



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2020 – 09:39 AM BST

PDB ID : 4DX9
Title : ICAP1 in complex with integrin beta 1 cytoplasmic tail
Authors : Liu, W.; Draheim, K.; Zhang, R.; Calderwood, D.A.; Boggon, T.J.
Deposited on : 2012-02-27
Resolution : 2.99 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.3.dev2
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) : 2.14.3.dev2

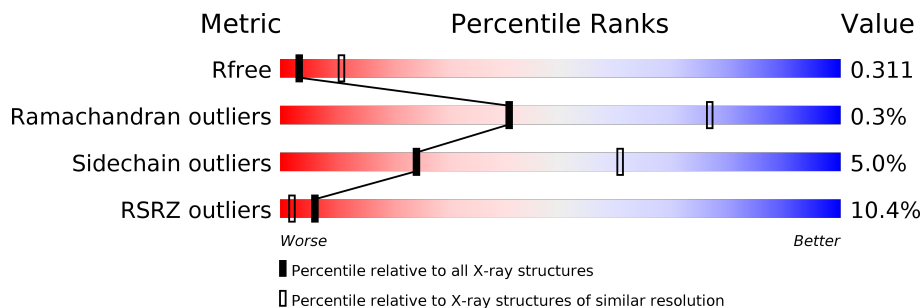
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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.






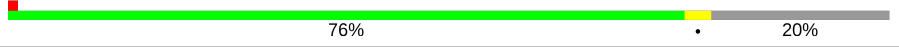
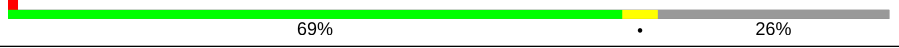


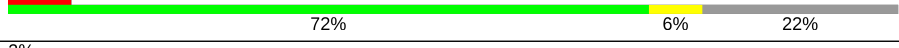






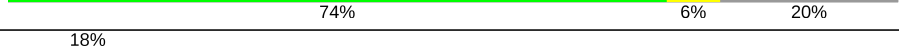
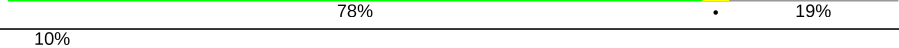

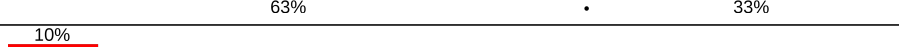
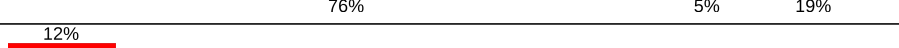
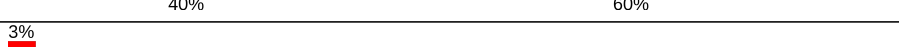
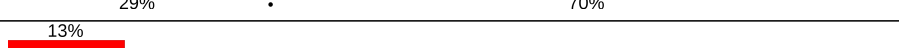
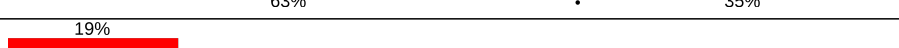
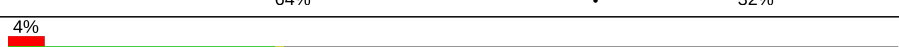
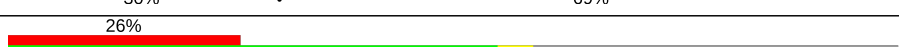
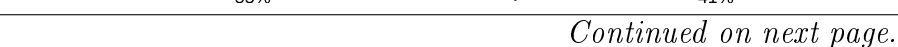
| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 2092 (3.00-3.00) |
| Ramachandran outliers | 138981 | 2333 (3.00-3.00) |
| Sidechain outliers | 138945 | 2336 (3.00-3.00) |
| RSRZ outliers | 127900 | 1990 (3.00-3.00) |

