1:F:493:ARG:CZ | 2.45 | 0.46 |
| 1:G:269:LEU:HD23 | 1:G:294:ALA:N | 2.31 | 0.46 |
| 1:F:60:ASP:OD2 | 1:F:63:THR:OG1 | 2.19 | 0.46 |
| 1:F:344:GLU:CD | 1:F:346:ARG:HH11 | 2.14 | 0.46 |
| 1:G:37:SER:HG | 1:G:46:LYS:NZ | 2.13 | 0.46 |
| 1:A:213:LEU:HD13 | 1:A:355:PHE:CD1 | 2.50 | 0.46 |
| 1:A:450:LEU:HD12 | 1:A:473:LEU:HD21 | 1.97 | 0.46 |
| 1:D:123:GLY:HA3 | 1:D:429:ALA:HB3 | 1.97 | 0.46 |
| 1:F:178:VAL:HG22 | 1:F:388:VAL:HG13 | 1.98 | 0.46 |
| 1:A:86:GLU:HB2 | 1:A:497:GLN:NE2 | 2.31 | 0.46 |
| 1:C:138:ILE:HG13 | 1:C:469:LYS:HD3 | 1.98 | 0.46 |
| 1:D:370:ARG:C | 1:D:377:ILE:HD11 | 2.36 | 0.46 |
| 1:F:232:ILE:HD12 | 1:F:321:THR:HG21 | 1.98 | 0.46 |
| 1:A:46:LYS:HZ3 | 1:B:513:ASP:CG | 2.18 | 0.46 |
| 1:D:164:GLU:HA | 1:D:167:LYS:HE3 | 1.97 | 0.46 |
| 1:D:508:MET:HB3 | 1:D:508:MET:HE2 | 1.79 | 0.46 |
| 1:E:46:LYS:HE2 | 1:F:513:ASP:OD1 | 2.15 | 0.46 |
| 1:F:31:ILE:HG13 | 1:F:75:ALA:HB1 | 1.98 | 0.46 |
| 1:G:29:ARG:NH2 | 1:H:9:PRO:HD2 | 2.31 | 0.46 |
| 1:H:218:ARG:NH2 | 1:H:225:LYS:NZ | 2.53 | 0.46 |
| 1:A:22:ARG:HH22 | 1:A:111:LEU:HB2 | 1.80 | 0.45 |
| 1:B:34:THR:HG22 | 1:C:13:LYS:HE2 | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:D:269:LEU:HD23 | 1:D:294:ALA:N | 2.31 | 0.45 |
| 1:H:288:LYS:O | 1:H:308:ARG:HG2 | 2.16 | 0.45 |
| 1:C:139:ALA:HB2 | 1:C:492:LEU:HD13 | 1.98 | 0.45 |
| 1:C:438:GLU:CD | 1:C:460:ARG:HH21 | 2.11 | 0.45 |
| 1:D:70:VAL:HG12 | 1:D:76:LYS:HG3 | 1.98 | 0.45 |
| 1:E:19:ASP:O | 1:E:23:MET:HG2 | 2.16 | 0.45 |
| 1:E:20:ALA:HB1 | 1:E:515:VAL:HG22 | 1.97 | 0.45 |
| 1:B:254:ASP:HB3 | 1:B:257:LYS:HG2 | 1.98 | 0.45 |
| 1:D:47:MET:HB3 | 1:E:515:VAL:HG12 | 1.98 | 0.45 |
| 1:E:10:GLU:H | 1:E:10:GLU:HG2 | 1.46 | 0.45 |
| 1:E:213:LEU:HD21 | 1:E:353:MET:HE1 | 1.98 | 0.45 |
| 1:G:94:THR:HB | 2:G:601:SO4:O1 | 2.16 | 0.45 |
| 1:G:180:ALA:O | 1:G:363:LYS:HD2 | 2.16 | 0.45 |
| 1:G:198:LYS:HZ3 | 1:G:348:ILE:HD11 | 1.80 | 0.45 |
| 1:G:273:VAL:HG13 | 1:G:298:LEU:HD23 | 1.98 | 0.45 |
| 1:A:416:ARG:HH12 | 1:A:460:ARG:NH2 | 2.13 | 0.45 |
| 1:C:370:ARG:C | 1:C:377:ILE:HD11 | 2.36 | 0.45 |
| 1:F:346:ARG:NH2 | 1:F:355:PHE:HD2 | 2.11 | 0.45 |
| 1:E:218:ARG:NH1 | 1:E:225:LYS:HG2 | 2.32 | 0.45 |
| 1:A:516:ILE:HD11 | 1:H:64:ILE:HG23 | 1.98 | 0.45 |
| 1:B:45:ASP:O | 1:C:512:ILE:HA | 2.17 | 0.45 |
| 1:E:195:ILE:HG13 | 1:E:385:ASP:OD1 | 2.16 | 0.45 |
| 1:G:252:ILE:HB | 1:H:250:ILE:HG12 | 1.99 | 0.45 |
| 1:H:218:ARG:NH1 | 1:H:225:LYS:HG2 | 2.32 | 0.45 |
| 1:D:199:SER:O | 1:D:370:ARG:NH2 | 2.43 | 0.45 |
