

Full wwPDB X-ray Structure Validation Report (i)

Nov 19, 2023 – 09:37 PM JST

| PDB ID | : | 7BW2 |
|--------------|---|---------------------------------------------------------------------------|
| Title | : | Crystal Structure of Cyanobacterial PSI Monomer from T.elongatus at 6.5 A |
| | | Resolution |
| Authors | : | Kurisu, G.; Coruh, O.; Tanaka, H.; Eithar, E.M.; Mian, Y. |
| Deposited on | : | 2020-04-13 |
| Resolution | : | 6.50 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 (1)) 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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 6.50 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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$ |
|-----------------------|----------------------------------------------------------------------|---------------------------------------------------------------------------|
| R_{free} | 130704 | 1000 (9.00-3.90) |
| Clashscore | 141614 | 1064 (9.00-3.90) |
| Ramachandran outliers | 138981 | 1012 (9.00-3.88) |
| Sidechain outliers | 138945 | 1010 (9.00-3.84) |
| RSRZ outliers | 127900 | 1002 (9.00-3.80) |

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 o | f chain |
|-----|-------|--------|-----------|-----------|
| 1 | А | 755 | 73% | 25% •• |
| 2 | В | 740 | 73% | 27% |
| 3 | С | 81 | 47% | 49% •• |
| 4 | D | 139 | 59% | 39% •• |
| 5 | Е | 76 | 5% | 29% 9% |
| 6 | F | 164 | 43% | 42% · 14% |



| Contr | nued from | <i>i</i> previous | page | |
|-------|-----------|-------------------|------------------|-----------|
| Mol | Chain | Length | Quality of cl | nain |
| 7 | T | 38 | 61% | 34% |
| • | - | | 2% | J-+ 0 . • |
| 8 | J | 41 | 80% | 20% |
| 0 | 17 | 0.0 | 11% | |
| 9 | K | 83 | 53% • | 43% |
| 10 | T. | 155 | 10% | 00/ 170/ |
| 10 | | 100 | 12% | 876 1776 |
| 11 | М | 31 | 77% | 23% |
| 12 | х | 39 | <u>3%</u> 67% | 8% 26% |
| | | - | | |

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$7\mathrm{BW2}$

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 17345 atoms, of which 111 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 Photosystem I P700 chlorophyll a apoprotein A1.

| Mol | Chain | Residues | | | Aton | ns | ZeroOcc | AltConf | Trace | | |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|-------|---|---|
| 1 | А | 743 | Total 5914 | C 3807 | Н 111 | N 991 | O 979 | S 26 | 0 | 0 | 0 |

• Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

| Mol | Chain | Residues | | At | toms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|-----------|----------|-----------|---------|---------|-------|---|
| 2 | В | 739 | Total 5879 | C 3867 | N 986 | O 1005 | S 21 | 0 | 0 | 0 |

• Molecule 3 is a protein called Photosystem I iron-sulfur center.

| Mol | Chain | Residues | | A | toms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|--------------|----------|----------|----------|---------|---------|-------|---|
| 3 | С | 80 | Total 598 | C 367 | N 103 | O 117 | S 11 | 0 | 0 | 0 |

• Molecule 4 is a protein called Photosystem I reaction center subunit II.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|-----------------|---------|---------|-------|
| 4 | D | 138 | Total 1075 | C 682 | N 186 | O 204 | ${ m S} { m 3}$ | 0 | 0 | 0 |

• Molecule 5 is a protein called Photosystem I reaction center subunit IV.

| Mol | Chain | Residues | | Ator | \mathbf{ns} | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------------|----------|---------|---------|-------|
| 5 | Е | 69 | Total 539 | C 342 | N 93 | O 104 | 0 | 0 | 0 |

• Molecule 6 is a protein called Photosystem I reaction center subunit III.

| Mol | Chain | Residues | | At | oms | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|---|
| 6 | F | 141 | Total 1065 | C 680 | N 184 | 0 197 | ${S \atop 4}$ | 0 | 0 | 0 |



• Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

| Mol | Chain | Residues | | Ato | \mathbf{ms} | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------------|---------|----------------|---------|---------|-------|
| 7 | Ι | 38 | Total 301 | C 208 | N 40 | 0 48 | ${ m S}{ m 5}$ | 0 | 0 | 0 |

• Molecule 8 is a protein called Photosystem I reaction center subunit IX.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|---------|---------|-----------------|-------|---|---|
| 8 | J | 41 | Total 338 | C 231 | N 51 | O 54 | ${ m S} { m 2}$ | 0 | 0 | 0 |

• Molecule 9 is a protein called Photosystem I reaction center subunit PsaK.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|---|
| 9 | K | 47 | Total 227 | C 133 | N 47 | O 47 | 0 | 0 | 0 |

• Molecule 10 is a protein called Photosystem I reaction center subunit XI.

| Mol | Chain | Residues | | At | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|---------|---------|-------|
| 10 | L | 128 | Total 936 | C 609 | N 154 | 0 170 | ${ m S} { m 3}$ | 0 | 0 | 0 |

• Molecule 11 is a protein called Photosystem I reaction center subunit XII.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|---|---|
| 11 | М | 31 | Total 241 | C 161 | N 36 | O 43 | S 1 | 0 | 0 | 0 |

• Molecule 12 is a protein called Photosystem I 4.8K protein.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|--------------|----------|---------|---------|---------|-------|---|
| 12 | Х | 29 | Total 232 | C 163 | N 34 | O 35 | 0 | 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: Photosystem I P700 chlorophyll a apoprotein A1









4 Data and refinement statistics (i)

| Property | Value | Source |
|---------------------------------------------|--------------------------------------------------|-----------|
| Space group | P 32 2 1 | Depositor |
| Cell constants | 187.03Å 187.03Å 233.81Å | Deperitor |
| a, b, c, α , β , γ | 90.00° 90.00° 120.00° | Depositor |
| \mathbf{D} and \mathbf{D} | 49.57 - 6.50 | Depositor |
| Resolution (A) | 49.57 - 6.50 | EDS |
| % Data completeness | 98.6 (49.57-6.50) | Depositor |
| (in resolution range) | $98.9 \ (49.57 - 6.50)$ | EDS |
| R _{merge} | 0.05 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | $8.76 (at 6.68 \text{\AA})$ | Xtriage |
| Refinement program | REFMAC 5.8.0238 | Depositor |
| D D | 0.409 , 0.486 | Depositor |
| Λ, Λ_{free} | 0.407 , 0.469 | DCC |
| R_{free} test set | 479 reflections $(5.00%)$ | wwPDB-VP |
| Wilson B-factor $(Å^2)$ | 296.5 | Xtriage |
| Anisotropy | 0.123 | Xtriage |
| Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$ | 0.26, 193.1 | EDS |
| L-test for twinning ² | $< L >=0.52, < L^2>=0.36$ | Xtriage |
| Estimated twinning fraction | 0.000 for -h,-k,l | Xtriage |
| F_o, F_c correlation | 0.71 | EDS |
| Total number of atoms | 17345 | wwPDB-VP |
| Average B, all atoms $(Å^2)$ | 274.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

| Mal | Chain | Bond | lengths | Bo | ond angles |
|-----|---------|------|----------|------|-------------------------------|
| | Ullalli | RMSZ | # Z > 5 | RMSZ | # Z > 5 |
| 1 | А | 0.54 | 0/6003 | 0.65 | 2/8188~(0.0%) |
| 2 | В | 0.55 | 0/6096 | 0.62 | 0/8332 |
| 3 | С | 0.70 | 0/608 | 0.78 | 0/824 |
| 4 | D | 0.59 | 0/1101 | 0.79 | 2/1492~(0.1%) |
| 5 | Е | 0.64 | 0/551 | 0.74 | 0/750 |
| 6 | F | 0.66 | 0/1087 | 0.71 | 0/1476 |
| 7 | Ι | 0.55 | 0/312 | 0.74 | 1/425~(0.2%) |
| 8 | J | 0.47 | 0/350 | 0.62 | 0/477 |
| 9 | Κ | 0.86 | 0/225 | 0.87 | 0/307 |
| 10 | L | 0.58 | 0/960 | 0.61 | 0/1304 |
| 11 | М | 0.53 | 0/244 | 0.57 | 0/332 |
| 12 | Х | 0.55 | 0/241 | 0.68 | 0/330 |
| All | All | 0.57 | 0/17778 | 0.67 | $5/2\overline{4237}\ (0.0\%)$ |

There are no bond length outliers.

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-----------|--------|------------------|---------------|
| 4 | D | 109 | ARG | NE-CZ-NH2 | -10.02 | 115.29 | 120.30 |
| 1 | А | 587 | CYS | N-CA-CB | 9.01 | 126.81 | 110.60 |
| 4 | D | 109 | ARG | NE-CZ-NH1 | 5.91 | 123.25 | 120.30 |
| 7 | Ι | 20 | TRP | C-N-CA | -5.45 | 108.07 | 121.70 |
| 1 | А | 587 | CYS | CB-CA-C | -5.30 | 99.81 | 110.40 |

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



| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | А | 5803 | 111 | 5664 | 270 | 0 |
| 2 | В | 5879 | 0 | 5634 | 323 | 0 |
| 3 | С | 598 | 0 | 588 | 101 | 0 |
| 4 | D | 1075 | 0 | 1077 | 76 | 0 |
| 5 | Е | 539 | 0 | 527 | 40 | 0 |
| 6 | F | 1065 | 0 | 1076 | 134 | 0 |
| 7 | Ι | 301 | 0 | 306 | 56 | 0 |
| 8 | J | 338 | 0 | 347 | 10 | 0 |
| 9 | Κ | 227 | 0 | 116 | 1 | 0 |
| 10 | L | 936 | 0 | 944 | 19 | 0 |
| 11 | М | 241 | 0 | 264 | 3 | 0 |
| 12 | X | 232 | 0 | 220 | 2 | 0 |
| All | All | 17234 | 111 | 16763 | 877 | 0 |

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.

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 26.

All (877) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom 1 | Atom 2 | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 2:B:562:ALA:HB2 | 2:B:579:TRP:CB | 1.34 | 1.53 |
| 1:A:44:THR:CG2 | 1:A:717:ILE:HB | 1.33 | 1.52 |
| 3:C:26:GLU:C | 4:D:109:ARG:HH22 | 1.07 | 1.51 |
| 1:A:264:VAL:HG23 | 1:A:268:PHE:CE1 | 1.48 | 1.48 |
| 7:I:20:TRP:HA | 7:I:23:PRO:CG | 1.44 | 1.47 |
| 6:F:6:VAL:HG13 | 6:F:12:PRO:CD | 1.44 | 1.44 |
| 1:A:49:TRP:CE3 | 1:A:726:GLN:OE1 | 1.70 | 1.42 |
| 2:B:16:THR:CG2 | 2:B:702:LYS:HB2 | 1.47 | 1.41 |
| 2:B:562:ALA:CB | 2:B:579:TRP:HB3 | 1.54 | 1.38 |
| 2:B:11:LEU:HD13 | 2:B:23:ALA:CB | 1.56 | 1.35 |
| 1:A:44:THR:CB | 1:A:717:ILE:HB | 1.58 | 1.34 |
| 2:B:4:PHE:CG | 2:B:5:PRO:HD3 | 1.65 | 1.32 |
| 2:B:16:THR:HG22 | 2:B:702:LYS:CB | 1.59 | 1.32 |
| 1:A:122:GLY:HA2 | 6:F:24:THR:OG1 | 1.31 | 1.31 |
| 2:B:4:PHE:CD2 | 2:B:5:PRO:HD3 | 1.64 | 1.30 |
| 5:E:36:VAL:O | 5:E:59:ASN:HB2 | 1.12 | 1.29 |
| 3:C:26:GLU:C | 4:D:109:ARG:NH2 | 1.82 | 1.29 |
| 1:A:122:GLY:CA | 6:F:24:THR:OG1 | 1.83 | 1.26 |
| 1:A:578:CYS:SG | 1:A:724:ILE:HG21 | 1.76 | 1.25 |



| | | Interatomic | Clash | |
|------------------|------------------|--------------|-------------|--|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:A:44:THR:CG2 | 1:A:717:ILE:CB | 2.14 | 1.24 | |
| 1:A:578:CYS:SG | 1:A:724:ILE:HD13 | 1.78 | 1.24 | |
| 1:A:44:THR:HB | 1:A:717:ILE:CD1 | 1.67 | 1.22 | |
| 1:A:44:THR:HG21 | 1:A:717:ILE:CA | 1.71 | 1.21 | |
| 7:I:19:CYS:O | 7:I:23:PRO:HG3 | 1.39 | 1.21 | |
| 2:B:674:ARG:HD2 | 2:B:707:SER:C | 1.63 | 1.19 | |
| 3:C:22:THR:HA | 4:D:65:LEU:HD13 | 1.23 | 1.19 | |
| 1:A:414:ILE:HG12 | 1:A:574:PHE:CZ | 1.77 | 1.18 | |
| 3:C:26:GLU:HB3 | 4:D:109:ARG:NH2 | 1.58 | 1.18 | |
| 3:C:26:GLU:CA | 4:D:109:ARG:HH22 | 1.59 | 1.16 | |
| 2:B:16:THR:HB | 2:B:702:LYS:O | 1.46 | 1.16 | |
| 1:A:44:THR:HB | 1:A:717:ILE:HD12 | 1.19 | 1.16 | |
| 1:A:49:TRP:CZ3 | 1:A:726:GLN:OE1 | 2.00 | 1.14 | |
| 1:A:246:PRO:HB3 | 1:A:258:TRP:O | 1.46 | 1.14 | |
| 2:B:568:PRO:HA | 2:B:572:GLY:HA2 | 1.30 | 1.14 | |
| 1:A:44:THR:HB | 1:A:717:ILE:CG1 | 1.80 | 1.12 | |
| 1:A:578:CYS:SG | 1:A:724:ILE:CD1 | 2.38 | 1.11 | |
| 6:F:6:VAL:CG1 | 6:F:12:PRO:HD2 | 1.81 | 1.11 | |
| 7:I:20:TRP:CA | 7:I:23:PRO:HG2 | 1.80 | 1.11 | |
| 1:A:44:THR:HG22 | 1:A:717:ILE:HB | 1.25 | 1.11 | |
| 1:A:267:PHE:HB2 | 1:A:275:TYR:OH | 1.49 | 1.10 | |
| 2:B:11:LEU:HD13 | 2:B:23:ALA:HB2 | 1.17 | 1.10 | |
| 2:B:4:PHE:CE1 | 2:B:12:ALA:HA | 1.87 | 1.09 | |
| 1:A:414:ILE:HG12 | 1:A:574:PHE:CE2 | 1.87 | 1.09 | |
| 7:I:20:TRP:C | 7:I:23:PRO:HD2 | 1.72 | 1.08 | |
| 7:I:35:GLU:HB3 | 10:L:99:VAL:HB | 1.27 | 1.08 | |
| 2:B:570:ARG:N | 5:E:47:GLY:O | 1.85 | 1.08 | |
| 2:B:11:LEU:HD13 | 2:B:23:ALA:CA | 1.83 | 1.08 | |
| 1:A:264:VAL:CG2 | 1:A:268:PHE:CE1 | 2.36 | 1.08 | |
| 5:E:36:VAL:O | 5:E:59:ASN:CB | 2.00 | 1.08 | |
| 2:B:709:VAL:HG22 | 2:B:712:ARG:NH2 | 1.69 | 1.07 | |
| 1:A:43:GLN:HG3 | 1:A:47:TRP:HB2 | 1.32 | 1.06 | |
| 6:F:6:VAL:HG13 | 6:F:12:PRO:HD3 | 1.36 | 1.06 | |
| 1:A:49:TRP:CE3 | 1:A:726:GLN:CD | 2.29 | 1.06 | |
| 7:I:20:TRP:CA | 7:I:23:PRO:CG | 2.34 | 1.06 | |
| 3:C:26:GLU:O | 4:D:109:ARG:NH2 | 1.88 | 1.04 | |
| 6:F:6:VAL:HG13 | 6:F:12:PRO:HD2 | 1.08 | 1.04 | |
| 1:A:44:THR:HB | 1:A:717:ILE:CB | 1.88 | 1.04 | |
| 2:B:568:PRO:HA | 2:B:572:GLY:CA | 1.87 | 1.03 | |
| 2:B:563:PHE:O | 2:B:577:SER:HB3 | 1.58 | 1.03 | |
| 6:F:33:LYS:O | 6:F:37:ARG:N | 1.91 | 1.03 | |