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 on 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 $\leq 5\%$. 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 | 0 | 157 | |
| 1 | 1 | 157 | |
| 1 | 2 | 157 | |
| 1 | 3 | 157 | |
| 1 | 4 | 157 | |
| 1 | 5 | 157 | |
| 1 | A | 157 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | C | 157 |  |
| 1 | E | 157 |  |
| 1 | G | 157 |  |
| 1 | I | 157 |  |
| 1 | K | 157 |  |
| 1 | M | 157 |  |
| 1 | O | 157 |  |
| 1 | Q | 157 |  |
| 1 | S | 157 |  |
| 1 | U | 157 |  |
| 1 | W | 157 |  |
| 1 | Y | 157 |  |
| 1 | a | 157 |  |
| 1 | c | 157 |  |
| 1 | e | 157 |  |
| 1 | g | 157 |  |
| 1 | i | 157 |  |
| 1 | k | 157 |  |
| 1 | m | 157 |  |
| 1 | o | 157 |  |
| 1 | q | 157 |  |
| 1 | s | 157 |  |
| 1 | u | 157 |  |
| 1 | w | 157 |  |
| 1 | y | 157 |  |


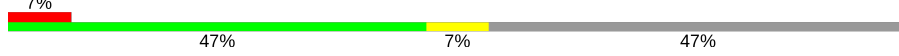
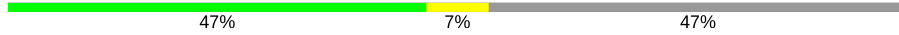


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2 | 6 | 15 | 73% 27% |
| 2 | 7 | 15 | 73% 27% |
| 2 | 8 | 15 | 7% 47% 7% 47% |
| 2 | 9 | 15 | 53% 47% |
| 2 | B | 15 | 7% 60% 7% 33% |
| 2 | D | 15 | 73% 27% |
| 2 | F | 15 | 67% 7% 27% |
| 2 | H | 15 | 67% 7% 27% |
| 2 | J | 15 | 7% 73% 27% |
| 2 | L | 15 | 73% 27% |
| 2 | N | 15 | 60% 13% 27% |
| 2 | P | 15 | 60% 13% 27% |
| 2 | R | 15 | 7% 67% 7% 27% |
| 2 | T | 15 | 73% 27% |
| 2 | V | 15 | 60% 7% 33% |
| 2 | X | 15 | 73% 7% 20% |
| 2 | Z | 15 | 73% 27% |
| 2 | b | 15 | 67% 33% |
| 2 | d | 15 | 73% 27% |
| 2 | f | 15 | 7% 67% 7% 27% |
| 2 | h | 15 | 7% 60% 7% 33% |
| 2 | j | 15 | 27% 73% |
| 2 | l | 15 | 47% 53% |
| 2 | n | 15 | 13% 73% 27% |
| 2 | p | 15 | 13% 33% 67% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 2 | r | 15 |  13% 87% |
| 2 | t | 15 |  7% 47% 7% 47% |
| 2 | v | 15 |  47% 7% 47% |
| 2 | x | 15 |  27% 73% |
| 2 | z | 15 |  33% 67% |

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29306 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 Integrin beta-1-binding protein 1.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|--------|---------|---------|---------|-------|
| | | | Total | C | N | O | S | Se | | | |
| 1 | A | 106 | Total 844 | C 547 | N 134 | O 157 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 0 | 110 | Total 858 | C 558 | N 138 | O 156 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | k | 105 | Total 827 | C 535 | N 133 | O 153 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | m | 127 | Total 991 | C 635 | N 158 | O 192 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 1 | 118 | Total 919 | C 591 | N 147 | O 175 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | C | 127 | Total 997 | C 640 | N 158 | O 193 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 2 | 91 | Total 716 | C 465 | N 117 | O 128 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | E | 113 | Total 875 | C 565 | N 140 | O 164 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 3 | 104 | Total 810 | C 523 | N 132 | O 149 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | G | 127 | Total 995 | C 639 | N 157 | O 193 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | o | 63 | Total 489 | C 319 | N 73 | O 92 | S 3 | Se 2 | 0 | 0 | 0 |
| 1 | q | 47 | Total 359 | C 234 | N 57 | O 62 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | I | 125 | Total 979 | C 627 | N 155 | O 191 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 4 | 129 | Total 1000 | C 641 | N 158 | O 195 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | K | 116 | Total 905 | C 584 | N 144 | O 171 | S 4 | Se 2 | 0 | 0 | 0 |
| 1 | 5 | 128 | Total 1000 | C 642 | N 158 | O 194 | S 4 | Se 2 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|----|---------|---------|-------|
| 1 | M | 124 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 970 | 623 | 154 | 187 | 4 | 2 | | | |
| 1 | O | 102 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 812 | 528 | 127 | 151 | 4 | 2 | | | |
| 1 | a | 99 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 777 | 507 | 124 | 140 | 4 | 2 | | | |
| 1 | s | 102 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 813 | 529 | 130 | 148 | 4 | 2 | | | |
| 1 | u | 106 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 831 | 536 | 135 | 154 | 4 | 2 | | | |
| 1 | c | 120 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 934 | 603 | 149 | 176 | 4 | 2 | | | |
| 1 | e | 126 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 987 | 633 | 156 | 192 | 4 | 2 | | | |
| 1 | g | 127 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 994 | 636 | 157 | 195 | 4 | 2 | | | |
| 1 | i | 101 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 779 | 506 | 126 | 141 | 4 | 2 | | | |
| 1 | Q | 122 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 945 | 606 | 150 | 183 | 4 | 2 | | | |
| 1 | S | 126 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 987 | 633 | 156 | 192 | 4 | 2 | | | |
| 1 | U | 101 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 811 | 528 | 129 | 148 | 4 | 2 | | | |
| 1 | W | 128 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 1005 | 647 | 159 | 193 | 4 | 2 | | | |
| 1 | w | 49 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 378 | 248 | 59 | 66 | 3 | 2 | | | |
| 1 | Y | 129 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 1013 | 651 | 161 | 195 | 4 | 2 | | | |
| 1 | y | 93 | Total | C | N | O | S | Se | 0 | 0 | 0 |
| | | | 738 | 488 | 111 | 133 | 4 | 2 | | | |