| 1:D:235:LEU:O | 1:D:286:VAL:HA | 2.16 | 0.45 |
| 1:H:80:GLU:O | 1:H:84:THR:HG23 | 2.16 | 0.45 |
| 1:A:49:VAL:HG22 | 1:A:55:VAL:HG12 | 1.99 | 0.45 |
| 1:C:449:GLY:O | 1:D:425:ARG:NH2 | 2.46 | 0.45 |
| 1:F:141:GLU:HG2 | 1:F:399:ARG:HG2 | 1.98 | 0.45 |
| 1:A:235:LEU:HG | 1:A:237:GLU:H | 1.82 | 0.45 |
| 1:B:180:ALA:O | 1:B:363:LYS:HD2 | 2.15 | 0.45 |
| 1:G:286:VAL:HG22 | 1:G:288:LYS:H | 1.81 | 0.45 |
| 1:A:291:ASP:OD1 | 1:A:292:ASP:N | 2.50 | 0.45 |
| 1:C:142:VAL:HG21 | 1:C:149:ILE:HG21 | 1.99 | 0.45 |
| 1:B:25:ILE:HG23 | 1:B:104:LEU:HB3 | 1.98 | 0.44 |
| 1:B:89:VAL:HG12 | 1:B:389:GLY:HA2 | 1.98 | 0.44 |
| 1:C:227:VAL:HG11 | 1:C:282:ASN:HB3 | 1.99 | 0.44 |
| 1:D:18:ARG:O | 1:D:22:ARG:HG2 | 2.17 | 0.44 |
| 1:E:135:LEU:HD11 | 1:E:499:ILE:HD12 | 2.00 | 0.44 |
| 1:E:142:VAL:HG11 | 1:E:149:ILE:HG21 | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:F:291:ASP:OD1 | 1:F:292:ASP:N | 2.49 | 0.44 |
| 1:G:313:ASP:HA | 1:G:316:LYS:HE2 | 1.99 | 0.44 |
| 1:H:254:ASP:HB3 | 1:H:257:LYS:HG3 | 1.99 | 0.44 |
| 1:A:131:ALA:HB1 | 1:A:499:ILE:HD13 | 1.98 | 0.44 |
| 1:A:218:ARG:NH1 | 1:A:225:LYS:HG2 | 2.32 | 0.44 |
| 1:A:380:VAL:O | 1:A:384:VAL:HG23 | 2.16 | 0.44 |
| 1:B:235:LEU:HG | 1:B:237:GLU:H | 1.82 | 0.44 |
| 1:E:313:ASP:OD1 | 1:E:316:LYS:HE2 | 2.17 | 0.44 |
| 1:H:29:ARG:HH11 | 1:H:108:GLU:CD | 2.20 | 0.44 |
| 1:C:18:ARG:HD2 | 1:C:22:ARG:HE | 1.81 | 0.44 |
| 1:B:195:ILE:HA | 1:B:367:MET:HB2 | 1.98 | 0.44 |
| 1:D:128:ALA:O | 1:D:132:GLN:HG2 | 2.18 | 0.44 |
| 1:H:377:ILE:HD13 | 1:H:377:ILE:HA | 1.83 | 0.44 |
| 1:A:269:LEU:HD21 | 1:A:291:ASP:OD2 | 2.18 | 0.44 |
| 1:C:123:GLY:HA3 | 1:C:429:ALA:HB3 | 1.98 | 0.44 |
| 1:F:313:ASP:HA | 1:F:316:LYS:HE2 | 1.99 | 0.44 |
| 1:G:14:ARG:O | 1:G:18:ARG:HG2 | 2.17 | 0.44 |
| 1:H:232:ILE:HD12 | 1:H:321:THR:HG21 | 2.00 | 0.44 |
| 1:A:119:ILE:HG12 | 1:A:425:ARG:HD2 | 1.99 | 0.44 |
| 1:A:511:ARG:O | 1:A:511:ARG:HG2 | 2.17 | 0.44 |
| 1:C:25:ILE:HG23 | 1:C:104:LEU:HB3 | 1.98 | 0.44 |
| 1:E:150:LEU:HD22 | 1:E:391:VAL:HG13 | 2.00 | 0.44 |
| 1:H:241:ILE:HD13 | 1:H:241:ILE:HA | 1.86 | 0.44 |
| 1:A:178:VAL:HA | 1:A:193:ILE:HD11 | 2.00 | 0.44 |
| 1:A:321:THR:HG22 | 1:A:359:VAL:HG23 | 1.99 | 0.44 |
| 1:C:29:ARG:HH11 | 1:C:108:GLU:CD | 2.21 | 0.44 |
| 1:D:19:ASP:O | 1:D:23:MET:HG2 | 2.16 | 0.44 |
| 1:E:119:ILE:CD1 | 1:E:425:ARG:HE | 2.31 | 0.44 |
| 1:G:313:ASP:HA | 1:G:316:LYS:HG2 | 1.99 | 0.44 |
| 1:H:161:LYS:NZ | 3:H:701:HOH:O | 2.41 | 0.44 |