| | | Interatomic | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 3:C:26:GLU:CB | 4:D:109:ARG:NH2 | 2.21 | 1.02 |
| 1:A:44:THR:CB | 1:A:717:ILE:HD12 | 1.90 | 1.02 |
| 1:A:264:VAL:CG2 | 1:A:268:PHE:HE1 | 1.71 | 1.02 |
| 2:B:4:PHE:CG | 2:B:5:PRO:CD | 2.42 | 1.02 |
| 2:B:11:LEU:CD1 | 2:B:23:ALA:HA | 1.90 | 1.02 |
| 2:B:568:PRO:CA | 2:B:572:GLY:HA2 | 1.91 | 1.01 |
| 1:A:44:THR:HB | 1:A:717:ILE:HB | 1.37 | 1.00 |
| 2:B:570:ARG:HD2 | 5:E:45:TYR:O | 1.62 | 1.00 |
| 2:B:566:ASP:HB3 | 2:B:573:THR:HG21 | 1.42 | 1.00 |
| 1:A:122:GLY:H | 6:F:24:THR:HG21 | 1.28 | 0.98 |
| 2:B:15:PRO:HD2 | 3:C:72:THR:HA | 1.45 | 0.98 |
| 6:F:6:VAL:CG1 | 6:F:12:PRO:CD | 2.39 | 0.97 |
| 1:A:122:GLY:H | 6:F:24:THR:CG2 | 1.77 | 0.97 |
| 1:A:586:THR:O | 1:A:589:VAL:HG12 | 1.63 | 0.97 |
| 1:A:122:GLY:N | 6:F:24:THR:OG1 | 1.98 | 0.97 |
| 3:C:25:LEU:O | 3:C:42:PRO:CD | 2.14 | 0.96 |
| 1:A:49:TRP:HE3 | 1:A:726:GLN:OE1 | 1.40 | 0.96 |
| 1:A:578:CYS:HG | 1:A:724:ILE:HD13 | 1.15 | 0.95 |
| 2:B:11:LEU:CD1 | 2:B:23:ALA:CB | 2.44 | 0.95 |
| 2:B:569:GLY:HA2 | 3:C:55:THR:HG23 | 1.47 | 0.95 |
| 5:E:10:LEU:HB3 | 5:E:64:GLU:O | 1.66 | 0.94 |
| 1:A:44:THR:CG2 | 1:A:717:ILE:CA | 2.44 | 0.94 |
| 1:A:122:GLY:H | 6:F:24:THR:CB | 1.80 | 0.94 |
| 3:C:17:VAL:HA | 3:C:25:LEU:HD12 | 1.47 | 0.93 |
| 7:I:20:TRP:O | 7:I:23:PRO:HD2 | 1.66 | 0.93 |
| 1:A:720:ARG:HH21 | 5:E:45:TYR:HA | 1.30 | 0.93 |
| 7:I:20:TRP:HA | 7:I:23:PRO:HG2 | 0.94 | 0.93 |
| 2:B:4:PHE:CD1 | 2:B:5:PRO:HD3 | 2.04 | 0.93 |
| 1:A:264:VAL:HG23 | 1:A:268:PHE:HE1 | 1.13 | 0.92 |
| 1:A:46:THR:HG22 | 1:A:50:ASN:ND2 | 1.83 | 0.92 |
| 2:B:562:ALA:HB2 | 2:B:579:TRP:HB2 | 1.48 | 0.92 |
| 2:B:566:ASP:HB3 | 2:B:573:THR:CG2 | 2.00 | 0.92 |
| 5:E:37:ILE:HA | 5:E:59:ASN:HB3 | 1.52 | 0.91 |
| 2:B:481:LEU:HD11 | 2:B:500:LEU:HD11 | 1.52 | 0.91 |
| 1:A:44:THR:HG21 | 1:A:718:GLN:N | 1.86 | 0.91 |
| 2:B:4:PHE:HZ | 2:B:11:LEU:O | 1.53 | 0.91 |
| 7:I:20:TRP:O | 7:I:23:PRO:CD | 2.18 | 0.91 |
| 2:B:709:VAL:HG22 | 2:B:712:ARG:HH22 | 1.29 | 0.91 |
| 3:C:8:ASP:O | 3:C:9:THR:HG22 | 1.69 | 0.91 |
| 1:A:414:ILE:CG1 | 1:A:574:PHE:CZ | 2.54 | 0.91 |
| 1:A:49:TRP:CZ3 | 1:A:726:GLN:CD | 2.44 | 0.90 |



| | | Interatomic | Clash |
|------------------|------------------|-------------------------|-------------|
| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 2:B:4:PHE:CD2 | 2:B:5:PRO:CD | 2.53 | 0.90 |
| 1:A:44:THR:CB | 1:A:717:ILE:CB | 2.39 | 0.90 |
| 2:B:4:PHE:CE2 | 2:B:5:PRO:HD3 | 2.07 | 0.90 |
| 6:F:61:GLY:O | 6:F:66:PRO:HD3 | 1.71 | 0.90 |
| 3:C:71:GLU:O | 3:C:75:SER:HB2 | 1.72 | 0.89 |
| 1:A:122:GLY:N | 6:F:24:THR:HG21 | 1.88 | 0.89 |
| 2:B:116:TYR:HA | 2:B:370:THR:HG22 | 1.52 | 0.89 |
| 2:B:700:LYS:HE2 | 7:I:37:GLU:HG3 | 1.55 | 0.89 |
| 1:A:44:THR:HG21 | 1:A:717:ILE:HA | 1.54 | 0.88 |
| 2:B:562:ALA:CB | 2:B:579:TRP:CB | 2.29 | 0.88 |
| 1:A:720:ARG:HH21 | 5:E:45:TYR:CA | 1.87 | 0.88 |
| 2:B:674:ARG:HD2 | 2:B:708:ILE:N | 1.87 | 0.87 |
| 1:A:268:PHE:HD1 | 1:A:268:PHE:H | 1.22 | 0.87 |
| 2:B:566:ASP:HB3 | 2:B:573:THR:CB | 2.06 | 0.86 |
| 2:B:566:ASP:CB | 2:B:573:THR:HG21 | 2.05 | 0.86 |
| 7:I:37:GLU:O | 10:L:102:GLN:CB | 2.23 | 0.86 |
| 4:D:10:TYR:CE1 | 4:D:12:GLY:CA | 2.58 | 0.86 |
| 4:D:10:TYR:HE1 | 4:D:12:GLY:CA | 1.89 | 0.85 |
| 2:B:562:ALA:HB2 | 2:B:579:TRP:CG | 2.12 | 0.85 |
| 3:C:26:GLU:HB3 | 4:D:109:ARG:CZ | 2.06 | 0.84 |
| 2:B:353:GLN:HA | 2:B:356:TYR:CE2 | 2.12 | 0.84 |
| 4:D:10:TYR:HE1 | 4:D:12:GLY:HA2 | 1.43 | 0.84 |
| 7:I:35:GLU:CB | 10:L:99:VAL:HB | 2.05 | 0.84 |
| 1:A:44:THR:HG21 | 1:A:717:ILE:C | 1.97 | 0.83 |
| 2:B:11:LEU:CD1 | 2:B:23:ALA:HB2 | 2.06 | 0.83 |
| 3:C:22:THR:CA | 4:D:65:LEU:HD13 | 2.06 | 0.83 |
| 1:A:27:LYS:O | 1:A:30:LYS:N | 2.13 | 0.82 |
| 2:B:562:ALA:HB2 | 2:B:579:TRP:HB3 | 0.83 | 0.82 |
| 2:B:570:ARG:CA | 5:E:47:GLY:O | 2.26 | 0.82 |
| 7:I:35:GLU:O | 7:I:37:GLU:HG2 | 1.80 | 0.82 |
| 6:F:60:ALA:O | 6:F:64:LEU:HB3 | 1.79 | 0.82 |
| 2:B:457:LEU:O | 6:F:50:HIS:HA | 1.78 | 0.81 |
| 1:A:583:ARG:NE | 3:C:48:VAL:HG11 | 1.96 | 0.81 |
| 2:B:573:THR:CG2 | 2:B:576:ILE:HG12 | 2.11 | 0.81 |
| 2:B:691:THR:HG23 | 2:B:694:ALA:HB3 | 1.60 | 0.81 |
| 3:C:6:ILE:HG21 | 3:C:39:ALA:HB3 | 1.63 | 0.81 |
| 3:C:27:MET:O | 4:D:109:ARG:CZ | 2.30 | 0.80 |
| 2:B:16:THR:HG22 | 2:B:702:LYS:HB2 | 0.81 | 0.80 |
| 1:A:576:PHE:HE2 | 1:A:579:ASP:HB2 | 1.47 | 0.80 |
| 6:F:31:GLY:O | 6:F:35:PHE:HD2 | 1.64 | 0.80 |
| 1:A:44:THR:CB | 1:A:717:ILE:CG1 | 2.60 | 0.80 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:122:GLY:N | 6:F:24:THR:CG2 | 2.44 | 0.80 |
| 7:I:37:GLU:O | 10:L:102:GLN:HB3 | 1.82 | 0.80 |
| 1:A:122:GLY:N | 6:F:24:THR:CB | 2.44 | 0.79 |
| 1:A:264:VAL:HB | 1:A:267:PHE:HB3 | 1.65 | 0.79 |
| 2:B:15:PRO:CD | 3:C:72:THR:HA | 2.13 | 0.79 |
| 2:B:22:TYR:CE1 | 2:B:707:SER:HB3 | 2.17 | 0.79 |
| 1:A:578:CYS:SG | 1:A:724:ILE:HD12 | 2.21 | 0.79 |
| 6:F:23:ASN:OD1 | 6:F:23:ASN:O | 2.00 | 0.79 |
| 4:D:36:GLU:HA | 4:D:49:MET:O | 1.83 | 0.78 |
| 6:F:23:ASN:HD22 | 6:F:31:GLY:H | 1.31 | 0.78 |
| 1:A:246:PRO:CB | 1:A:258:TRP:O | 2.29 | 0.78 |
| 1:A:43:GLN:CG | 1:A:47:TRP:HB2 | 2.13 | 0.78 |
| 2:B:674:ABG:CZ | 2:B:707:SEB:HA | 2.14 | 0.78 |
| 7:I:20:TRP:O | 7:I:21:LEU:C | 2.16 | 0.78 |
| 6:F:60:ALA:O | 6:F:64:LEU:N | 2.16 | 0.78 |
| 7:I:20:TRP:C | 7:I:23:PRO:CD | 2.52 | 0.78 |
| 3:C:9:THR:HB | 5:E:34:TYB:CE1 | 2.18 | 0.77 |
| 1:A:414:ILE:CG1 | 1:A:574:PHE:CE2 | 2.66 | 0.77 |
| 7:I:37:GLU:O | 10:L:102:GLN:HB2 | 1.84 | 0.77 |
| 3·C·28·VAL·HG12 | 4·D·109·ARG·HB3 | 1.64 | 0.77 |
| 7:I:20:TRP:CA | 7:I:23:PRO:CD | 2.63 | 0.77 |
| 1:A:122:GLY:HA2 | 6:F:24:THR:CB | 2.15 | 0.77 |
| 6:F:8:CYS:HB3 | 6:F:41:ALA:O | 1.84 | 0.77 |
| 2:B:200:GLU:OE1 | 2:B:205:HIS:HA | 1.85 | 0.76 |
| 2:B:11:LEU:HD11 | 2:B:23:ALA:HA | 1.65 | 0.76 |
| 2:B:16:THR:HG21 | 2:B:702:LYS:HB2 | 1.63 | 0.76 |
| 2:B:461:VAL:HG11 | 6:F:52:VAL:CG2 | 2.15 | 0.76 |
| 2:B:469:ALA:HA | 2:B:480:LEU:O | 1.85 | 0.76 |
| 7:I:20:TRP:HA | 7:I:23:PRO:CD | 2.16 | 0.76 |
| 1:A:414:ILE:HG12 | 1:A:574:PHE:CE1 | 2.19 | 0.76 |
| 3:C:25:LEU:O | 3:C:42:PRO:HD2 | 1.82 | 0.76 |
| 2:B:4:PHE:CZ | 2:B:11:LEU:O | 2.38 | 0.76 |
| 1:A:416:MET:CE | 1:A:561:ARG:HB2 | 2.15 | 0.76 |
| 2:B:708:ILE:HG22 | 2:B:712:ARG:HH12 | 1.49 | 0.76 |
| 8:J:38:PHE:HE1 | 8:J:40:PRO:HA | 1.50 | 0.76 |
| 2:B:552:LEU:HD23 | 2:B:576:ILE:HG21 | 1.68 | 0.75 |
| 2:B:562:ALA:HA | 2:B:577:SER:HB2 | 1.68 | 0.75 |
| 1:A:265:ILE:N | 1:A:266:PRO:HD2 | 2.01 | 0.75 |
| 3:C:32:GLY:O | 5:E:32:VAL:HA | 1.87 | 0.75 |
| 2:B:4:PHE:HE1 | 2:B:12:ALA:HA | 1.50 | 0.75 |
| 3:C:28:VAL:HG12 | 4:D:109:ARG:CB | 2.16 | 0.74 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 4:D:10:TYR:CE1 | 4:D:12:GLY:HA2 | 2.23 | 0.74 |
| 1:A:217:ILE:HA | 1:A:221:LEU:HD12 | 1.69 | 0.74 |
| 7:I:20:TRP:CA | 7:I:23:PRO:HD2 | 2.17 | 0.74 |
| 2:B:458:ILE:HA | 6:F:50:HIS:HB2 | 1.69 | 0.73 |
| 5:E:46:THR:HB | 5:E:54:GLY:HA3 | 1.69 | 0.73 |
| 6:F:60:ALA:O | 6:F:64:LEU:CB | 2.36 | 0.73 |
| 6:F:31:GLY:O | 6:F:35:PHE:CD2 | 2.42 | 0.73 |
| 3:C:14:THR:O | 3:C:18:ARG:HB2 | 1.89 | 0.73 |
| 3:C:62:LEU:HB2 | 3:C:65:ARG:NE | 2.04 | 0.73 |
| 5:E:37:ILE:HA | 5:E:59:ASN:CB | 2.18 | 0.72 |
| 6:F:61:GLY:HA2 | 6:F:65:ILE:CG1 | 2.18 | 0.72 |
| 2:B:4:PHE:CD1 | 2:B:5:PRO:CD | 2.69 | 0.72 |
| 2:B:8:SER:OG | 2:B:11:LEU:HG | 1.88 | 0.72 |
| 2:B:17:THR:O | 2:B:20:ILE:HG22 | 1.89 | 0.72 |
| 4:D:10:TYR:CE1 | 4:D:12:GLY:N | 2.57 | 0.72 |
| 1:A:44:THR:HG22 | 1:A:717:ILE:CB | 2.00 | 0.72 |
| 1:A:583:ARG:CZ | 3:C:48:VAL:HG11 | 2.18 | 0.72 |
| 1:A:46:THR:HG22 | 1:A:50:ASN:HD21 | 1.50 | 0.72 |
| 2:B:16:THR:HG22 | 2:B:702:LYS:CG | 2.19 | 0.72 |
| 3:C:26:GLU:CA | 4:D:109:ARG:NH2 | 2.33 | 0.72 |
| 1:A:144:PHE:HA | 1:A:147:TRP:HD1 | 1.53 | 0.72 |
| 1:A:420:TYR:CE2 | 1:A:561:ARG:NE | 2.58 | 0.72 |
| 1:A:583:ARG:HG2 | 3:C:77:GLY:HA3 | 1.70 | 0.72 |
| 3:C:17:VAL:CA | 3:C:25:LEU:HD12 | 2.20 | 0.71 |
| 1:A:20:PRO:HD2 | 1:A:181:HIS:O | 1.90 | 0.71 |
| 1:A:561:ARG:NH2 | 4:D:40:GLU:OE1 | 2.23 | 0.71 |
| 3:C:24:VAL:CG1 | 3:C:46:ASP:HB2 | 2.19 | 0.71 |
| 1:A:471:PRO:O | 1:A:474:MET:HG2 | 1.90 | 0.71 |
| 2:B:353:GLN:HA | 2:B:356:TYR:HE2 | 1.51 | 0.71 |
| 1:A:44:THR:HG21 | 1:A:717:ILE:CB | 1.93 | 0.71 |
| 1:A:49:TRP:CE3 | 1:A:726:GLN:NE2 | 2.58 | 0.71 |
| 2:B:17:THR:HB | 2:B:701:ASP:CB | 2.20 | 0.71 |
| 2:B:674:ARG:HH11 | 2:B:708:ILE:H | 1.38 | 0.71 |
| 2:B:457:LEU:O | 6:F:50:HIS:CA | 2.39 | 0.71 |
| 2:B:570:ARG:HA | 5:E:47:GLY:O | 1.91 | 0.71 |
| 2:B:486:SER:O | 2:B:490:THR:HG23 | 1.90 | 0.70 |
| 6:F:61:GLY:O | 6:F:66:PRO:CD | 2.39 | 0.70 |
| 1:A:44:THR:CG2 | 1:A:717:ILE:HA | 2.15 | 0.70 |
| 1:A:44:THR:HG21 | 1:A:718:GLN:H | 1.53 | 0.70 |
| 2:B:573:THR:HG23 | 2:B:576:ILE:HG12 | 1.73 | 0.70 |
| 2:B:461:VAL:CG1 | 6:F:52:VAL:CG2 | 2.70 | 0.70 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance $(Å)$ | overlap (Å) |
| 1:A:586:THR:O | 1:A:589:VAL:CG1 | 2.37 | 0.70 |
| 1:A:34:PHE:HB3 | 1:A:61:HIS:CG | 2.27 | 0.70 |
| 2:B:570:ARG:CD | 5:E:45:TYR:O | 2.38 | 0.70 |
| 3:C:25:LEU:O | 3:C:42:PRO:CG | 2.40 | 0.70 |
| 11:M:25:LEU:O | 11:M:29:LEU:HG | 1.92 | 0.70 |
| 1:A:47:TRP:CH2 | 1:A:51:LEU:HD22 | 2.26 | 0.69 |
| 2:B:569:GLY:CA | 3:C:55:THR:HG23 | 2.22 | 0.69 |
| 3:C:59:THR:HB | 3:C:61:PHE:CE2 | 2.27 | 0.69 |
| 2:B:11:LEU:CD1 | 2:B:23:ALA:CA | 2.52 | 0.69 |
| 3:C:27:MET:O | 4:D:109:ARG:NH1 | 2.25 | 0.69 |
| 2:B:481:LEU:HA | 2:B:489:SER:OG | 1.91 | 0.69 |
| 2:B:579:TRP:HZ3 | 2:B:712:ARG:HE | 1.39 | 0.69 |
| 1:A:718:GLN:HG3 | 5:E:44:ASN:HB2 | 1.74 | 0.69 |
| 2:B:461:VAL:HA | 2:B:464:GLN:HG2 | 1.72 | 0.69 |
| 7:I:19:CYS:HB2 | 7:I:20:TRP:CD1 | 2.27 | 0.69 |
| 6:F:14:PHE:HA | 6:F:17:ARG:HD2 | 1.75 | 0.69 |
| 9:K:32:TYR:HA | 9:K:35:GLN:CB | 2.22 | 0.69 |
| 1:A:221:LEU:HB2 | 1:A:222:PRO:HD3 | 1.75 | 0.69 |
| 1:A:695:GLY:CA | 2:B:576:ILE:CG2 | 2.71 | 0.69 |
| 2:B:674:ARG:CD | 2:B:708:ILE:N | 2.56 | 0.69 |
| 3:C:26:GLU:HG2 | 4:D:102:PRO:HB3 | 1.75 | 0.69 |
| 2:B:457:LEU:O | 6:F:50:HIS:CB | 2.41 | 0.68 |
| 2:B:197:ALA:O | 2:B:201:SER:HB2 | 1.93 | 0.68 |
| 2:B:553:MET:CE | 2:B:566:ASP:HB2 | 2.23 | 0.68 |
| 2:B:568:PRO:C | 2:B:572:GLY:HA2 | 2.12 | 0.68 |
| 2:B:461:VAL:HG21 | 6:F:54:ASP:HB3 | 1.75 | 0.68 |
| 1:A:168:MET:O | 1:A:172:MET:HG2 | 1.94 | 0.68 |
| 1:A:471:PRO:HA | 1:A:474:MET:HE2 | 1.74 | 0.68 |
| 3:C:22:THR:HA | 4:D:65:LEU:CD1 | 2.14 | 0.68 |
| 1:A:122:GLY:CA | 6:F:24:THR:CB | 2.71 | 0.67 |
| 1:A:202:ALA:HB2 | 1:A:312:GLY:HA3 | 1.76 | 0.67 |
| 2:B:16:THR:HA | 2:B:702:LYS:H | 1.59 | 0.67 |
| 4:D:6:GLN:O | 4:D:55:LEU:HG | 1.93 | 0.67 |
| 2:B:2:THR:HG23 | 7:I:37:GLU:H | 1.60 | 0.67 |
| 3:C:71:GLU:O | 3:C:75:SER:CB | 2.42 | 0.67 |
| 6:F:43:CYS:HB3 | 6:F:48:LEU:O | 1.95 | 0.67 |
| 3:C:9:THR:HB | 5:E:34:TYR:CD1 | 2.29 | 0.67 |
| 1:A:261:PHE:O | 1:A:268:PHE:HZ | 1.76 | 0.67 |
| 6:F:32:GLN:O | 6:F:36:GLU:N | 2.25 | 0.67 |
| 7:I:35:GLU:HG3 | 10:L:99:VAL:HG21 | 1.77 | 0.67 |
| 1:A:576:PHE:O | 1:A:590:SER:HB2 | 1.95 | 0.67 |