There are 160 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 44 | GLY | - | expression tag | UNP O14713 |
| A | 45 | PRO | - | expression tag | UNP O14713 |
| A | 46 | LEU | - | expression tag | UNP O14713 |
| A | 47 | GLY | - | expression tag | UNP O14713 |
| A | 48 | SER | - | expression tag | UNP O14713 |
| 0 | 44 | GLY | - | expression tag | UNP O14713 |
| 0 | 45 | PRO | - | expression tag | UNP O14713 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| 0 | 46 | LEU | - | expression tag | UNP O14713 |
| 0 | 47 | GLY | - | expression tag | UNP O14713 |
| 0 | 48 | SER | - | expression tag | UNP O14713 |
| k | 44 | GLY | - | expression tag | UNP O14713 |
| k | 45 | PRO | - | expression tag | UNP O14713 |
| k | 46 | LEU | - | expression tag | UNP O14713 |
| k | 47 | GLY | - | expression tag | UNP O14713 |
| k | 48 | SER | - | expression tag | UNP O14713 |
| m | 44 | GLY | - | expression tag | UNP O14713 |
| m | 45 | PRO | - | expression tag | UNP O14713 |
| m | 46 | LEU | - | expression tag | UNP O14713 |
| m | 47 | GLY | - | expression tag | UNP O14713 |
| m | 48 | SER | - | expression tag | UNP O14713 |
| 1 | 44 | GLY | - | expression tag | UNP O14713 |
| 1 | 45 | PRO | - | expression tag | UNP O14713 |
| 1 | 46 | LEU | - | expression tag | UNP O14713 |
| 1 | 47 | GLY | - | expression tag | UNP O14713 |
| 1 | 48 | SER | - | expression tag | UNP O14713 |
| C | 44 | GLY | - | expression tag | UNP O14713 |
| C | 45 | PRO | - | expression tag | UNP O14713 |
| C | 46 | LEU | - | expression tag | UNP O14713 |
| C | 47 | GLY | - | expression tag | UNP O14713 |
| C | 48 | SER | - | expression tag | UNP O14713 |
| 2 | 44 | GLY | - | expression tag | UNP O14713 |
| 2 | 45 | PRO | - | expression tag | UNP O14713 |
| 2 | 46 | LEU | - | expression tag | UNP O14713 |
| 2 | 47 | GLY | - | expression tag | UNP O14713 |
| 2 | 48 | SER | - | expression tag | UNP O14713 |
| E | 44 | GLY | - | expression tag | UNP O14713 |
| E | 45 | PRO | - | expression tag | UNP O14713 |
| E | 46 | LEU | - | expression tag | UNP O14713 |
| E | 47 | GLY | - | expression tag | UNP O14713 |
| E | 48 | SER | - | expression tag | UNP O14713 |
| 3 | 44 | GLY | - | expression tag | UNP O14713 |
| 3 | 45 | PRO | - | expression tag | UNP O14713 |
| 3 | 46 | LEU | - | expression tag | UNP O14713 |
| 3 | 47 | GLY | - | expression tag | UNP O14713 |
| 3 | 48 | SER | - | expression tag | UNP O14713 |
| G | 44 | GLY | - | expression tag | UNP O14713 |
| G | 45 | PRO | - | expression tag | UNP O14713 |
| G | 46 | LEU | - | expression tag | UNP O14713 |
| G | 47 | GLY | - | expression tag | UNP O14713 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| G | 48 | SER | - | expression tag | UNP O14713 |
| o | 44 | GLY | - | expression tag | UNP O14713 |
| o | 45 | PRO | - | expression tag | UNP O14713 |
| o | 46 | LEU | - | expression tag | UNP O14713 |
| o | 47 | GLY | - | expression tag | UNP O14713 |
| o | 48 | SER | - | expression tag | UNP O14713 |
| q | 44 | GLY | - | expression tag | UNP O14713 |
| q | 45 | PRO | - | expression tag | UNP O14713 |
| q | 46 | LEU | - | expression tag | UNP O14713 |
| q | 47 | GLY | - | expression tag | UNP O14713 |
| q | 48 | SER | - | expression tag | UNP O14713 |
| I | 44 | GLY | - | expression tag | UNP O14713 |
| I | 45 | PRO | - | expression tag | UNP O14713 |
| I | 46 | LEU | - | expression tag | UNP O14713 |
| I | 47 | GLY | - | expression tag | UNP O14713 |
| I | 48 | SER | - | expression tag | UNP O14713 |
| 4 | 44 | GLY | - | expression tag | UNP O14713 |
| 4 | 45 | PRO | - | expression tag | UNP O14713 |
| 4 | 46 | LEU | - | expression tag | UNP O14713 |
| 4 | 47 | GLY | - | expression tag | UNP O14713 |
| 4 | 48 | SER | - | expression tag | UNP O14713 |
| K | 44 | GLY | - | expression tag | UNP O14713 |
| K | 45 | PRO | - | expression tag | UNP O14713 |
| K | 46 | LEU | - | expression tag | UNP O14713 |
| K | 47 | GLY | - | expression tag | UNP O14713 |
| K | 48 | SER | - | expression tag | UNP O14713 |
| 5 | 44 | GLY | - | expression tag | UNP O14713 |
| 5 | 45 | PRO | - | expression tag | UNP O14713 |
| 5 | 46 | LEU | - | expression tag | UNP O14713 |
| 5 | 47 | GLY | - | expression tag | UNP O14713 |