| 1:F:29:ARG:HH11 | 1:F:108:GLU:CD | 2.21 | 0.44 |
| 1:F:237:GLU:OE1 | 1:F:328:ASN:HA | 2.18 | 0.44 |
| 1:H:514:ASP:OD1 | 1:H:515:VAL:N | 2.51 | 0.44 |
| 1:A:266:GLU:HG2 | 1:A:293:LEU:HD21 | 2.00 | 0.43 |
| 1:B:90:GLY:HA2 | 1:B:494:VAL:HG22 | 1.99 | 0.43 |
| 1:B:293:LEU:O | 1:B:296:HIS:HB3 | 2.17 | 0.43 |
| 1:C:135:LEU:HD21 | 1:C:411:LEU:HD11 | 1.99 | 0.43 |
| 1:C:277:LYS:HD3 | 1:C:303:ILE:HD11 | 2.00 | 0.43 |
| 1:E:31:ILE:HG13 | 1:E:75:ALA:HB1 | 2.00 | 0.43 |
| 1:E:78:LEU:HB2 | 1:E:509:LEU:HD21 | 2.00 | 0.43 |
| 1:F:45:ASP:O | 1:G:512:ILE:HA | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:B:218:ARG:NH1 | 1:B:225:LYS:HG2 | 2.34 | 0.43 |
| 1:B:250:ILE:HG21 | 1:C:246:THR:HG23 | 2.00 | 0.43 |
| 1:C:218:ARG:HD2 | 1:C:223:MET:HB2 | 1.99 | 0.43 |
| 1:B:31:ILE:HG13 | 1:B:75:ALA:HB1 | 2.00 | 0.43 |
| 1:D:149:ILE:HD13 | 1:D:149:ILE:HA | 1.88 | 0.43 |
| 1:G:45:ASP:O | 1:H:512:ILE:HA | 2.19 | 0.43 |
| 1:G:89:VAL:CG1 | 1:G:190:LYS:HD2 | 2.48 | 0.43 |
| 1:D:89:VAL:HG22 | 1:D:393:SER:HB2 | 2.00 | 0.43 |
| 1:E:218:ARG:NH1 | 1:E:225:LYS:NZ | 2.63 | 0.43 |
| 1:G:213:LEU:HD13 | 1:G:355:PHE:CD1 | 2.53 | 0.43 |
| 1:D:29:ARG:NH2 | 1:E:10:GLU:OE2 | 2.47 | 0.43 |
| 1:E:123:GLY:HA3 | 1:E:429:ALA:HB3 | 2.00 | 0.43 |
| 1:G:508:MET:HE2 | 1:G:509:LEU:HD22 | 1.99 | 0.43 |
| 1:H:252:ILE:HG12 | 1:H:261:PHE:CE2 | 2.53 | 0.43 |
| 1:A:29:ARG:NH1 | 1:A:108:GLU:OE1 | 2.51 | 0.43 |
| 1:A:34:THR:O | 1:A:46:LYS:HE3 | 2.18 | 0.43 |
| 1:A:235:LEU:HD11 | 1:A:237:GLU:HB3 | 2.01 | 0.43 |
| 1:A:415:LEU:O | 1:A:419:ALA:N | 2.49 | 0.43 |
| 1:C:34:THR:HG22 | 1:D:13:LYS:HE2 | 2.01 | 0.43 |
| 1:E:266:GLU:HG2 | 1:E:293:LEU:HD21 | 1.99 | 0.43 |
| 1:G:35:VAL:O | 1:G:38:THR:OG1 | 2.32 | 0.43 |
| 1:B:218:ARG:HD2 | 1:B:223:MET:HB2 | 1.99 | 0.43 |
| 1:B:241:ILE:HD13 | 1:C:245:GLU:HG2 | 2.00 | 0.43 |
| 1:B:252:ILE:HG12 | 1:B:261:PHE:CE2 | 2.54 | 0.43 |
| 1:C:387:ALA:HA | 1:C:390:VAL:HG22 | 2.00 | 0.43 |
| 1:E:29:ARG:HH11 | 1:E:108:GLU:CD | 2.22 | 0.43 |
| 1:H:219:VAL:HG23 | 1:H:307:ARG:HD3 | 2.01 | 0.43 |
| 1:E:219:VAL:HG22 | 1:E:295:GLN:NE2 | 2.34 | 0.43 |
| 1:G:44:MET:CE | 1:H:116:HIS:HE1 | 2.32 | 0.43 |
| 1:H:283:VAL:HA | 1:H:304:MET:O | 2.19 | 0.43 |
| 1:C:18:ARG:O | 1:C:22:ARG:HG2 | 2.18 | 0.43 |
| 1:C:321:THR:HG22 | 1:C:359:VAL:HG23 | 2.00 | 0.43 |
| 1:D:89:VAL:HG23 | 1:D:389:GLY:CA | 2.49 | 0.43 |
| 1:D:284:LEU:O | 1:D:305:ALA:HA | 2.19 | 0.43 |
| 1:D:377:ILE:HD13 | 1:D:377:ILE:HA | 1.74 | 0.43 |