| | A L O | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 2:B:568:PRO:HA | 2:B:572:GLY:HA3 | 1.75 | 0.67 |
| 1:A:576:PHE:HE2 | 1:A:579:ASP:CB | 2.07 | 0.67 |
| 1:A:385:THR:HG21 | 1:A:520:VAL:HB | 1.76 | 0.66 |
| 1:A:578:CYS:O | 2:B:568:PRO:HB3 | 1.96 | 0.66 |
| 2:B:16:THR:HA | 2:B:702:LYS:N | 2.09 | 0.66 |
| 2:B:7:PHE:HZ | 2:B:23:ALA:O | 1.79 | 0.66 |
| 6:F:53:VAL:HG11 | 6:F:63:PHE:HB3 | 1.76 | 0.66 |
| 1:A:695:GLY:CA | 2:B:576:ILE:HG22 | 2.26 | 0.66 |
| 6:F:34:ARG:O | 6:F:38:TYR:CD2 | 2.49 | 0.65 |
| 1:A:583:ARG:HG3 | 3:C:48:VAL:HB | 1.79 | 0.65 |
| 3:C:27:MET:CE | 3:C:37:GLN:HB2 | 2.26 | 0.65 |
| 6:F:21:ALA:HB3 | 6:F:35:PHE:CZ | 2.31 | 0.65 |
| 4:D:11:GLY:O | 10:L:7:PRO:HD3 | 1.96 | 0.65 |
| 6:F:107:ILE:O | 6:F:111:LEU:HG | 1.96 | 0.65 |
| 1:A:43:GLN:HG3 | 1:A:47:TRP:CB | 2.19 | 0.65 |
| 1:A:560:ALA:O | 1:A:569:LYS:CG | 2.45 | 0.65 |
| 1:A:281:PHE:CZ | 1:A:299:HIS:CE1 | 2.84 | 0.65 |
| 1:A:143:LEU:HD22 | 1:A:147:TRP:CZ2 | 2.31 | 0.65 |
| 1:A:695:GLY:HA3 | 2:B:576:ILE:HG23 | 1.78 | 0.65 |
| 3:C:17:VAL:HA | 3:C:25:LEU:CD1 | 2.25 | 0.65 |
| 3:C:25:LEU:O | 3:C:42:PRO:HG2 | 1.97 | 0.65 |
| 2:B:562:ALA:CA | 2:B:579:TRP:HB3 | 2.26 | 0.65 |
| 3:C:62:LEU:HD12 | 3:C:65:ARG:NH1 | 2.12 | 0.65 |
| 2:B:304:MET:HG3 | 2:B:322:HIS:O | 1.97 | 0.64 |
| 2:B:457:LEU:O | 6:F:50:HIS:HB2 | 1.96 | 0.64 |
| 4:D:60:ARG:HG3 | 4:D:62:GLU:H | 1.63 | 0.64 |
| 4:D:68:ALA:HB1 | 4:D:80:TYR:CZ | 2.32 | 0.64 |
| 6:F:6:VAL:N | 6:F:7:PRO:CD | 2.59 | 0.64 |
| 2:B:22:TYR:HE1 | 2:B:707:SER:HB3 | 1.63 | 0.64 |
| 1:A:120:ILE:HG12 | 1:A:121:VAL:HG13 | 1.79 | 0.64 |
| 1:A:471:PRO:HA | 1:A:474:MET:CE | 2.26 | 0.64 |
| 1:A:564:ARG:HD2 | 2:B:682:GLU:HB3 | 1.79 | 0.64 |
| 3:C:17:VAL:HG23 | 3:C:25:LEU:HB2 | 1.80 | 0.64 |
| 3:C:28:VAL:O | 3:C:38:ILE:HG22 | 1.98 | 0.64 |
| 1:A:249:MET:O | 1:A:252:LEU:O | 2.17 | 0.63 |
| 2:B:461:VAL:CG1 | 6:F:52:VAL:HG21 | 2.27 | 0.63 |
| 1:A:264:VAL:CB | 1:A:268:PHE:HE1 | 2.11 | 0.63 |
| 6:F:18:ALA:HA | 6:F:35:PHE:CD1 | 2.34 | 0.63 |
| 2:B:569:GLY:HA3 | 3:C:55:THR:HA | 1.79 | 0.63 |
| 6:F:60:ALA:C | 6:F:64:LEU:HB3 | 2.18 | 0.63 |
| 6:F:60:ALA:HB1 | 6:F:64:LEU:HD13 | 1.79 | 0.63 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 7:I:35:GLU:O | 7:I:37:GLU:N | 2.32 | 0.63 |
| 3:C:27:MET:N | 4:D:109:ARG:HH22 | 1.91 | 0.63 |
| 2:B:439:LEU:HD22 | 2:B:456:ILE:HG21 | 1.81 | 0.63 |
| 1:A:41:GLY:N | 1:A:42:PRO:HD2 | 2.13 | 0.63 |
| 2:B:444:ASP:OD2 | 2:B:622:LEU:N | 2.26 | 0.63 |
| 1:A:16:VAL:HG12 | 1:A:185:PRO:HA | 1.81 | 0.62 |
| 6:F:21:ALA:HB3 | 6:F:35:PHE:HZ | 1.64 | 0.62 |
| 1:A:224:ASN:HA | 1:A:227:LEU:HD12 | 1.81 | 0.62 |
| 2:B:699:TRP:HE1 | 2:B:702:LYS:HD3 | 1.65 | 0.62 |
| 1:A:122:GLY:CA | 6:F:24:THR:CG2 | 2.77 | 0.62 |
| 2:B:458:ILE:HD11 | 6:F:52:VAL:HA | 1.82 | 0.62 |
| 1:A:583:ARG:HG2 | 3:C:77:GLY:CA | 2.29 | 0.62 |
| 2:B:456:ILE:O | 2:B:457:LEU:HD23 | 1.98 | 0.62 |
| 2:B:704:VAL:HG21 | 3:C:76:MET:HE1 | 1.81 | 0.62 |
| 2:B:222:ALA:HB3 | 2:B:223:PRO:HD3 | 1.81 | 0.62 |
| 6:F:61:GLY:HA2 | 6:F:65:ILE:HG12 | 1.81 | 0.62 |
| 1:A:43:GLN:CB | 5:E:52:ALA:HB3 | 2.30 | 0.62 |
| 2:B:235:ASN:O | 2:B:252:ALA:CB | 2.47 | 0.62 |
| 1:A:414:ILE:CD1 | 1:A:574:PHE:CE2 | 2.83 | 0.62 |
| 2:B:459:GLU:HG2 | 2:B:519:GLY:HA2 | 1.81 | 0.61 |
| 2:B:506:ALA:O | 2:B:512:ASN:ND2 | 2.22 | 0.61 |
| 2:B:708:ILE:HG22 | 2:B:712:ARG:NH1 | 2.14 | 0.61 |
| 1:A:577:PRO:HB3 | 1:A:725:ILE:HD11 | 1.83 | 0.61 |
| 4:D:10:TYR:CD1 | 4:D:12:GLY:N | 2.69 | 0.61 |
| 1:A:472:GLN:CD | 1:A:472:GLN:H | 2.04 | 0.61 |
| 2:B:22:TYR:CE1 | 2:B:707:SER:CB | 2.84 | 0.60 |
| 3:C:6:ILE:HD13 | 3:C:39:ALA:HB1 | 1.82 | 0.60 |
| 8:J:38:PHE:CE1 | 8:J:40:PRO:HA | 2.34 | 0.60 |
| 2:B:21:TRP:CE3 | 2:B:710:GLN:NE2 | 2.70 | 0.60 |
| 3:C:9:THR:HG23 | 3:C:61:PHE:CZ | 2.35 | 0.60 |
| 6:F:8:CYS:CB | 6:F:41:ALA:O | 2.49 | 0.60 |
| 1:A:417:VAL:HG11 | 1:A:574:PHE:N | 2.15 | 0.60 |
| 2:B:674:ARG:HD3 | 2:B:708:ILE:HG13 | 1.82 | 0.60 |
| 2:B:384:PHE:O | 2:B:387:VAL:HG12 | 2.01 | 0.60 |
| 1:A:695:GLY:HA3 | 2:B:576:ILE:CG2 | 2.32 | 0.60 |
| 3:C:14:THR:HG22 | 3:C:27:MET:HG3 | 1.81 | 0.60 |
| 5:E:46:THR:HB | 5:E:54:GLY:CA | 2.31 | 0.60 |
| 2:B:198:ILE:O | 2:B:202:ARG:HG3 | 2.02 | 0.60 |
| 2:B:321:PRO:HB2 | 2:B:409:ASN:HA | 1.82 | 0.60 |
| 2:B:461:VAL:HB | 12:X:30:TYR:OH | 2.02 | 0.60 |
| 2:B:491:ALA:HB1 | 2:B:494:ASN:HB3 | 1.83 | 0.60 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 2:B:461:VAL:HG11 | 6:F:52:VAL:HG21 | 1.83 | 0.60 |
| 2:B:567:GLY:O | 2:B:573:THR:N | 2.34 | 0.60 |
| 5:E:36:VAL:C | 5:E:59:ASN:HB2 | 2.13 | 0.60 |
| 2:B:22:TYR:CZ | 2:B:707:SER:HB3 | 2.37 | 0.60 |
| 2:B:700:LYS:HE3 | 7:I:37:GLU:CD | 2.22 | 0.60 |
| 2:B:22:TYR:OH | 2:B:707:SER:HB3 | 2.01 | 0.60 |
| 1:A:576:PHE:CE2 | 1:A:579:ASP:HB2 | 2.33 | 0.59 |
| 1:A:718:GLN:HB3 | 5:E:44:ASN:ND2 | 2.17 | 0.59 |
| 2:B:14:ASP:HB2 | 2:B:19:ARG:HG3 | 1.84 | 0.59 |
| 8:J:39:HIS:CG | 8:J:41:LEU:HG | 2.37 | 0.59 |
| 1:A:420:TYR:CD2 | 1:A:561:ARG:CZ | 2.85 | 0.59 |
| 2:B:459:GLU:OE1 | 2:B:464:GLN:OE1 | 2.20 | 0.59 |
| 8:J:33:TYR:HB3 | 8:J:36:LEU:HD11 | 1.85 | 0.59 |
| 2:B:678:GLN:OE1 | 2:B:704:VAL:HG13 | 2.03 | 0.59 |
| 6:F:14:PHE:HE2 | 6:F:39:SER:HA | 1.67 | 0.59 |
| 2:B:4:PHE:HZ | 2:B:11:LEU:C | 2.05 | 0.59 |
| 1:A:25:PHE:HA | 1:A:28:TRP:CD1 | 2.38 | 0.59 |
| 1:A:43:GLN:HB3 | 5:E:52:ALA:HB3 | 1.84 | 0.59 |
| 6:F:9:LYS:CA | 6:F:39:SER:O | 2.50 | 0.59 |
| 1:A:695:GLY:CA | 2:B:576:ILE:HG23 | 2.33 | 0.59 |
| 12:X:7:PRO:N | 12:X:9:TYR:HH | 1.99 | 0.59 |
| 1:A:223:ILE:O | 1:A:227:LEU:HG | 2.02 | 0.59 |
| 3:C:24:VAL:HG12 | 3:C:46:ASP:HB2 | 1.84 | 0.59 |
| 6:F:7:PRO:O | 6:F:11:SER:N | 2.35 | 0.59 |
| 6:F:60:ALA:O | 6:F:64:LEU:CA | 2.50 | 0.59 |
| 1:A:144:PHE:HA | 1:A:147:TRP:CD1 | 2.37 | 0.58 |
| 6:F:14:PHE:CE2 | 6:F:39:SER:HA | 2.38 | 0.58 |
| 7:I:19:CYS:CB | 7:I:20:TRP:CD1 | 2.86 | 0.58 |
| 1:A:414:ILE:HG12 | 1:A:574:PHE:CD2 | 2.38 | 0.58 |
| 2:B:553:MET:HE2 | 2:B:566:ASP:HB2 | 1.84 | 0.58 |
| 1:A:19:ASP:HA | 1:A:181:HIS:O | 2.04 | 0.58 |
| 1:A:260:PHE:O | 1:A:262:SER:N | 2.36 | 0.58 |
| 2:B:553:MET:HE1 | 2:B:566:ASP:OD1 | 2.03 | 0.58 |
| 2:B:702:LYS:CE | 3:C:80:TYR:OXT | 2.51 | 0.58 |
| 4:D:37:GLN:O | 4:D:38:VAL:HB | 2.04 | 0.58 |
| 6:F:33:LYS:O | 6:F:37:ARG:HB2 | 2.03 | 0.58 |
| 2:B:256:PHE:CD1 | 2:B:499:TRP:HB3 | 2.39 | 0.58 |
| 1:A:416:MET:HE2 | 1:A:561:ARG:HB2 | 1.86 | 0.58 |
| 1:A:577:PRO:HB3 | 1:A:725:ILE:CD1 | 2.33 | 0.58 |
| 1:A:577:PRO:HG3 | 1:A:725:ILE:HG12 | 1.86 | 0.58 |
| 1:A:264:VAL:HG23 | 1:A:268:PHE:CZ | 2.29 | 0.58 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance $(Å)$ | overlap (Å) |
| 2:B:17:THR:N | 2:B:701:ASP:HB3 | 2.18 | 0.58 |
| 6:F:23:ASN:HB3 | 6:F:31:GLY:CA | 2.34 | 0.58 |
| 1:A:46:THR:CG2 | 1:A:50:ASN:HD21 | 2.15 | 0.58 |
| 1:A:237:PRO:HG2 | 1:A:248:LEU:HD21 | 1.86 | 0.58 |
| 2:B:481:LEU:O | 2:B:481:LEU:HG | 2.03 | 0.58 |
| 2:B:481:LEU:CD1 | 2:B:500:LEU:HD11 | 2.31 | 0.58 |
| 2:B:568:PRO:O | 2:B:572:GLY:N | 2.37 | 0.58 |
| 1:A:35:ASP:HB3 | 1:A:38:LEU:HB2 | 1.86 | 0.57 |
| 3:C:14:THR:O | 3:C:18:ARG:CB | 2.51 | 0.57 |
| 6:F:60:ALA:CB | 6:F:64:LEU:HD13 | 2.33 | 0.57 |
| 2:B:197:ALA:O | 2:B:201:SER:CB | 2.52 | 0.57 |
| 2:B:4:PHE:CZ | 2:B:11:LEU:C | 2.77 | 0.57 |
| 1:A:560:ALA:O | 1:A:569:LYS:HG3 | 2.04 | 0.57 |
| 1:A:264:VAL:CA | 1:A:268:PHE:HE1 | 2.10 | 0.57 |
| 1:A:265:ILE:N | 1:A:266:PRO:CD | 2.68 | 0.57 |
| 1:A:383:LEU:HG | 1:A:390:GLN:OE1 | 2.05 | 0.57 |
| 2:B:4:PHE:CE1 | 2:B:5:PRO:HD3 | 2.40 | 0.57 |
| 2:B:688:HIS:O | 2:B:691:THR:HG22 | 2.04 | 0.57 |
| 7:I:31:PHE:CZ | 10:L:99:VAL:HG21 | 2.40 | 0.57 |
| 2:B:67:VAL:O | 2:B:71:GLY:O | 2.23 | 0.57 |
| 2:B:446:VAL:HG13 | 2:B:454:LYS:HB2 | 1.85 | 0.57 |
| 2:B:171:GLU:OE2 | 2:B:299:SER:HA | 2.05 | 0.56 |
| 1:A:237:PRO:CG | 1:A:248:LEU:HD21 | 2.35 | 0.56 |
| 2:B:469:ALA:O | 2:B:480:LEU:O | 2.23 | 0.56 |
| 2:B:674:ARG:NH1 | 2:B:708:ILE:H | 2.04 | 0.56 |
| 3:C:27:MET:HE3 | 3:C:37:GLN:HB2 | 1.88 | 0.56 |
| 3:C:37:GLN:HB3 | 4:D:105:VAL:CG2 | 2.36 | 0.56 |
| 1:A:49:TRP:CD2 | 1:A:726:GLN:NE2 | 2.74 | 0.56 |
| 1:A:750:ARG:O | 1:A:754:VAL:HG22 | 2.05 | 0.56 |
| 1:A:86:TRP:O | 1:A:90:MET:HG2 | 2.04 | 0.56 |
| 1:A:578:CYS:CB | 1:A:724:ILE:HD12 | 2.36 | 0.56 |
| 10:L:62:TRP:O | 10:L:66:GLY:N | 2.36 | 0.56 |
| 2:B:567:GLY:O | 2:B:572:GLY:HA2 | 2.06 | 0.55 |
| 7:I:35:GLU:O | 7:I:36:GLY:C | 2.45 | 0.55 |
| 2:B:702:LYS:HD2 | 3:C:80:TYR:OXT | 2.07 | 0.55 |
| 6:F:88:VAL:HG12 | 6:F:94:ALA:HA | 1.89 | 0.55 |
| 1:A:552:ILE:HG12 | 2:B:676:TYR:OH | 2.07 | 0.55 |
| 2:B:67:VAL:O | 2:B:71:GLY:N | 2.38 | 0.55 |
| 2:B:461:VAL:HA | 2:B:464:GLN:CG | 2.36 | 0.55 |
| 1:A:43:GLN:CB | 5:E:52:ALA:CB | 2.84 | 0.55 |
| 1:A:583:ARG:NH2 | 4:D:62:GLU:OE1 | 2.40 | 0.55 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 6:F:111:LEU:O | 6:F:114:PHE:CE2 | 2.59 | 0.55 |
| 2:B:4:PHE:N | 2:B:5:PRO:HD2 | 2.21 | 0.55 |
| 5:E:36:VAL:O | 5:E:59:ASN:CA | 2.55 | 0.55 |
| 6:F:59:ARG:NE | 6:F:59:ARG:HA | 2.22 | 0.55 |
| 1:A:47:TRP:CZ3 | 1:A:51:LEU:HD22 | 2.41 | 0.55 |
| 7:I:20:TRP:CD1 | 7:I:20:TRP:N | 2.74 | 0.55 |
| 7:I:35:GLU:CB | 10:L:99:VAL:CB | 2.81 | 0.55 |
| 4:D:10:TYR:OH | 4:D:13:SER:HB3 | 2.07 | 0.55 |
| 1:A:560:ALA:O | 1:A:569:LYS:HG2 | 2.07 | 0.55 |
| 2:B:700:LYS:HE2 | 7:I:37:GLU:CG | 2.35 | 0.55 |
| 2:B:179:ALA:HB2 | 2:B:287:GLY:HA3 | 1.88 | 0.55 |
| 2:B:562:ALA:CA | 2:B:577:SER:HB2 | 2.35 | 0.55 |
| 4:D:41:MET:HB3 | 4:D:42:PRO:HD2 | 1.89 | 0.55 |
| 2:B:4:PHE:CZ | 2:B:5:PRO:HD3 | 2.42 | 0.54 |
| 2:B:731:LEU:O | 2:B:735:THR:HG22 | 2.07 | 0.54 |
| 1:A:120:ILE:C | 6:F:24:THR:HG21 | 2.28 | 0.54 |
| 3:C:17:VAL:CB | 3:C:25:LEU:HD12 | 2.36 | 0.54 |
| 2:B:67:VAL:O | 2:B:71:GLY:CA | 2.56 | 0.54 |
| 2:B:398:VAL:CG2 | 2:B:547:ALA:HB1 | 2.38 | 0.54 |
| 2:B:568:PRO:CA | 2:B:572:GLY:CA | 2.67 | 0.54 |
| 3:C:14:THR:HA | 3:C:17:VAL:HG12 | 1.90 | 0.54 |
| 1:A:43:GLN:HB3 | 5:E:52:ALA:CB | 2.37 | 0.54 |
| 1:A:566:ILE:CG2 | 1:A:568:ASP:OD1 | 2.56 | 0.54 |
| 1:A:356:LEU:O | 1:A:360:LEU:HG | 2.08 | 0.54 |
| 2:B:566:ASP:HB3 | 2:B:573:THR:HB | 1.89 | 0.54 |
| 2:B:674:ARG:CD | 2:B:707:SER:C | 2.57 | 0.54 |
| 2:B:700:LYS:CE | 7:I:37:GLU:HG3 | 2.33 | 0.54 |
| 4:D:40:GLU:HG2 | 4:D:71:GLN:OE1 | 2.07 | 0.54 |
| 7:I:19:CYS:CB | 7:I:20:TRP:HD1 | 2.20 | 0.54 |
| 2:B:7:PHE:O | 2:B:33:HIS:CD2 | 2.61 | 0.54 |
| 3:C:28:VAL:HG12 | 4:D:109:ARG:HB2 | 1.90 | 0.54 |
| 7:I:22:MET:N | 7:I:23:PRO:HD2 | 2.22 | 0.54 |
| 2:B:563:PHE:CE1 | 2:B:565:CYS:O | 2.61 | 0.54 |
| 4:D:55:LEU:O | 4:D:55:LEU:HD12 | 2.08 | 0.54 |
| 2:B:4:PHE:CD2 | 2:B:20:ILE:HG13 | 2.43 | 0.54 |
| 2:B:461:VAL:HG21 | 6:F:54:ASP:CB | 2.38 | 0.54 |
| 1:A:91:TYR:CE2 | 1:A:161:THR:HG21 | 2.44 | 0.53 |
| 1:A:584:GLY:O | 2:B:674:ARG:NH2 | 2.41 | 0.53 |
| 3:C:41:SER:HB2 | 4:D:113:ASN:HD22 | 1.72 | 0.53 |
| 2:B:14:ASP:CB | 2:B:19:ARG:HG3 | 2.37 | 0.53 |
| 2:B:468:ALA:HB1 | 2:B:477:PHE:HB3 | 1.89 | 0.53 |