| 5 | 48 | SER | - | expression tag | UNP O14713 |
| M | 44 | GLY | - | expression tag | UNP O14713 |
| M | 45 | PRO | - | expression tag | UNP O14713 |
| M | 46 | LEU | - | expression tag | UNP O14713 |
| M | 47 | GLY | - | expression tag | UNP O14713 |
| M | 48 | SER | - | expression tag | UNP O14713 |
| O | 44 | GLY | - | expression tag | UNP O14713 |
| O | 45 | PRO | - | expression tag | UNP O14713 |
| O | 46 | LEU | - | expression tag | UNP O14713 |
| O | 47 | GLY | - | expression tag | UNP O14713 |
| O | 48 | SER | - | expression tag | UNP O14713 |
| a | 44 | GLY | - | expression tag | UNP O14713 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| a | 45 | PRO | - | expression tag | UNP O14713 |
| a | 46 | LEU | - | expression tag | UNP O14713 |
| a | 47 | GLY | - | expression tag | UNP O14713 |
| a | 48 | SER | - | expression tag | UNP O14713 |
| s | 44 | GLY | - | expression tag | UNP O14713 |
| s | 45 | PRO | - | expression tag | UNP O14713 |
| s | 46 | LEU | - | expression tag | UNP O14713 |
| s | 47 | GLY | - | expression tag | UNP O14713 |
| s | 48 | SER | - | expression tag | UNP O14713 |
| u | 44 | GLY | - | expression tag | UNP O14713 |
| u | 45 | PRO | - | expression tag | UNP O14713 |
| u | 46 | LEU | - | expression tag | UNP O14713 |
| u | 47 | GLY | - | expression tag | UNP O14713 |
| u | 48 | SER | - | expression tag | UNP O14713 |
| c | 44 | GLY | - | expression tag | UNP O14713 |
| c | 45 | PRO | - | expression tag | UNP O14713 |
| c | 46 | LEU | - | expression tag | UNP O14713 |
| c | 47 | GLY | - | expression tag | UNP O14713 |
| c | 48 | SER | - | expression tag | UNP O14713 |
| e | 44 | GLY | - | expression tag | UNP O14713 |
| e | 45 | PRO | - | expression tag | UNP O14713 |
| e | 46 | LEU | - | expression tag | UNP O14713 |
| e | 47 | GLY | - | expression tag | UNP O14713 |
| e | 48 | SER | - | expression tag | UNP O14713 |
| g | 44 | GLY | - | expression tag | UNP O14713 |
| g | 45 | PRO | - | expression tag | UNP O14713 |
| g | 46 | LEU | - | expression tag | UNP O14713 |
| g | 47 | GLY | - | expression tag | UNP O14713 |
| g | 48 | SER | - | expression tag | UNP O14713 |
| i | 44 | GLY | - | expression tag | UNP O14713 |
| i | 45 | PRO | - | expression tag | UNP O14713 |
| i | 46 | LEU | - | expression tag | UNP O14713 |
| i | 47 | GLY | - | expression tag | UNP O14713 |
| i | 48 | SER | - | expression tag | UNP O14713 |
| Q | 44 | GLY | - | expression tag | UNP O14713 |
| Q | 45 | PRO | - | expression tag | UNP O14713 |
| Q | 46 | LEU | - | expression tag | UNP O14713 |
| Q | 47 | GLY | - | expression tag | UNP O14713 |
| Q | 48 | SER | - | expression tag | UNP O14713 |
| S | 44 | GLY | - | expression tag | UNP O14713 |
| S | 45 | PRO | - | expression tag | UNP O14713 |
| S | 46 | LEU | - | expression tag | UNP O14713 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| S | 47 | GLY | - | expression tag | UNP O14713 |
| S | 48 | SER | - | expression tag | UNP O14713 |
| U | 44 | GLY | - | expression tag | UNP O14713 |
| U | 45 | PRO | - | expression tag | UNP O14713 |
| U | 46 | LEU | - | expression tag | UNP O14713 |
| U | 47 | GLY | - | expression tag | UNP O14713 |
| U | 48 | SER | - | expression tag | UNP O14713 |
| W | 44 | GLY | - | expression tag | UNP O14713 |
| W | 45 | PRO | - | expression tag | UNP O14713 |
| W | 46 | LEU | - | expression tag | UNP O14713 |
| W | 47 | GLY | - | expression tag | UNP O14713 |
| W | 48 | SER | - | expression tag | UNP O14713 |
| w | 44 | GLY | - | expression tag | UNP O14713 |
| w | 45 | PRO | - | expression tag | UNP O14713 |
| w | 46 | LEU | - | expression tag | UNP O14713 |
| w | 47 | GLY | - | expression tag | UNP O14713 |
| w | 48 | SER | - | expression tag | UNP O14713 |
| Y | 44 | GLY | - | expression tag | UNP O14713 |
| Y | 45 | PRO | - | expression tag | UNP O14713 |
| Y | 46 | LEU | - | expression tag | UNP O14713 |
| Y | 47 | GLY | - | expression tag | UNP O14713 |
| Y | 48 | SER | - | expression tag | UNP O14713 |
| y | 44 | GLY | - | expression tag | UNP O14713 |
| y | 45 | PRO | - | expression tag | UNP O14713 |
| y | 46 | LEU | - | expression tag | UNP O14713 |
| y | 47 | GLY | - | expression tag | UNP O14713 |
| y | 48 | SER | - | expression tag | UNP O14713 |