| 1:E:94:THR:HB | 2:E:601:SO4:O1 | 2.19 | 0.43 |
| 1:E:313:ASP:HA | 1:E:316:LYS:HE2 | 2.00 | 0.43 |
| 1:D:135:LEU:HD11 | 1:D:499:ILE:HD12 | 2.00 | 0.42 |
| 1:D:348:ILE:HD11 | 1:D:355:PHE:CZ | 2.54 | 0.42 |
| 1:B:208:LEU:HD12 | 1:B:366:THR:O | 2.19 | 0.42 |
| 1:D:293:LEU:O | 1:D:296:HIS:HB3 | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:427:GLN:HG3 | 1:G:428:LEU:HD12 | 2.01 | 0.42 |
| 1:A:241:ILE:HD13 | 1:A:241:ILE:HA | 1.89 | 0.42 |
| 1:C:346:ARG:HD2 | 1:C:355:PHE:CD2 | 2.54 | 0.42 |
| 1:D:213:LEU:HD21 | 1:D:353:MET:HE1 | 2.00 | 0.42 |
| 1:E:514:ASP:OD1 | 1:E:515:VAL:N | 2.51 | 0.42 |
| 1:F:401:VAL:HG21 | 1:F:495:LYS:HG3 | 2.01 | 0.42 |
| 1:H:154:ALA:O | 1:H:158:ILE:HG12 | 2.19 | 0.42 |
| 1:A:346:ARG:HD2 | 1:A:355:PHE:CD2 | 2.54 | 0.42 |
| 1:C:284:LEU:O | 1:C:305:ALA:HA | 2.20 | 0.42 |
| 1:D:37:SER:HG | 1:D:46:LYS:NZ | 2.17 | 0.42 |
| 1:E:284:LEU:O | 1:E:305:ALA:HA | 2.19 | 0.42 |
| 1:E:291:ASP:OD1 | 1:E:292:ASP:N | 2.52 | 0.42 |
| 1:H:183:ASP:OD1 | 1:H:187:LYS:N | 2.52 | 0.42 |
| 1:A:119:ILE:CD1 | 1:H:449:GLY:HA3 | 2.50 | 0.42 |
| 1:C:373:THR:HB | 1:C:376:VAL:HG22 | 2.02 | 0.42 |
| 1:D:266:GLU:HG2 | 1:D:293:LEU:CD2 | 2.49 | 0.42 |
| 1:E:29:ARG:NH2 | 1:F:9:PRO:HD2 | 2.34 | 0.42 |
| 1:F:201:ALA:HB1 | 1:F:205:ASP:OD2 | 2.20 | 0.42 |
| 1:B:116:HIS:CG | 1:B:117:PRO:HD2 | 2.55 | 0.42 |
| 1:B:226:LYS:HE3 | 1:B:342:LEU:HD11 | 2.01 | 0.42 |
| 1:B:313:ASP:OD1 | 1:B:316:LYS:HE2 | 2.18 | 0.42 |
| 1:C:49:VAL:HG22 | 1:C:55:VAL:HG12 | 2.00 | 0.42 |
| 1:C:455:ILE:HG21 | 1:C:473:LEU:HD13 | 2.01 | 0.42 |
| 1:G:346:ARG:O | 1:G:352:SER:OG | 2.21 | 0.42 |
| 1:H:87:LYS:HB3 | 1:H:493:ARG:NH1 | 2.35 | 0.42 |
| 1:B:206:THR:HG23 | 1:B:368:LEU:O | 2.20 | 0.42 |
| 1:C:252:ILE:HG12 | 1:C:261:PHE:CE2 | 2.55 | 0.42 |
| 1:C:105:ARG:HD2 | 1:D:10:GLU:OE2 | 2.20 | 0.42 |
| 1:H:293:LEU:O | 1:H:296:HIS:HB3 | 2.19 | 0.42 |
| 1:A:29:ARG:NH2 | 1:B:10:GLU:OE2 | 2.48 | 0.42 |
| 1:A:394:THR:OG1 | 1:A:491:PRO:HG3 | 2.20 | 0.42 |
| 1:C:91:ASP:OD1 | 1:C:386:ASP:HB3 | 2.20 | 0.42 |
| 1:E:269:LEU:HD23 | 1:E:294:ALA:N | 2.35 | 0.42 |
| 1:F:13:LYS:HD2 | 1:F:13:LYS:HA | 1.89 | 0.42 |
| 1:F:147:LYS:O | 1:F:151:THR:HG23 | 2.20 | 0.42 |
| 1:F:438:GLU:CD | 1:F:460:ARG:HH21 | 2.19 | 0.42 |
| 1:D:320:ALA:HB1 | 1:D:359:VAL:HG21 | 2.01 | 0.42 |
| 1:A:84:THR:OG1 | 1:H:373:THR:HG22 | 2.20 | 0.41 |
| 1:C:89:VAL:CG2 | 1:C:493:ARG:HH11 | 2.33 | 0.41 |
| 1:D:313:ASP:OD1 | 1:D:316:LYS:HE2 | 2.20 | 0.41 |