| | A h o | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 1:A:567:PRO:HB2 | 4:D:66:ALA:CB | 2.38 | 0.53 |
| 1:A:676:PHE:HE2 | 2:B:626:LEU:HD21 | 1.73 | 0.53 |
| 1:A:44:THR:CG2 | 1:A:718:GLN:H | 2.20 | 0.53 |
| 2:B:520:PRO:O | 2:B:523:PHE:HB3 | 2.08 | 0.53 |
| 3:C:24:VAL:HG11 | 3:C:46:ASP:HB2 | 1.88 | 0.53 |
| 6:F:103:VAL:HB | 6:F:104:PRO:HD3 | 1.89 | 0.53 |
| 2:B:9:GLN:OE1 | 2:B:9:GLN:HA | 2.08 | 0.53 |
| 1:A:253:TYR:CE1 | 1:A:278:PHE:HB3 | 2.44 | 0.53 |
| 1:A:590:SER:HB3 | 1:A:593:ASP:OD2 | 2.09 | 0.53 |
| 4:D:6:GLN:HG2 | 4:D:53:GLU:HB2 | 1.91 | 0.53 |
| 1:A:244:LEU:O | 1:A:246:PRO:HD3 | 2.09 | 0.53 |
| 2:B:22:TYR:OH | 2:B:707:SER:CB | 2.57 | 0.53 |
| 4:D:10:TYR:OH | 4:D:13:SER:CB | 2.56 | 0.53 |
| 2:B:461:VAL:CA | 2:B:464:GLN:HG2 | 2.39 | 0.53 |
| 1:A:651:ARG:HB2 | 2:B:638:ILE:HG23 | 1.90 | 0.53 |
| 6:F:61:GLY:HA2 | 6:F:65:ILE:HB | 1.90 | 0.53 |
| 1:A:583:ARG:HA | 3:C:76:MET:C | 2.30 | 0.53 |
| 2:B:674:ARG:NE | 2:B:707:SER:HA | 2.23 | 0.53 |
| 2:B:382:ALA:O | 2:B:386:MET:HG2 | 2.09 | 0.52 |
| 3:C:11:ILE:O | 3:C:35:ALA:CB | 2.57 | 0.52 |
| 1:A:114:ALA:HB3 | 1:A:139:ILE:HG21 | 1.91 | 0.52 |
| 1:A:265:ILE:H | 1:A:266:PRO:HD2 | 1.73 | 0.52 |
| 1:A:283:GLY:O | 1:A:508:THR:O | 2.28 | 0.52 |
| 2:B:555:ASP:OD2 | 2:B:559:PHE:CE2 | 2.62 | 0.52 |
| 2:B:456:ILE:C | 2:B:457:LEU:HD23 | 2.30 | 0.52 |
| 4:D:41:MET:HB3 | 4:D:42:PRO:CD | 2.40 | 0.52 |
| 5:E:61:ALA:HB3 | 5:E:64:GLU:HG2 | 1.91 | 0.52 |
| 7:I:20:TRP:O | 7:I:23:PRO:N | 2.43 | 0.52 |
| 1:A:577:PRO:CB | 1:A:725:ILE:HG12 | 2.40 | 0.52 |
| 1:A:268:PHE:CD1 | 1:A:268:PHE:N | 2.71 | 0.52 |
| 2:B:138:ALA:O | 2:B:142:LEU:HG | 2.09 | 0.52 |
| 4:D:50:ARG:HB3 | 4:D:54:ASN:OD1 | 2.10 | 0.52 |
| 4:D:125:PRO:HA | 4:D:128:LEU:HD12 | 1.90 | 0.52 |
| 6:F:6:VAL:HG12 | 6:F:6:VAL:O | 2.10 | 0.52 |
| 1:A:257:ASP:O | 1:A:258:TRP:HB2 | 2.10 | 0.52 |
| 1:A:577:PRO:HB3 | 1:A:725:ILE:HG12 | 1.91 | 0.52 |
| 2:B:235:ASN:O | 2:B:252:ALA:HB2 | 2.10 | 0.52 |
| 6:F:33:LYS:O | 6:F:37:ARG:CB | 2.57 | 0.52 |
| 6:F:60:ALA:HB1 | 6:F:64:LEU:HB3 | 1.92 | 0.52 |
| 3:C:30:TRP:CZ2 | 3:C:32:GLY:HA3 | 2.45 | 0.52 |
| 7:I:20:TRP:O | 7:I:23:PRO:CG | 2.58 | 0.52 |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) |
| 2:B:18:ARG:HD3 | 2:B:705:ALA:O | 2.10 | 0.51 |
| 2:B:20:ILE:HD11 | 7:I:34:ILE:HG22 | 1.91 | 0.51 |
| 4:D:2:THR:O | 4:D:4:THR:HG23 | 2.10 | 0.51 |
| 5:E:55:VAL:HG22 | 5:E:57:THR:HG22 | 1.92 | 0.51 |
| 7:I:13:ILE:O | 7:I:16:PRO:HD2 | 2.10 | 0.51 |
| 1:A:35:ASP:HB3 | 1:A:38:LEU:HD22 | 1.92 | 0.51 |
| 5:E:10:LEU:HG | 5:E:10:LEU:O | 2.10 | 0.51 |
| 4:D:10:TYR:CE1 | 4:D:12:GLY:C | 2.84 | 0.51 |
| 2:B:702:LYS:NZ | 3:C:80:TYR:OXT | 2.43 | 0.51 |
| 2:B:461:VAL:O | 2:B:464:GLN:HG2 | 2.10 | 0.51 |
| 2:B:458:ILE:CD1 | 6:F:52:VAL:HA | 2.40 | 0.51 |
| 6:F:6:VAL:HG11 | 6:F:45:GLU:O | 2.11 | 0.51 |
| 6:F:53:VAL:HG23 | 6:F:59:ARG:O | 2.11 | 0.51 |
| 1:A:420:TYR:CD2 | 1:A:561:ARG:NE | 2.78 | 0.51 |
| 2:B:563:PHE:N | 2:B:577:SER:HB2 | 2.26 | 0.51 |
| 6:F:34:ARG:HH21 | 8:J:34:PRO:HB2 | 1.76 | 0.51 |
| 6:F:51:LEU:HB3 | 6:F:62:ASP:HB3 | 1.93 | 0.51 |
| 1:A:583:ARG:HG3 | 3:C:48:VAL:CG1 | 2.41 | 0.50 |
| 2:B:372:ALA:HA | 2:B:600:TRP:CZ3 | 2.46 | 0.50 |
| 2:B:674:ARG:HH11 | 2:B:708:ILE:N | 2.05 | 0.50 |
| 4:D:30:THR:O | 4:D:80:TYR:HA | 2.11 | 0.50 |
| 6:F:34:ARG:O | 6:F:38:TYR:CG | 2.65 | 0.50 |
| 1:A:44:THR:CB | 1:A:717:ILE:CD1 | 2.58 | 0.50 |
| 1:A:91:TYR:CE2 | 1:A:147:TRP:HZ3 | 2.30 | 0.50 |
| 1:A:410:ALA:O | 1:A:414:ILE:HG13 | 2.12 | 0.50 |
| 1:A:695:GLY:HA2 | 2:B:576:ILE:CG2 | 2.40 | 0.50 |
| 2:B:335:PHE:HB2 | 2:B:396:PHE:CD1 | 2.46 | 0.50 |
| 7:I:35:GLU:HB2 | 10:L:99:VAL:CG1 | 2.41 | 0.50 |
| 2:B:425:LEU:HD13 | 2:B:538:LEU:HA | 1.92 | 0.50 |
| 6:F:61:GLY:HA2 | 6:F:65:ILE:CB | 2.42 | 0.50 |
| 6:F:113:GLY:O | 6:F:116:TRP:HB3 | 2.11 | 0.50 |
| 2:B:332:SER:OG | 2:B:396:PHE:HD1 | 1.94 | 0.50 |
| 2:B:580:ASP:O | 2:B:583:TYR:HB3 | 2.12 | 0.50 |
| 3:C:30:TRP:CH2 | 3:C:32:GLY:HA3 | 2.46 | 0.50 |
| 6:F:88:VAL:CG1 | 6:F:94:ALA:HA | 2.42 | 0.50 |
| 5:E:37:ILE:HG12 | 5:E:59:ASN:HD22 | 1.77 | 0.50 |
| 1:A:44:THR:CA | 1:A:717:ILE:HD12 | 2.41 | 0.50 |
| 3:C:27:MET:N | 4:D:109:ARG:NH2 | 2.54 | 0.50 |
| 5:E:38:VAL:N | 5:E:58:ASN:O | 2.45 | 0.50 |
| 6:F:23:ASN:OD1 | 6:F:25:THR:O | 2.30 | 0.50 |
| 6:F:53:VAL:CG1 | 6:F:63:PHE:HB3 | 2.41 | 0.50 |



| | • • • • • • | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 2:B:425:LEU:HB3 | 2:B:538:LEU:HD13 | 1.92 | 0.49 |
| 1:A:694:ARG:HD3 | 2:B:571:GLY:O | 2.12 | 0.49 |
| 3:C:6:ILE:HD13 | 3:C:39:ALA:CB | 2.41 | 0.49 |
| 6:F:52:VAL:HG22 | 6:F:54:ASP:OD2 | 2.12 | 0.49 |
| 7:I:19:CYS:C | 7:I:23:PRO:HG3 | 2.26 | 0.49 |
| 3:C:11:ILE:O | 3:C:35:ALA:HB2 | 2.12 | 0.49 |
| 1:A:237:PRO:CB | 1:A:248:LEU:HD21 | 2.42 | 0.49 |
| 2:B:116:TYR:CA | 2:B:370:THR:HG22 | 2.34 | 0.49 |
| 1:A:677:LEU:HD11 | 2:B:623:MET:HB2 | 1.93 | 0.49 |
| 2:B:568:PRO:C | 2:B:572:GLY:CA | 2.80 | 0.49 |
| 6:F:6:VAL:N | 6:F:7:PRO:HD3 | 2.26 | 0.49 |
| 6:F:9:LYS:N | 6:F:39:SER:O | 2.45 | 0.49 |
| 8:J:39:HIS:ND1 | 8:J:41:LEU:HG | 2.28 | 0.49 |
| 1:A:253:TYR:CD1 | 1:A:277:ASP:HB3 | 2.47 | 0.49 |
| 2:B:562:ALA:C | 2:B:577:SER:HB2 | 2.33 | 0.49 |
| 1:A:25:PHE:HA | 1:A:28:TRP:HD1 | 1.78 | 0.49 |
| 2:B:477:PHE:CZ | 2:B:479:THR:HB | 2.47 | 0.49 |
| 1:A:257:ASP:HB2 | 1:A:263:GLY:O | 2.12 | 0.49 |
| 2:B:674:ARG:HG2 | 2:B:706:LEU:O | 2.13 | 0.49 |
| 10:L:62:TRP:O | 10:L:66:GLY:HA3 | 2.13 | 0.49 |
| 1:A:576:PHE:O | 1:A:590:SER:CB | 2.60 | 0.49 |
| 2:B:461:VAL:HA | 2:B:464:GLN:CD | 2.33 | 0.49 |
| 2:B:548:ARG:HB2 | 6:F:141:ARG:O | 2.13 | 0.49 |
| 2:B:566:ASP:HB2 | 2:B:573:THR:HG21 | 1.93 | 0.49 |
| 1:A:578:CYS:HB2 | 1:A:724:ILE:HD12 | 1.94 | 0.49 |
| 3:C:62:LEU:HD12 | 3:C:65:ARG:CZ | 2.43 | 0.49 |
| 7:I:35:GLU:O | 7:I:37:GLU:CG | 2.58 | 0.49 |
| 2:B:440:TYR:CZ | 2:B:524:LEU:HB3 | 2.48 | 0.48 |
| 2:B:491:ALA:O | 2:B:494:ASN:N | 2.45 | 0.48 |
| 6:F:6:VAL:CG1 | 6:F:12:PRO:HD3 | 2.23 | 0.48 |
| 2:B:465:PHE:CE1 | 2:B:477:PHE:CZ | 3.01 | 0.48 |
| 2:B:642:ASN:HB2 | 2:B:643:PRO:HD2 | 1.95 | 0.48 |
| 1:A:583:ARG:HG3 | 3:C:48:VAL:CB | 2.43 | 0.48 |
| 2:B:468:ALA:CB | 2:B:477:PHE:HB3 | 2.44 | 0.48 |
| 4:D:40:GLU:CG | 4:D:71:GLN:NE2 | 2.77 | 0.48 |
| 4:D:42:PRO:HG2 | 4:D:58:PHE:CE1 | 2.48 | 0.48 |
| 6:F:14:PHE:HE2 | 6:F:39:SER:CA | 2.25 | 0.48 |
| 6:F:114:PHE:CD1 | 6:F:115:ALA:N | 2.81 | 0.48 |
| 3:C:12:GLY:HA3 | 3:C:37:GLN:HG3 | 1.94 | 0.48 |
| 1:A:255:LYS:HD3 | 1:A:274:ALA:HA | 1.94 | 0.48 |
| 2:B:412:ASP:O | 2:B:416:GLN:HG2 | 2.14 | 0.48 |



| Interatomic Clash | | | | |
|-------------------|------------------|--------------|-------------|--|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 2:B:525:VAL:HG11 | 2:B:599:TYR:HB2 | 1.94 | 0.48 | |
| 6:F:9:LYS:HA | 6:F:39:SER:O | 2.12 | 0.48 | |
| 1:A:43:GLN:HB2 | 5:E:52:ALA:CB | 2.43 | 0.48 | |
| 1:A:475:PHE:HA | 1:A:480:ILE:O | 2.14 | 0.48 | |
| 2:B:4:PHE:HD2 | 2:B:20:ILE:HG13 | 1.78 | 0.48 | |
| 2:B:17:THR:HB | 2:B:701:ASP:HB2 | 1.92 | 0.48 | |
| 2:B:198:ILE:HB | 2:B:199:PRO:HD3 | 1.96 | 0.48 | |
| 2:B:199:PRO:O | 2:B:202:ARG:HB2 | 2.14 | 0.48 | |
| 1:A:260:PHE:C | 1:A:261:PHE:CD1 | 2.87 | 0.48 | |
| 1:A:711:LEU:O | 1:A:713:VAL:HG13 | 2.14 | 0.48 | |
| 4:D:95:HIS:HB3 | 4:D:96:PRO:HD3 | 1.95 | 0.48 | |
| 10:L:34:LEU:O | 10:L:38:ARG:N | 2.47 | 0.48 | |
| 2:B:461:VAL:HG13 | 6:F:52:VAL:HG23 | 1.96 | 0.48 | |
| 1:A:497:ALA:N | 1:A:498:PRO:CD | 2.77 | 0.48 | |
| 2:B:433:GLY:HA2 | 2:B:531:LEU:HD22 | 1.96 | 0.48 | |
| 2:B:460:PRO:HG2 | 2:B:518:ILE:HD12 | 1.95 | 0.48 | |
| 3:C:22:THR:CB | 4:D:65:LEU:CD1 | 2.92 | 0.48 | |
| 6:F:9:LYS:HA | 6:F:39:SER:OG | 2.14 | 0.48 | |
| 2:B:199:PRO:HB2 | 2:B:206:VAL:HG21 | 1.96 | 0.47 | |
| 4:D:43:THR:HG22 | 4:D:45:GLY:H | 1.78 | 0.47 | |
| 1:A:242:PHE:HB3 | 1:A:249:MET:SD | 2.54 | 0.47 | |
| 2:B:2:THR:OG1 | 7:I:37:GLU:CD | 2.53 | 0.47 | |
| 2:B:90:ILE:HB | 2:B:111:PRO:HB2 | 1.96 | 0.47 | |
| 2:B:559:PHE:HB3 | 2:B:563:PHE:CD2 | 2.49 | 0.47 | |
| 4:D:37:GLN:O | 4:D:38:VAL:CB | 2.61 | 0.47 | |
| 2:B:709:VAL:CG2 | 2:B:712:ARG:HH22 | 2.15 | 0.47 | |
| 3:C:25:LEU:HA | 3:C:42:PRO:HD2 | 1.97 | 0.47 | |
| 1:A:143:LEU:HB3 | 1:A:147:TRP:NE1 | 2.29 | 0.47 | |
| 1:A:567:PRO:HG2 | 4:D:63:GLN:HA | 1.95 | 0.47 | |
| 1:A:577:PRO:HB3 | 1:A:725:ILE:CG1 | 2.43 | 0.47 | |
| 2:B:8:SER:CB | 2:B:11:LEU:HD12 | 2.44 | 0.47 | |
| 2:B:17:THR:HB | 2:B:701:ASP:HB3 | 1.93 | 0.47 | |
| 6:F:108:LYS:HA | 6:F:111:LEU:HD12 | 1.95 | 0.47 | |
| 2:B:7:PHE:HA | 2:B:33:HIS:NE2 | 2.29 | 0.47 | |
| 2:B:479:THR:HG22 | 2:B:480:LEU:N | 2.29 | 0.47 | |
| 1:A:203:GLY:O | 1:A:207:LEU:HB2 | 2.15 | 0.47 | |
| 1:A:345:TYR:O | 1:A:349:THR:HG23 | 2.15 | 0.47 | |
| 1:A:372:GLN:HA | 1:A:375:TYR:CE2 | 2.50 | 0.47 | |
| 1:A:433:VAL:HG13 | 1:A:440:ILE:HD12 | 1.97 | 0.47 | |
| 2:B:439:LEU:HD22 | 2:B:456:ILE:CG2 | 2.44 | 0.47 | |
| 7:I:19:CYS:O | 7:I:23:PRO:CG | 2.28 | 0.47 | |



| | | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 8:J:39:HIS:CE1 | 8:J:41:LEU:HG | 2.50 | 0.47 | |
| 1:A:420:TYR:CE2 | 1:A:561:ARG:CZ | 2.97 | 0.47 | |
| 6:F:60:ALA:CA | 6:F:64:LEU:HB3 | 2.45 | 0.47 | |
| 1:A:414:ILE:CD1 | 1:A:574:PHE:CZ | 2.97 | 0.47 | |
| 1:A:416:MET:HE3 | 1:A:561:ARG:HB2 | 1.97 | 0.47 | |
| 1:A:568:ASP:HB2 | 1:A:571:ASN:HB2 | 1.97 | 0.47 | |
| 1:A:445:ASN:ND2 | 2:B:684:LEU:HD21 | 2.30 | 0.47 | |
| 1:A:578:CYS:SG | 1:A:724:ILE:CG2 | 2.72 | 0.47 | |
| 2:B:22:TYR:CZ | 2:B:707:SER:CB | 2.98 | 0.47 | |
| 1:A:253:TYR:HD1 | 1:A:277:ASP:HB3 | 1.78 | 0.46 | |
| 2:B:553:MET:HE1 | 2:B:566:ASP:HB2 | 1.96 | 0.46 | |
| 3:C:17:VAL:HG23 | 3:C:25:LEU:HD12 | 1.96 | 0.46 | |
| 4:D:10:TYR:HE1 | 4:D:12:GLY:C | 2.19 | 0.46 | |
| 6:F:14:PHE:HE2 | 6:F:39:SER:CB | 2.28 | 0.46 | |
| 1:A:642:SER:O | 1:A:648:GLY:HA3 | 2.15 | 0.46 | |
| 2:B:674:ARG:HH11 | 2:B:708:ILE:HG13 | 1.79 | 0.46 | |
| 1:A:335:PRO:O | 10:L:4:LEU:N | 2.48 | 0.46 | |
| 2:B:4:PHE:CD1 | 2:B:5:PRO:HD2 | 2.49 | 0.46 | |
| 2:B:553:MET:CE | 2:B:566:ASP:CG | 2.84 | 0.46 | |
| 5:E:10:LEU:CB | 5:E:64:GLU:O | 2.50 | 0.46 | |
| 6:F:8:CYS:HB2 | 6:F:43:CYS:N | 2.30 | 0.46 | |
| 7:I:13:ILE:C | 7:I:16:PRO:HD2 | 2.36 | 0.46 | |
| 6:F:2:VAL:HG12 | 6:F:2:VAL:O | 2.16 | 0.46 | |
| 6:F:14:PHE:HZ | 6:F:35:PHE:O | 1.99 | 0.46 | |
| 1:A:564:ARG:HB2 | 2:B:682:GLU:OE1 | 2.16 | 0.46 | |
| 2:B:479:THR:HG22 | 2:B:480:LEU:HG | 1.97 | 0.46 | |
| 3:C:60:ASP:HB3 | 5:E:58:ASN:ND2 | 2.31 | 0.46 | |
| 6:F:65:ILE:HG21 | 8:J:39:HIS:HB3 | 1.97 | 0.46 | |
| 1:A:356:LEU:HD23 | 1:A:411:HIS:CE1 | 2.51 | 0.46 | |
| 2:B:387:VAL:HG22 | 2:B:582:PHE:CE2 | 2.50 | 0.46 | |
| 2:B:18:ARG:CD | 2:B:705:ALA:O | 2.64 | 0.46 | |
| 2:B:461:VAL:HG13 | 6:F:52:VAL:CG2 | 2.45 | 0.46 | |
| 3:C:40:SER:HB2 | 4:D:112:VAL:H | 1.79 | 0.46 | |
| 6:F:112:THR:O | 6:F:112:THR:HG22 | 2.15 | 0.46 | |
| 1:A:581:PRO:HA | 1:A:585:GLY:HA2 | 1.98 | 0.46 | |
| 3:C:24:VAL:HB | 3:C:43:ARG:O | 2.16 | 0.46 | |
| 4:D:34:PRO:O | 4:D:51:GLU:HG3 | 2.16 | 0.46 | |
| 1:A:473:ASP:HA | 10:L:69:ARG:HH22 | 1.80 | 0.46 | |
| 2:B:553:MET:CE | 2:B:566:ASP:CB | 2.92 | 0.46 | |
| 2:B:685:VAL:HG21 | 3:C:80:TYR:CE2 | 2.51 | 0.46 | |
| 3:C:27:MET:HE2 | 3:C:37:GLN:HB2 | 1.97 | 0.46 | |



| | | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (\AA) | overlap (Å) | |
| 7:I:20:TRP:C | 7:I:23:PRO:HG2 | 2.36 | 0.46 | |
| 2:B:4:PHE:CE2 | 2:B:5:PRO:CD | 2.92 | 0.46 | |
| 2:B:469:ALA:O | 2:B:481:LEU:HB3 | 2.15 | 0.46 | |
| 2:B:601:HIS:O | 2:B:605:LEU:HD13 | 2.16 | 0.46 | |
| 6:F:53:VAL:HG23 | 6:F:59:ARG:C | 2.36 | 0.46 | |
| 1:A:27:LYS:O | 1:A:28:TRP:C | 2.53 | 0.45 | |
| 2:B:2:THR:HG1 | 7:I:37:GLU:CD | 2.19 | 0.45 | |
| 2:B:465:PHE:HE1 | 2:B:477:PHE:CZ | 2.33 | 0.45 | |
| 8:J:38:PHE:CD1 | 8:J:38:PHE:C | 2.88 | 0.45 | |
| 1:A:686:SER:HB3 | 1:A:734:HIS:CB | 2.46 | 0.45 | |
| 2:B:536:THR:OG1 | 2:B:588:TRP:HB3 | 2.16 | 0.45 | |
| 3:C:29:PRO:HG3 | 4:D:105:VAL:CG1 | 2.47 | 0.45 | |
| 4:D:40:GLU:HG3 | 4:D:40:GLU:O | 2.16 | 0.45 | |
| 6:F:53:VAL:CG2 | 6:F:60:ALA:HA | 2.46 | 0.45 | |
| 1:A:43:GLN:HB2 | 5:E:52:ALA:HB3 | 1.98 | 0.45 | |
| 1:A:261:PHE:O | 1:A:268:PHE:CZ | 2.63 | 0.45 | |
| 1:A:422:PRO:HB3 | 4:D:46:ALA:HB2 | 1.98 | 0.45 | |
| 2:B:8:SER:HB3 | 2:B:11:LEU:HD12 | 1.98 | 0.45 | |
| 2:B:110:ASN:HB3 | 7:I:3:GLY:HA2 | 1.99 | 0.45 | |
| 2:B:369:THR:HG23 | 2:B:735:THR:HG23 | 1.98 | 0.45 | |
| 4:D:39:PHE:CD1 | 4:D:47:ALA:O | 2.69 | 0.45 | |
| 6:F:23:ASN:HD21 | 6:F:28:PRO:HA | 1.80 | 0.45 | |
| 10:L:26:LEU:O | 10:L:30:PHE:CD2 | 2.70 | 0.45 | |
| 1:A:91:TYR:CD2 | 1:A:147:TRP:HZ3 | 2.34 | 0.45 | |
| 2:B:563:PHE:HE1 | 2:B:565:CYS:O | 2.00 | 0.45 | |
| 6:F:51:LEU:HD23 | 6:F:62:ASP:HB3 | 1.98 | 0.45 | |
| 1:A:583:ARG:CG | 3:C:77:GLY:HA3 | 2.45 | 0.45 | |
| 1:A:577:PRO:CG | 1:A:725:ILE:HG12 | 2.46 | 0.45 | |
| 1:A:226:LEU:HD13 | 1:A:236:ILE:HG23 | 1.99 | 0.45 | |
| 1:A:686:SER:CB | 1:A:734:HIS:HB2 | 2.47 | 0.45 | |
| 1:A:695:GLY:C | 2:B:576:ILE:HG22 | 2.37 | 0.45 | |
| 2:B:129:ARG:HG3 | 2:B:200:GLU:OE2 | 2.16 | 0.45 | |
| 2:B:634:SER:O | 2:B:638:ILE:HB | 2.17 | 0.45 | |
| 6:F:93:GLU:OE1 | 6:F:93:GLU:HA | 2.16 | 0.45 | |
| 2:B:425:LEU:CB | 2:B:538:LEU:HD13 | 2.46 | 0.45 | |
| 2:B:556:LYS:HE2 | 2:B:576:ILE:HD12 | 1.99 | 0.45 | |
| 1:A:253:TYR:CD1 | 1:A:278:PHE:HB3 | 2.52 | 0.45 | |
| 2:B:2:THR:HG21 | 7:I:34:ILE:O | 2.16 | 0.45 | |
| 2:B:7:PHE:CZ | 2:B:23:ALA:O | 2.65 | 0.45 | |
| 2:B:291:ARG:HA | 2:B:296:ILE:O | 2.17 | 0.45 | |
| 2:B:554:PRO:HB3 | 6:F:140:PRO:HG2 | 1.99 | 0.45 | |



| Intera | | | Clash |
|------------------|------------------|--------------|-------------|
| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 6:F:65:ILE:HB | 6:F:66:PRO:HD3 | 1.98 | 0.45 |
| 2:B:15:PRO:HD2 | 3:C:72:THR:CA | 2.30 | 0.44 |
| 2:B:446:VAL:CG1 | 2:B:454:LYS:HB2 | 2.46 | 0.44 |
| 6:F:116:TRP:CG | 6:F:117:PRO:HD3 | 2.52 | 0.44 |
| 2:B:70:GLN:NE2 | 2:B:89:ALA:HB3 | 2.32 | 0.44 |
| 3:C:28:VAL:CG1 | 4:D:109:ARG:HB3 | 2.39 | 0.44 |
| 4:D:39:PHE:CE1 | 4:D:47:ALA:O | 2.70 | 0.44 |
| 2:B:16:THR:CG2 | 2:B:702:LYS:CB | 2.42 | 0.44 |
| 2:B:642:ASN:HB2 | 2:B:643:PRO:CD | 2.47 | 0.44 |
| 6:F:52:VAL:HG13 | 6:F:52:VAL:O | 2.18 | 0.44 |
| 6:F:79:TRP:CH2 | 6:F:120:ALA:HA | 2.52 | 0.44 |
| 1:A:420:TYR:HD2 | 1:A:561:ARG:CZ | 2.27 | 0.44 |
| 2:B:77:VAL:HG13 | 2:B:124:TYR:CE1 | 2.52 | 0.44 |
| 2:B:547:ALA:O | 2:B:556:LYS:HD2 | 2.17 | 0.44 |
| 4:D:73:ARG:HB2 | 4:D:74:PRO:HD3 | 1.99 | 0.44 |
| 1:A:372:GLN:HE21 | 1:A:398:MET:CE | 2.30 | 0.44 |
| 1:A:377:MET:N | 1:A:378:PRO:HD3 | 2.33 | 0.44 |
| 1:A:716:ALA:HB3 | 6:F:98:GLU:OE1 | 2.18 | 0.44 |
| 1:A:718:GLN:CG | 5:E:44:ASN:HB2 | 2.47 | 0.44 |
| 2:B:492:TRP:HB3 | 2:B:493:PRO:HD3 | 1.99 | 0.44 |
| 5:E:55:VAL:HG13 | 5:E:57:THR:H | 1.83 | 0.44 |
| 6:F:60:ALA:HB1 | 6:F:64:LEU:CB | 2.46 | 0.44 |
| 7:I:35:GLU:HB2 | 10:L:99:VAL:HG11 | 1.99 | 0.44 |
| 2:B:72:ASN:N | 2:B:72:ASN:HD22 | 2.16 | 0.44 |
| 1:A:44:THR:C | 1:A:717:ILE:HD12 | 2.38 | 0.44 |
| 1:A:695:GLY:O | 2:B:576:ILE:HG22 | 2.18 | 0.44 |
| 3:C:71:GLU:C | 3:C:75:SER:HB2 | 2.36 | 0.44 |
| 2:B:74:GLU:HA | 2:B:77:VAL:HB | 1.99 | 0.43 |
| 2:B:674:ARG:HD2 | 2:B:707:SER:CA | 2.45 | 0.43 |
| 3:C:26:GLU:CG | 4:D:102:PRO:HB3 | 2.47 | 0.43 |
| 2:B:561:TYR:CE2 | 2:B:579:TRP:HB2 | 2.53 | 0.43 |
| 2:B:702:LYS:CD | 3:C:80:TYR:OXT | 2.65 | 0.43 |
| 2:B:235:ASN:HB3 | 2:B:251:THR:H | 1.83 | 0.43 |
| 4:D:83:TYR:CE2 | 4:D:93:LEU:HG | 2.53 | 0.43 |
| 2:B:553:MET:HE2 | 2:B:566:ASP:CB | 2.48 | 0.43 |
| 7:I:20:TRP:O | 7:I:22:MET:N | 2.51 | 0.43 |
| 4:D:10:TYR:OH | 4:D:13:SER:OG | 2.37 | 0.43 |
| 5:E:8:LYS:HE3 | 5:E:18:ASN:HA | 1.99 | 0.43 |
| 10:L:62:TRP:O | 10:L:66:GLY:CA | 2.66 | 0.43 |
| 2:B:379:GLN:HA | 2:B:379:GLN:OE1 | 2.18 | 0.43 |
| 1:A:315:TYR:HE2 | 1:A:325:LEU:HD21 | 1.84 | 0.43 |