- Molecule 2 is a protein called Integrin beta-1.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2 | l | 7 | Total | C | N | O | 0 | 0 | 0 |
| | | | 49 | 31 | 9 | 9 | | | |
| 2 | n | 11 | Total | C | N | O | 0 | 0 | 0 |
| | | | 79 | 50 | 14 | 15 | | | |
| 2 | x | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 25 | 15 | 4 | 6 | | | |
| 2 | D | 11 | Total | C | N | O | 0 | 0 | 0 |
| | | | 79 | 50 | 14 | 15 | | | |
| 2 | 8 | 8 | Total | C | N | O | 0 | 0 | 0 |
| | | | 55 | 35 | 9 | 11 | | | |
| 2 | H | 11 | Total | C | N | O | 0 | 0 | 0 |
| | | | 79 | 50 | 14 | 15 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 2 | p | 5 | 38 | 25 | 7 | 6 | 0 | 0 | 0 |
| 2 | B | 10 | 70 | 44 | 12 | 14 | 0 | 0 | 0 |
| 2 | 9 | 8 | 54 | 33 | 9 | 12 | 0 | 0 | 0 |
| 2 | F | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | r | 2 | 15 | 9 | 3 | 3 | 0 | 0 | 0 |
| 2 | J | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | 7 | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | L | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | 6 | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | N | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | P | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | t | 8 | 58 | 37 | 11 | 10 | 0 | 0 | 0 |
| 2 | v | 8 | 55 | 35 | 9 | 11 | 0 | 0 | 0 |
| 2 | b | 10 | 70 | 44 | 12 | 14 | 0 | 0 | 0 |
| 2 | d | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | f | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | h | 10 | 70 | 44 | 12 | 14 | 0 | 0 | 0 |
| 2 | j | 4 | 27 | 17 | 5 | 5 | 0 | 0 | 0 |
| 2 | R | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | T | 11 | 79 | 50 | 14 | 15 | 0 | 0 | 0 |
| 2 | V | 10 | 70 | 44 | 12 | 14 | 0 | 0 | 0 |