| 1:H:164:GLU:H | 1:H:164:GLU:HG2 | 1.55 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:513:ASP:OD1 | 1:H:46:LYS:HE2 | 2.21 | 0.41 |
| 1:B:208:LEU:HD11 | 1:B:365:VAL:HG22 | 2.02 | 0.41 |
| 1:H:95:THR:HG23 | 1:H:440:ILE:HD12 | 2.02 | 0.41 |
| 1:C:30:ILE:O | 1:C:34:THR:HG23 | 2.20 | 0.41 |
| 1:C:418:TYR:CZ | 1:C:422:ILE:HD11 | 2.55 | 0.41 |
| 1:F:348:ILE:HG22 | 1:F:349:SER:N | 2.36 | 0.41 |
| 1:G:119:ILE:HD11 | 1:G:425:ARG:HH21 | 1.84 | 0.41 |
| 1:G:237:GLU:OE1 | 1:G:329:ILE:HG13 | 2.20 | 0.41 |
| 1:B:29:ARG:NH2 | 1:C:9:PRO:HD2 | 2.35 | 0.41 |
| 1:C:206:THR:HG23 | 1:C:369:ILE:HA | 2.02 | 0.41 |
| 1:C:313:ASP:OD1 | 1:C:316:LYS:HE2 | 2.20 | 0.41 |
| 1:C:409:VAL:HG11 | 1:C:459:VAL:HG12 | 2.01 | 0.41 |
| 1:G:218:ARG:HD2 | 1:G:223:MET:HB2 | 2.01 | 0.41 |
| 1:H:18:ARG:HA | 1:H:18:ARG:HD2 | 1.74 | 0.41 |
| 1:B:313:ASP:HA | 1:B:316:LYS:HG2 | 2.03 | 0.41 |
| 1:B:418:TYR:CE2 | 1:B:422:ILE:HD11 | 2.56 | 0.41 |
| 1:D:255:PRO:HG3 | 1:E:260:GLU:HB3 | 2.03 | 0.41 |
| 1:F:313:ASP:HA | 1:F:316:LYS:HG2 | 2.02 | 0.41 |
| 1:G:164:GLU:HA | 1:G:167:LYS:HB2 | 2.01 | 0.41 |
| 1:H:18:ARG:HH12 | 1:H:111:LEU:HD13 | 1.86 | 0.41 |
| 1:H:235:LEU:HB3 | 1:H:286:VAL:HG22 | 2.01 | 0.41 |
| 1:H:475:VAL:HG23 | 1:H:476:PHE:CD1 | 2.55 | 0.41 |
| 1:C:462:ALA:O | 1:C:467:GLY:HA3 | 2.20 | 0.41 |
| 1:D:9:PRO:O | 1:D:12:MET:HB3 | 2.20 | 0.41 |
| 1:E:219:VAL:HG22 | 1:E:295:GLN:CD | 2.41 | 0.41 |
| 1:E:418:TYR:CE2 | 1:E:422:ILE:HD11 | 2.55 | 0.41 |
| 1:G:41:PRO:HB3 | 1:G:159:THR:HG22 | 2.01 | 0.41 |
| 1:G:321:THR:HG22 | 1:G:359:VAL:HG23 | 2.02 | 0.41 |
| 1:F:147:LYS:HE3 | 1:F:179:SER:OG | 2.20 | 0.41 |
| 1:F:377:ILE:HA | 1:F:377:ILE:HD13 | 1.81 | 0.41 |
| 1:G:287:GLN:CG | 1:G:314:MET:HG3 | 2.49 | 0.41 |
| 1:H:508:MET:HE2 | 1:H:508:MET:HB3 | 1.86 | 0.41 |
| 1:B:348:ILE:HG13 | 1:B:348:ILE:O | 2.21 | 0.41 |
| 1:B:509:LEU:HD13 | 1:B:509:LEU:HA | 1.92 | 0.41 |
| 1:C:64:ILE:HG23 | 1:D:516:ILE:HD11 | 2.03 | 0.41 |
| 1:D:475:VAL:HG23 | 1:D:476:PHE:CD1 | 2.56 | 0.41 |
| 1:E:188:VAL:HG12 | 1:E:396:GLU:OE2 | 2.21 | 0.41 |
| 1:E:508:MET:HB3 | 1:E:508:MET:HE2 | 1.92 | 0.41 |
| 1:F:420:GLU:OE2 | 1:F:431:ARG:NH2 | 2.54 | 0.41 |
| 1:F:455:ILE:HG21 | 1:F:473:LEU:HD22 | 2.03 | 0.41 |
| 1:G:77:MET:HB3 | 1:G:508:MET:SD | 2.61 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:H:10:GLU:H | 1:H:10:GLU:HG2 | 1.54 | 0.41 |
| 1:A:164:GLU:O | 1:A:165:LYS:C | 2.59 | 0.41 |
| 1:A:267:LYS:HD2 | 1:A:270:LYS:HE3 | 2.02 | 0.41 |
| 1:C:66:ARG:NH1 | 1:C:67:GLU:OE2 | 2.53 | 0.41 |