| | | Interatomic | Clash | |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) | |
| 1:A:575:ARG:HG2 | 1:A:592:TRP:HB2 | 2.00 | 0.43 | |
| 2:B:479:THR:O | 2:B:482:SER:HB3 | 2.19 | 0.43 | |
| 7:I:8:SER:O | 7:I:11:PRO:HD2 | 2.19 | 0.43 | |
| 7:I:31:PHE:CE2 | 10:L:99:VAL:HG21 | 2.54 | 0.43 | |
| 4:D:40:GLU:O | 4:D:71:GLN:HG3 | 2.19 | 0.43 | |
| 6:F:34:ARG:HB3 | 6:F:38:TYR:CE2 | 2.54 | 0.43 | |
| 2:B:709:VAL:CG2 | 2:B:712:ARG:NH2 | 2.61 | 0.43 | |
| 1:A:114:ALA:HB3 | 1:A:139:ILE:CG2 | 2.49 | 0.42 | |
| 2:B:203:GLY:HA2 | 2:B:244:GLY:O | 2.19 | 0.42 | |
| 2:B:479:THR:HG22 | 2:B:480:LEU:H | 1.83 | 0.42 | |
| 3:C:48:VAL:HG23 | 3:C:50:CYS:H | 1.84 | 0.42 | |
| 3:C:59:THR:CB | 3:C:61:PHE:CE2 | 3.00 | 0.42 | |
| 1:A:47:TRP:CE3 | 1:A:47:TRP:C | 2.93 | 0.42 | |
| 2:B:11:LEU:HD23 | 2:B:19:ARG:CZ | 2.48 | 0.42 | |
| 2:B:235:ASN:O | 2:B:252:ALA:HB3 | 2.18 | 0.42 | |
| 1:A:34:PHE:HB3 | 1:A:61:HIS:CB | 2.49 | 0.42 | |
| 1:A:41:GLY:N | 1:A:42:PRO:CD | 2.80 | 0.42 | |
| 1:A:74:SER:OG | 1:A:180:TYR:HB2 | 2.18 | 0.42 | |
| 1:A:231:VAL:O | 1:A:232:ALA:HB3 | 2.18 | 0.42 | |
| 2:B:637:LEU:HD13 | 2:B:733:ALA:HB3 | 2.01 | 0.42 | |
| 11:M:27:THR:O | 11:M:31:LYS:N | 2.52 | 0.42 | |
| 1:A:300:HIS:O | 1:A:304:ILE:HG12 | 2.19 | 0.42 | |
| 2:B:479:THR:CG2 | 2:B:480:LEU:H | 2.32 | 0.42 | |
| 1:A:43:GLN:HG3 | 1:A:47:TRP:CD1 | 2.55 | 0.42 | |
| 6:F:32:GLN:O | 6:F:36:GLU:CB | 2.68 | 0.42 | |
| 1:A:44:THR:CG2 | 1:A:718:GLN:N | 2.70 | 0.42 | |
| 1:A:233:ALA:HA | 1:A:236:ILE:HB | 2.01 | 0.42 | |
| 1:A:476:SER:HA | 1:A:533:THR:HG21 | 2.00 | 0.42 | |
| 3:C:9:THR:CB | 5:E:34:TYR:CD1 | 2.99 | 0.42 | |
| 4:D:38:VAL:HA | 4:D:48:VAL:HA | 2.01 | 0.42 | |
| 6:F:111:LEU:O | 6:F:114:PHE:CD2 | 2.73 | 0.42 | |
| 1:A:483:GLN:HA | 1:A:484:PRO:HD3 | 1.90 | 0.42 | |
| 2:B:614:GLN:O | 2:B:618:SER:HB2 | 2.19 | 0.42 | |
| 6:F:6:VAL:HG13 | 6:F:12:PRO:CG | 2.34 | 0.42 | |
| 2:B:11:LEU:HD23 | 2:B:19:ARG:NE | 2.35 | 0.42 | |
| 2:B:469:ALA:CA | 2:B:480:LEU:O | 2.60 | 0.42 | |
| 4:D:70:GLN:HG2 | 4:D:71:GLN:NE2 | 2.35 | 0.42 | |
| 2:B:459:GLU:CG | 2:B:519:GLY:HA2 | 2.49 | 0.42 | |
| 3:C:28:VAL:HG23 | 3:C:38:ILE:CG2 | 2.50 | 0.42 | |
| 4:D:29:ILE:HA | 4:D:81:LYS:O | 2.20 | 0.42 | |
| 7:I:19:CYS:HB3 | 7:I:20:TRP:HD1 | 1.83 | 0.42 | |



| | | Interatomic | Clash |
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| Atom-1 | Atom-2 | distance (Å) | overlap (Å) |
| 1:A:122:GLY:HA2 | 6:F:24:THR:CG2 | 2.49 | 0.41 |
| 1:A:395:THR:HG22 | 1:A:610:ILE:HB | 2.01 | 0.41 |
| 1:A:417:VAL:HG11 | 1:A:574:PHE:CA | 2.51 | 0.41 |
| 1:A:724:ILE:CD1 | 2:B:574:CYS:HB2 | 2.49 | 0.41 |
| 4:D:68:ALA:HB1 | 4:D:80:TYR:CE1 | 2.55 | 0.41 |
| 6:F:62:ASP:O | 6:F:66:PRO:HG2 | 2.20 | 0.41 |
| 1:A:26:GLU:HA | 8:J:3:HIS:CG | 2.55 | 0.41 |
| 1:A:143:LEU:O | 1:A:147:TRP:CD1 | 2.73 | 0.41 |
| 2:B:50:PHE:HB3 | 2:B:148:ALA:O | 2.20 | 0.41 |
| 3:C:17:VAL:CG2 | 3:C:25:LEU:HB2 | 2.48 | 0.41 |
| 3:C:71:GLU:HB3 | 3:C:76:MET:HG3 | 2.01 | 0.41 |
| 1:A:343:GLY:O | 1:A:347:VAL:HG23 | 2.20 | 0.41 |
| 2:B:561:TYR:CZ | 2:B:579:TRP:HA | 2.55 | 0.41 |
| 6:F:23:ASN:ND2 | 6:F:27:ASP:O | 2.53 | 0.41 |
| 6:F:53:VAL:HG13 | 6:F:54:ASP:N | 2.36 | 0.41 |
| 2:B:553:MET:HE1 | 2:B:566:ASP:CG | 2.41 | 0.41 |
| 5:E:8:LYS:CE | 5:E:18:ASN:HA | 2.50 | 0.41 |
| 6:F:73:ILE:O | 6:F:76:TRP:HB3 | 2.20 | 0.41 |
| 2:B:479:THR:H | 2:B:482:SER:HB3 | 1.85 | 0.41 |
| 6:F:44:GLY:N | 6:F:48:LEU:O | 2.42 | 0.41 |
| 7:I:36:GLY:O | 7:I:37:GLU:C | 2.59 | 0.41 |
| 1:A:154:ASN:OD1 | 1:A:156:PHE:HB3 | 2.21 | 0.41 |
| 1:A:588:GLN:HB2 | 2:B:673:TRP:HB2 | 2.03 | 0.41 |
| 2:B:7:PHE:O | 2:B:33:HIS:NE2 | 2.54 | 0.41 |
| 2:B:460:PRO:HD3 | 2:B:523:PHE:HB2 | 2.01 | 0.41 |
| 2:B:565:CYS:SG | 2:B:574:CYS:HA | 2.61 | 0.41 |
| 3:C:61:PHE:CE1 | 3:C:63:SER:OG | 2.74 | 0.41 |
| 5:E:17:TYR:CD2 | 6:F:138:VAL:HG22 | 2.55 | 0.41 |
| 6:F:80:VAL:HG23 | 6:F:113:GLY:HA2 | 2.03 | 0.41 |
| 1:A:32:GLY:HA3 | 1:A:51:LEU:CD1 | 2.50 | 0.41 |
| 1:A:225:LYS:CE | 1:A:252:LEU:HD22 | 2.51 | 0.41 |
| 1:A:281:PHE:CE2 | 1:A:299:HIS:CE1 | 3.09 | 0.41 |
| 2:B:446:VAL:HG13 | 2:B:451:THR:O | 2.20 | 0.41 |
| 3:C:14:THR:HG22 | 3:C:27:MET:CG | 2.50 | 0.41 |
| 6:F:60:ALA:HA | 6:F:64:LEU:HB2 | 2.02 | 0.41 |
| 1:A:433:VAL:HA | 1:A:436:HIS:CE1 | 2.55 | 0.41 |
| 2:B:76:TRP:CZ3 | 2:B:120:TYR:HB3 | 2.56 | 0.41 |
| 2:B:243:PHE:CD2 | 2:B:264:THR:HG21 | 2.55 | 0.41 |
| 2:B:535:THR:HG21 | 2:B:588:TRP:CE2 | 2.56 | 0.41 |
| 4:D:8:PRO:HG3 | 4:D:54:ASN:HB3 | 2.02 | 0.41 |
| 11:M:28:GLU:O | 11:M:30:TYR:N | 2.48 | 0.41 |



| Atom-1 | Atom-2 | Interatomic | Clash | |
|------------------|------------------|-------------|-------------|--|
| | | | overlap (A) | |
| 1:A:47:TRP:HE3 | 1:A:48:ILE:N | 2.18 | 0.41 | |
| 1:A:502:ALA:N | 1:A:503:PRO:HD3 | 2.36 | 0.41 | |
| 1:A:720:ARG:HH22 | 2:B:570:ARG:HB2 | 1.86 | 0.41 | |
| 2:B:7:PHE:HA | 2:B:33:HIS:HE2 | 1.85 | 0.41 | |
| 2:B:700:LYS:CE | 7:I:37:GLU:CD | 2.88 | 0.41 | |
| 3:C:25:LEU:O | 3:C:42:PRO:HD3 | 2.12 | 0.41 | |
| 6:F:60:ALA:O | 6:F:65:ILE:N | 2.52 | 0.41 | |
| 7:I:20:TRP:O | 7:I:23:PRO:HG2 | 2.19 | 0.41 | |
| 1:A:283:GLY:O | 1:A:507:ALA:HB3 | 2.21 | 0.41 | |
| 4:D:55:LEU:HD12 | 4:D:55:LEU:C | 2.42 | 0.41 | |
| 6:F:102:ASP:OD2 | 6:F:105:LEU:HD12 | 2.20 | 0.41 | |
| 1:A:87:LEU:O | 1:A:91:TYR:HD1 | 2.03 | 0.40 | |
| 1:A:514:GLY:HA2 | 1:A:528:PRO:HB3 | 2.03 | 0.40 | |
| 2:B:261:HIS:CE1 | 2:B:263:GLN:HB2 | 2.57 | 0.40 | |
| 2:B:732:ILE:O | 2:B:735:THR:HG22 | 2.21 | 0.40 | |
| 1:A:152:ILE:HG21 | 1:A:158:LEU:CD2 | 2.51 | 0.40 | |
| 1:A:346:GLU:HA | 1:A:349:THR:OG1 | 2.20 | 0.40 | |
| 2:B:4:PHE:N | 2:B:5:PRO:CD | 2.83 | 0.40 | |
| 2:B:337:LEU:HD23 | 2:B:392:HIS:CE1 | 2.56 | 0.40 | |
| 6:F:63:PHE:C | 6:F:66:PRO:HD2 | 2.42 | 0.40 | |
| 6:F:76:TRP:CZ3 | 6:F:114:PHE:HB3 | 2.56 | 0.40 | |
| 1:A:43:GLN:NE2 | 1:A:47:TRP:HA | 2.37 | 0.40 | |
| 1:A:244:LEU:C | 1:A:246:PRO:HD3 | 2.41 | 0.40 | |
| 2:B:535:THR:HG21 | 2:B:588:TRP:CZ2 | 2.56 | 0.40 | |
| 2:B:580:ASP:O | 2:B:583:TYR:N | 2.55 | 0.40 | |
| 6:F:27:ASP:OD1 | 6:F:28:PRO:HD2 | 2.21 | 0.40 | |
| 1:A:686:SER:HB3 | 1:A:734:HIS:HB3 | 2.03 | 0.40 | |
| 2:B:22:TYR:CE1 | 2:B:710:GLN:HB2 | 2.57 | 0.40 | |
| 2:B:85:PRO:HB3 | 2:B:120:TYR:CD2 | 2.56 | 0.40 | |
| 2:B:139:ILE:HD13 | 2:B:142:LEU:HD12 | 2.03 | 0.40 | |
| 2:B:199:PRO:HA | 2:B:202:ARG:HD3 | 2.03 | 0.40 | |
| 2:B:461:VAL:CG1 | 6:F:52:VAL:HG23 | 2.47 | 0.40 | |
| 2:B:674:ARG:HD3 | 2:B:708:ILE:CG1 | 2.49 | 0.40 | |
| 3:C:7:TYR:HD2 | 4:D:117:ARG:O | 2.04 | 0.40 | |
| 6:F:138:VAL:HG21 | 6:F:141:ARG:HH12 | 1.85 | 0.40 | |
| 1:A:455:SER:OG | 1:A:456:PHE:N | 2.55 | 0.40 | |
| 1:A:678:GLY:O | 1:A:681:PHE:HB3 | 2.21 | 0.40 | |
| 2:B:479:THR:CG2 | 2:B:480:LEU:N | 2.85 | 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 | Perce | entiles |
|-----|-------|-----------------|------------|----------|----------|-------|---------|
| 1 | А | 741/755~(98%) | 697 (94%) | 40 (5%) | 4 (0%) | 29 | 69 |
| 2 | В | 737/740~(100%) | 703~(95%) | 34~(5%) | 0 | 100 | 100 |
| 3 | С | 78/81~(96%) | 71 (91%) | 6 (8%) | 1 (1%) | 12 | 48 |
| 4 | D | 136/139~(98%) | 124 (91%) | 10 (7%) | 2(2%) | 10 | 46 |
| 5 | Е | 67/76~(88%) | 60 (90%) | 6 (9%) | 1 (2%) | 10 | 46 |
| 6 | F | 139/164~(85%) | 128 (92%) | 9~(6%) | 2(1%) | 11 | 46 |
| 7 | Ι | 36/38~(95%) | 32 (89%) | 3 (8%) | 1 (3%) | 5 | 30 |
| 8 | J | 39/41~(95%) | 37~(95%) | 2(5%) | 0 | 100 | 100 |
| 9 | Κ | 43/83~(52%) | 39 (91%) | 3~(7%) | 1 (2%) | 6 | 34 |
| 10 | L | 126/155~(81%) | 121 (96%) | 5(4%) | 0 | 100 | 100 |
| 11 | М | 29/31~(94%) | 27~(93%) | 2(7%) | 0 | 100 | 100 |
| 12 | Х | 27/39~(69%) | 24 (89%) | 3 (11%) | 0 | 100 | 100 |
| All | All | 2198/2342 (94%) | 2063 (94%) | 123 (6%) | 12 (0%) | 29 | 69 |