| 1:C:241:ILE:HD11 | 1:C:268:MET:SD | 2.61 | 0.41 |
| 1:C:269:LEU:HD21 | 1:C:291:ASP:OD2 | 2.21 | 0.41 |
| 1:D:397:ASP:OD2 | 1:D:493:ARG:NE | 2.51 | 0.41 |
| 1:F:155:MET:O | 1:F:159:THR:OG1 | 2.31 | 0.41 |
| 1:B:390:VAL:HG12 | 1:B:494:VAL:HG21 | 2.02 | 0.40 |
| 1:D:116:HIS:CG | 1:D:117:PRO:HD2 | 2.56 | 0.40 |
| 1:A:206:THR:HG23 | 1:A:369:ILE:HA | 2.03 | 0.40 |
| 1:D:105:ARG:HD3 | 1:E:10:GLU:OE2 | 2.21 | 0.40 |
| 1:F:103:LEU:HB2 | 1:F:506:THR:HG21 | 2.02 | 0.40 |
| 1:G:19:ASP:O | 1:G:23:MET:HG2 | 2.22 | 0.40 |
| 1:G:387:ALA:HA | 1:G:390:VAL:HG22 | 2.03 | 0.40 |
| 1:A:401:VAL:O | 1:A:489:VAL:HG23 | 2.22 | 0.40 |
| 1:D:31:ILE:HG13 | 1:D:75:ALA:HB1 | 2.03 | 0.40 |
| 1:D:87:LYS:O | 1:D:89:VAL:N | 2.54 | 0.40 |
| 1:D:89:VAL:CG2 | 1:D:393:SER:HB2 | 2.51 | 0.40 |
| 1:F:77:MET:HB3 | 1:F:508:MET:SD | 2.61 | 0.40 |
| 1:F:436:ALA:O | 1:F:439:VAL:HG12 | 2.21 | 0.40 |
| 1:C:235:LEU:O | 1:C:286:VAL:HA | 2.21 | 0.40 |
| 1:C:377:ILE:HD13 | 1:C:377:ILE:HA | 1.75 | 0.40 |
| 1:G:235:LEU:O | 1:G:286:VAL:HA | 2.21 | 0.40 |
| 1:A:339:ASP:HB2 | 1:A:360:LYS:HE2 | 2.04 | 0.40 |
| 1:A:512:ILE:HA | 1:H:45:ASP:O | 2.21 | 0.40 |
| 1:B:91:ASP:HB3 | 2:B:601:SO4:O4 | 2.22 | 0.40 |
| 1:B:401:VAL:HG21 | 1:B:495:LYS:HG3 | 2.03 | 0.40 |
| 1:E:18:ARG:HH11 | 1:E:22:ARG:HH11 | 1.66 | 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 | 513/543 (94%) | 501 (98%) | 12 (2%) | 0 | 100 | 100 |
| 1 | B | 513/543 (94%) | 499 (97%) | 13 (2%) | 1 (0%) | 47 | 79 |
| 1 | C | 513/543 (94%) | 504 (98%) | 9 (2%) | 0 | 100 | 100 |
| 1 | D | 513/543 (94%) | 502 (98%) | 9 (2%) | 2 (0%) | 34 | 68 |
| 1 | E | 513/543 (94%) | 503 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | F | 513/543 (94%) | 503 (98%) | 10 (2%) | 0 | 100 | 100 |
| 1 | G | 513/543 (94%) | 500 (98%) | 13 (2%) | 0 | 100 | 100 |
| 1 | H | 513/543 (94%) | 504 (98%) | 9 (2%) | 0 | 100 | 100 |
| All | All | 4104/4344 (94%) | 4016 (98%) | 85 (2%) | 3 (0%) | 51 | 83 |

All (3) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 88 | GLU |
| 1 | D | 350 | GLY |
| 1 | B | 353 | MET |

### 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 | 416/434 (96%) | 416 (100%) | 0 | 100 | 100 |
| 1 | B | 416/434 (96%) | 415 (100%) | 1 (0%) | 93 | 97 |
| 1 | C | 416/434 (96%) | 416 (100%) | 0 | 100 | 100 |
| 1 | D | 416/434 (96%) | 415 (100%) | 1 (0%) | 93 | 97 |
| 1 | E | 416/434 (96%) | 415 (100%) | 1 (0%) | 93 | 97 |
| 1 | F | 416/434 (96%) | 415 (100%) | 1 (0%) | 93 | 97 |
| 1 | G | 416/434 (96%) | 416 (100%) | 0 | 100 | 100 |
| 1 | H | 416/434 (96%) | 415 (100%) | 1 (0%) | 93 | 97 |
| All | All | 3328/3472 (96%) | 3323 (100%) | 5 (0%) | 93 | 97 |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 390 | VAL |
| 1 | D | 390 | VAL |
| 1 | E | 250 | ILE |
| 1 | F | 62 | VAL |
| 1 | H | 390 | VAL |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 287 | GLN |
| 1 | A | 361 | HIS |
| 1 | A | 486 | ASN |
| 1 | A | 497 | GLN |
| 1 | B | 24 | ASN |
| 1 | B | 497 | GLN |
| 1 | D | 497 | GLN |
| 1 | F | 497 | GLN |
| 1 | H | 287 | GLN |
| 1 | H | 486 | 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)

8 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 | SO4 | H | 601 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.07 | 0 |
| 2 | SO4 | B | 601 | - | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.18 | 0 |
| 2 | SO4 | G | 601 | - | 4,4,4 | 0.15 | 0 | 6,6,6 | 0.09 | 0 |
| 2 | SO4 | A | 601 | 1 | 4,4,4 | 0.17 | 0 | 6,6,6 | 0.11 | 0 |
| 2 | SO4 | E | 601 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.13 | 0 |
| 2 | SO4 | D | 601 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.05 | 0 |
| 2 | SO4 | C | 601 | - | 4,4,4 | 0.25 | 0 | 6,6,6 | 0.14 | 0 |
| 2 | SO4 | F | 601 | - | 4,4,4 | 0.16 | 0 | 6,6,6 | 0.11 | 0 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 601 | SO4 | 1 | 0 |
| 2 | G | 601 | SO4 | 1 | 0 |
| 2 | E | 601 | SO4 | 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 (i)

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

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 | 515/543 (94%) | 0.26 | 10 (1%) | 66 | 47 | 39, 59, 93, 102 | 0 |
| 1 | B | 515/543 (94%) | 0.25 | 11 (2%) | 63 | 43 | 39, 66, 96, 108 | 0 |
| 1 | C | 515/543 (94%) | 0.13 | 4 (0%) | 86 | 74 | 39, 64, 85, 100 | 0 |
| 1 | D | 515/543 (94%) | 0.11 | 5 (0%) | 82 | 69 | 36, 61, 83, 94 | 0 |
| 1 | E | 515/543 (94%) | 0.24 | 14 (2%) | 54 | 31 | 39, 67, 94, 106 | 0 |
| 1 | F | 515/543 (94%) | 0.11 | 4 (0%) | 86 | 74 | 41, 64, 82, 99 | 0 |
| 1 | G | 515/543 (94%) | 0.25 | 7 (1%) | 75 | 58 | 43, 68, 87, 100 | 0 |
| 1 | H | 515/543 (94%) | 0.17 | 11 (2%) | 63 | 43 | 40, 63, 87, 101 | 0 |
| All | All | 4120/4344 (94%) | 0.19 | 66 (1%) | 72 | 52 | 36, 64, 91, 108 | 0 |

All (66) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 11 | ASN | 4.3 |
| 1 | B | 324 | ASN | 4.0 |
| 1 | E | 234 | LEU | 3.9 |
| 1 | E | 86 | GLU | 3.9 |