All (12) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 261 | PHE |
| 4 | D | 38 | VAL |
| 7 | Ι | 36 | GLY |
| 9 | K | 41 | PRO |
| 3 | С | 61 | PHE |
| 6 | F | 14 | PHE |
| 4 | D | 7 | PRO |
| 1 | А | 258 | TRP |
| 1 | А | 273 | ALA |
| 1 | А | 577 | PRO |
| 5 | Е | 53 | SER |
| 6 | F | 49 | PRO |



5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Perce | ntiles |
|-----|-------|-----------------|------------|----------|-------|--------|
| 1 | А | 591/603~(98%) | 587~(99%) | 4 (1%) | 84 | 90 |
| 2 | В | 595/597~(100%) | 591 (99%) | 4 (1%) | 84 | 90 |
| 3 | С | 67/68~(98%) | 66~(98%) | 1 (2%) | 65 | 80 |
| 4 | D | 115/116~(99%) | 114 (99%) | 1 (1%) | 78 | 88 |
| 5 | Ε | 59/65~(91%) | 59~(100%) | 0 | 100 | 100 |
| 6 | F | 109/128~(85%) | 108 (99%) | 1 (1%) | 78 | 88 |
| 7 | Ι | 32/32~(100%) | 31~(97%) | 1 (3%) | 40 | 62 |
| 8 | J | 36/36~(100%) | 36 (100%) | 0 | 100 | 100 |
| 10 | L | 98/120~(82%) | 97~(99%) | 1 (1%) | 76 | 86 |
| 11 | М | 26/26~(100%) | 25~(96%) | 1 (4%) | 33 | 57 |
| 12 | Х | 20/31~(64%) | 20 (100%) | 0 | 100 | 100 |
| All | All | 1748/1822 (96%) | 1734 (99%) | 14 (1%) | 81 | 89 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 268 | PHE |
| 1 | А | 270 | PHE |
| 1 | А | 271 | ASN |
| 1 | А | 587 | CYS |
| 2 | В | 20 | ILE |
| 2 | В | 256 | PHE |
| 2 | В | 465 | PHE |
| 2 | В | 575 | ASP |
| 3 | С | 37 | GLN |
| 4 | D | 119 | ILE |
| 6 | F | 40 | GLN |
| 7 | Ι | 20 | TRP |
| 10 | L | 57 | PHE |
| 11 | М | 5 | ASP |



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | А | 50 | ASN |
| 1 | А | 372 | GLN |
| 1 | А | 445 | ASN |
| 1 | А | 588 | GLN |
| 2 | В | 43 | GLN |
| 2 | В | 72 | ASN |
| 2 | В | 274 | HIS |
| 2 | В | 497 | ASN |
| 2 | В | 614 | GLN |
| 4 | D | 113 | ASN |
| 6 | F | 23 | 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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ $>$ | #RSRZ>2 | $OWAB(Å^2)$ | Q<0.9 |
|-----|-------|-------------------------------|-----------|----------------|--------------------|-------|
| 1 | А | 743/755~(98%) | 0.20 | 37 (4%) 28 28 | 120, 234, 334, 449 | 0 |
| 2 | В | 739/740~(99%) | 0.50 | 80 (10%) 5 9 | 138, 283, 382, 480 | 0 |
| 3 | С | 80/81~(98%) | 0.67 | 12 (15%) 2 5 | 172, 259, 413, 481 | 0 |
| 4 | D | 138/139~(99%) | 0.56 | 16 (11%) 4 8 | 152, 275, 362, 380 | 0 |
| 5 | Е | 69/76~(90%) | 0.26 | 4 (5%) 23 23 | 206, 290, 382, 410 | 0 |
| 6 | F | 141/164 (85%) | -0.10 | 4 (2%) 53 46 | 178, 275, 373, 446 | 0 |
| 7 | Ι | 38/38~(100%) | 0.86 | 8 (21%) 1 3 | 274, 349, 476, 481 | 0 |
| 8 | J | 41/41 (100%) | -0.15 | 1 (2%) 59 52 | 165, 241, 310, 358 | 0 |
| 9 | K | 47/83~(56%) | 1.04 | 9(19%) 1 3 | 184, 298, 338, 354 | 0 |
| 10 | L | 128/155~(82%) | 0.62 | 16 (12%) 3 8 | 259, 361, 556, 628 | 0 |
| 11 | М | 31/31~(100%) | 0.12 | 0 100 100 | 210, 350, 450, 487 | 0 |
| 12 | X | 29/39~(74%) | -0.01 | 1 (3%) 45 40 | 166, 262, 394, 411 | 0 |
| All | All | $222\overline{4/2342}~(94\%)$ | 0.36 | 188 (8%) 10 13 | 120, 268, 391, 628 | 0 |

All (188) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | В | 110 | ASN | 7.8 |
| 3 | С | 47 | CYS | 7.6 |
| 2 | В | 566 | ASP | 7.4 |
| 2 | В | 91 | TRP | 7.4 |
| 4 | D | 6 | GLN | 6.9 |
| 2 | В | 567 | GLY | 6.7 |
| 2 | В | 111 | PRO | 6.7 |
| 2 | В | 90 | ILE | 6.5 |
| 7 | Ι | 3 | GLY | 6.4 |
| 2 | В | 129 | ARG | 6.3 |
| 10 | L | 12 | PRO | 6.1 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | В | 573 | THR | 5.9 |
| 4 | D | 5 | GLY | 5.9 |
| 7 | Ι | 4 | SER | 5.8 |
| 2 | В | 109 | SER | 5.7 |
| 6 | F | 1 | ASP | 5.2 |
| 9 | Κ | 23 | ASN | 5.1 |
| 2 | В | 312 | THR | 5.1 |
| 2 | В | 255 | THR | 4.9 |
| 2 | В | 292 | THR | 4.9 |
| 2 | В | 565 | CYS | 4.6 |
| 2 | В | 127 | GLY | 4.6 |
| 2 | В | 293 | GLN | 4.5 |
| 3 | С | 10 | CYS | 4.5 |
| 3 | С | 49 | GLY | 4.5 |
| 4 | D | 138 | PRO | 4.4 |
| 2 | В | 311 | GLY | 4.4 |
| 1 | А | 580 | GLY | 4.4 |
| 10 | L | 11 | ASP | 4.2 |
| 10 | L | 70 | ASP | 4.2 |
| 2 | В | 162 | PRO | 4.1 |
| 1 | А | 22 | PRO | 4.1 |
| 7 | Ι | 38 | ALA | 4.1 |
| 10 | L | 4 | LEU | 4.1 |
| 1 | А | 652 | ASP | 4.0 |
| 2 | В | 470 | HIS | 4.0 |
| 3 | С | 50 | CYS | 4.0 |
| 2 | В | 229 | TRP | 4.0 |
| 4 | D | 130 | PHE | 3.9 |
| 10 | L | 20 | PRO | 3.9 |
| 2 | В | 83 | THR | 3.9 |
| 2 | В | 89 | ALA | 3.8 |
| 2 | В | 128 | MET | 3.8 |
| 10 | L | 21 | ILE | 3.7 |
| 2 | В | 205 | HIS | 3.7 |
| 1 | A | 21 | VAL | 3.6 |
| 2 | В | 228 | ASN | 3.6 |
| 1 | А | 579 | ASP | 3.6 |
| 4 | D | 7 | PRO | 3.6 |
| 4 | D | 129 | LYS | 3.6 |
| 2 | В | 562 | ALA | 3.6 |
| 10 | L | 13 | PHE | 3.6 |
| 2 | В | 108 | ALA | 3.5 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10 | L | 5 | VAL | 3.5 |
| 3 | С | 48 | VAL | 3.5 |
| 10 | L | 80 | ILE | 3.5 |
| 3 | С | 12 | GLY | 3.5 |
| 2 | В | 576 | ILE | 3.5 |
| 2 | В | 256 | PHE | 3.4 |
| 2 | В | 130 | THR | 3.4 |
| 10 | L | 39 | GLN | 3.4 |
| 4 | D | 4 | THR | 3.4 |
| 4 | D | 55 | LEU | 3.4 |
| 1 | А | 17 | ASP | 3.3 |
| 1 | А | 653 | PHE | 3.3 |
| 7 | Ι | 5 | TYR | 3.3 |
| 2 | В | 563 | PHE | 3.3 |
| 2 | В | 471 | GLY | 3.3 |
| 2 | В | 84 | ARG | 3.2 |
| 12 | Х | 33 | ILE | 3.2 |
| 7 | Ι | 2 | MET | 3.2 |
| 1 | А | 318 | ASN | 3.2 |
| 3 | С | 46 | ASP | 3.2 |
| 10 | L | 107 | SER | 3.2 |
| 1 | А | 578 | CYS | 3.2 |
| 1 | А | 470 | ARG | 3.2 |
| 2 | В | 574 | CYS | 3.2 |
| 5 | Ε | 26 | VAL | 3.2 |
| 2 | В | 98 | ALA | 3.2 |
| 2 | В | 240 | SER | 3.2 |
| 1 | А | 28 | TRP | 3.2 |
| 1 | А | 29 | ALA | 3.1 |
| 3 | С | 43 | ARG | 3.1 |
| 1 | А | 16 | VAL | 3.1 |
| 2 | В | 206 | VAL | 3.0 |
| 1 | A | 341 | HIS | 3.0 |
| 1 | A | 20 | PRO | 3.0 |
| 2 | В | 99 | ALA | 3.0 |
| 2 | В | 472 | LYS | 3.0 |
| 9 | K | 22 | CYS | 2.9 |
| 4 | D | 57 | TYR | 2.9 |
| 9 | K | 71 | ALA | 2.9 |
| 1 | A | 319 | TRP | 2.9 |
| 7 | Ι | 1 | MET | 2.8 |
| 2 | В | 309 | PHE | 2.8 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10 | L | 69 | ARG | 2.8 |
| 2 | В | 124 | TYR | 2.8 |
| 1 | А | 469 | GLY | 2.8 |
| 2 | В | 233 | ALA | 2.7 |
| 4 | D | 8 | PRO | 2.7 |
| 2 | В | 257 | LEU | 2.7 |
| 2 | В | 568 | PRO | 2.7 |
| 10 | L | 76 | LEU | 2.7 |
| 1 | А | 23 | THR | 2.7 |
| 2 | В | 163 | SER | 2.7 |
| 7 | Ι | 37 | GLU | 2.7 |
| 2 | В | 96 | GLY | 2.6 |
| 3 | С | 24 | VAL | 2.6 |
| 1 | А | 577 | PRO | 2.6 |
| 10 | L | 40 | GLY | 2.5 |
| 2 | В | 78 | GLN | 2.5 |
| 1 | А | 96 | LYS | 2.5 |
| 2 | В | 412 | ASP | 2.5 |
| 3 | С | 44 | THR | 2.5 |
| 4 | D | 56 | VAL | 2.5 |
| 6 | F | 55 | GLY | 2.5 |
| 2 | В | 310 | PHE | 2.5 |
| 5 | Е | 50 | GLY | 2.5 |
| 1 | А | 235 | ASP | 2.5 |
| 1 | А | 472 | GLN | 2.5 |
| 1 | А | 581 | PRO | 2.5 |
| 2 | В | 564 | PRO | 2.5 |
| 2 | В | 507 | ILE | 2.5 |
| 1 | А | 642 | SER | 2.4 |
| 2 | В | 133 | ASP | 2.4 |
| 4 | D | 137 | ASP | 2.4 |
| 2 | B | 499 | TRP | 2.4 |
| 9 | K | 20 | ILE | 2.4 |
| 6 | F | 54 | ASP | 2.4 |
| 2 | В | 118 | GLY | 2.4 |
| 2 | В | 254 | LEU | 2.4 |
| 2 | B | 508 | ASN | 2.4 |
| 10 | L | 14 | VAL | 2.4 |
| 2 | В | 291 | ARG | 2.4 |
| 2 | В | 106 | ALA | 2.4 |
| 9 | К | 70 | ALA | 2.4 |
| 8 | J | 32 | PHE | 2.4 |



| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 10 | L | 81 | SER | 2.4 |
| 5 | Е | 49 | SER | 2.4 |
| 2 | В | 160 | PHE | 2.3 |
| 4 | D | 1 | THR | 2.3 |
| 4 | D | 107 | LYS | 2.3 |
| 9 | К | 57 | PRO | 2.3 |
| 5 | Е | 25 | SER | 2.3 |
| 1 | А | 643 | ALA | 2.3 |
| 1 | А | 31 | PRO | 2.2 |
| 1 | А | 58 | PHE | 2.2 |
| 1 | А | 18 | ASN | 2.2 |
| 1 | А | 529 | ILE | 2.2 |
| 3 | С | 2 | HIS | 2.2 |
| 2 | В | 44 | LYS | 2.2 |
| 1 | А | 473 | ASP | 2.2 |
| 2 | В | 239 | ALA | 2.2 |
| 2 | В | 575 | ASP | 2.2 |
| 9 | К | 24 | LEU | 2.2 |
| 1 | А | 25 | PHE | 2.2 |
| 2 | В | 243 | PHE | 2.2 |
| 2 | В | 230 | GLY | 2.2 |
| 7 | Ι | 6 | ALA | 2.2 |
| 2 | В | 218 | PRO | 2.2 |
| 2 | В | 308 | ASP | 2.2 |
| 2 | В | 247 | GLN | 2.2 |
| 2 | В | 303 | MET | 2.2 |
| 2 | В | 219 | ALA | 2.1 |
| 1 | А | 582 | GLY | 2.1 |
| 9 | K | 21 | LEU | 2.1 |
| 1 | А | 30 | LYS | 2.1 |
| 4 | D | 108 | GLY | 2.1 |
| 3 | C | 9 | THR | 2.1 |
| 2 | В | 299 | SER | 2.1 |
| 2 | B | 572 | GLY | 2.1 |
| 1 | A | 15 | VAL | 2.1 |
| 2 | В | 503 | TRP | 2.1 |
| 6 | F | 2 | VAL | 2.1 |
| 1 | А | 233 | ALA | 2.1 |
| 2 | В | 455 | GLN | 2.1 |
| 2 | В | 500 | LEU | 2.1 |
| 2 | В | 43 | GLN | 2.1 |
| 2 | В | 232 | TYR | 2.1 |



| | 3 | 1 | 1 5 | |
|-----|-------|-----|------|------|
| Mol | Chain | Res | Type | RSRZ |
| 9 | K | 26 | ALA | 2.0 |
| 1 | А | 385 | THR | 2.0 |
| 4 | D | 91 | THR | 2.0 |
| 2 | В | 39 | GLU | 2.0 |
| 2 | В | 241 | HIS | 2.0 |
| 1 | А | 755 | GLY | 2.0 |
| 2 | В | 155 | HIS | 2.0 |
| 2 | В | 82 | ASN | 2.0 |
| 2 | В | 161 | ARG | 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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