| 1 | H | 11 | ASN | 3.8 |
| 1 | C | 9 | PRO | 3.7 |
| 1 | B | 325 | VAL | 3.7 |
| 1 | H | 9 | PRO | 3.4 |
| 1 | H | 14 | ARG | 3.2 |
| 1 | A | 234 | LEU | 3.2 |
| 1 | C | 17 | GLY | 3.2 |
| 1 | E | 327 | THR | 3.1 |
| 1 | D | 11 | ASN | 3.0 |
| 1 | E | 233 | ALA | 2.9 |
| 1 | F | 11 | ASN | 2.9 |
| 1 | E | 332 | LEU | 2.9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | E | 335 | GLN | 2.8 |
| 1 | B | 351 | ASP | 2.8 |
| 1 | H | 235 | LEU | 2.8 |
| 1 | B | 10 | GLU | 2.8 |
| 1 | A | 222 | GLN | 2.8 |
| 1 | E | 90 | GLY | 2.8 |
| 1 | H | 87 | LYS | 2.8 |
| 1 | C | 14 | ARG | 2.8 |
| 1 | H | 12 | MET | 2.7 |
| 1 | H | 272 | MET | 2.6 |
| 1 | A | 246 | THR | 2.6 |
| 1 | A | 363 | LYS | 2.6 |
| 1 | H | 310 | LYS | 2.6 |
| 1 | H | 86 | GLU | 2.5 |
| 1 | D | 89 | VAL | 2.5 |
| 1 | G | 248 | ALA | 2.5 |
| 1 | B | 88 | GLU | 2.5 |
| 1 | G | 281 | ALA | 2.5 |
| 1 | G | 86 | GLU | 2.5 |
| 1 | E | 85 | GLN | 2.4 |
| 1 | A | 343 | VAL | 2.4 |
| 1 | E | 87 | LYS | 2.4 |
| 1 | D | 350 | GLY | 2.4 |
| 1 | D | 12 | MET | 2.4 |
| 1 | B | 285 | PHE | 2.4 |
| 1 | G | 11 | ASN | 2.4 |
| 1 | A | 232 | ILE | 2.4 |
| 1 | H | 8 | LEU | 2.3 |
| 1 | C | 16 | MET | 2.3 |
| 1 | H | 10 | GLU | 2.3 |
| 1 | E | 16 | MET | 2.3 |
| 1 | E | 331 | ASP | 2.2 |
| 1 | A | 213 | LEU | 2.2 |
| 1 | A | 276 | ILE | 2.2 |
| 1 | G | 16 | MET | 2.2 |
| 1 | E | 212 | VAL | 2.2 |
| 1 | G | 12 | MET | 2.2 |
| 1 | G | 145 | GLN | 2.1 |
| 1 | A | 303 | ILE | 2.1 |
| 1 | B | 339 | ASP | 2.1 |
| 1 | B | 8 | LEU | 2.1 |
| 1 | F | 89 | VAL | 2.1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | F | 373 | THR | 2.1 |
| 1 | E | 15 | TYR | 2.1 |
| 1 | D | 14 | ARG | 2.1 |
| 1 | F | 9 | PRO | 2.1 |
| 1 | B | 14 | ARG | 2.0 |
| 1 | E | 325 | VAL | 2.0 |
| 1 | A | 230 | ALA | 2.0 |
| 1 | B | 340 | ALA | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no 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 | SO4 | G | 601 | 5/5 | 0.78 | 0.27 | 71,72,72,73 | 0 |
| 2 | SO4 | E | 601 | 5/5 | 0.81 | 0.22 | 77,78,79,79 | 0 |
| 2 | SO4 | B | 601 | 5/5 | 0.84 | 0.25 | 73,74,75,76 | 0 |
| 2 | SO4 | H | 601 | 5/5 | 0.85 | 0.23 | 84,84,85,85 | 0 |
| 2 | SO4 | D | 601 | 5/5 | 0.89 | 0.23 | 75,76,77,77 | 0 |
| 2 | SO4 | A | 601 | 5/5 | 0.91 | 0.18 | 59,59,60,60 | 0 |
| 2 | SO4 | F | 601 | 5/5 | 0.93 | 0.14 | 67,67,69,69 | 0 |
| 2 | SO4 | C | 601 | 5/5 | 0.95 | 0.17 | 61,62,63,63 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.