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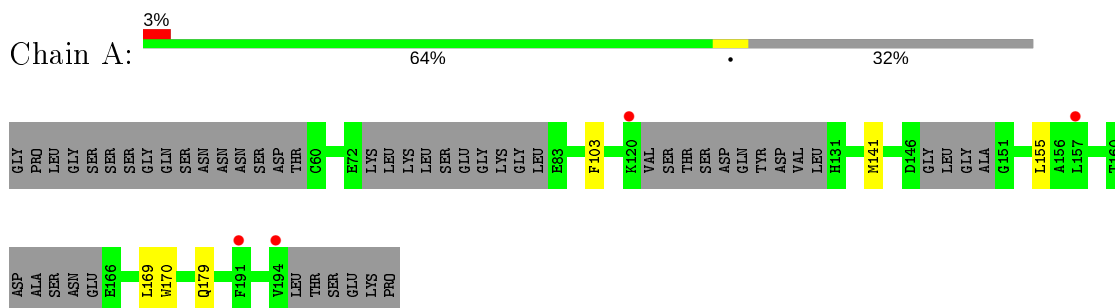
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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------------|---------|---------|---------|---------|---------|-------|
| | | | Total | C | N | O | | | |
| 2 | X | 12 | Total 91 | C 59 | N 15 | O 17 | 0 | 0 | 0 |
| 2 | Z | 11 | Total 79 | C 50 | N 14 | O 15 | 0 | 0 | 0 |
| 2 | z | 5 | Total 36 | C 23 | N 6 | O 7 | 0 | 0 | 0 |

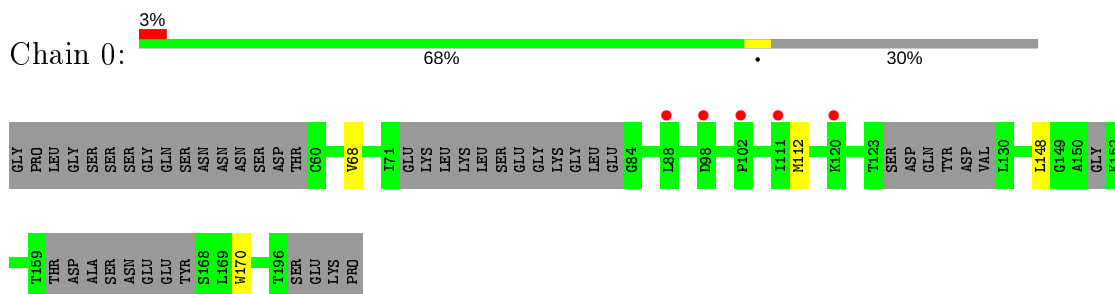
3 Residue-property plots [i](#)

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.

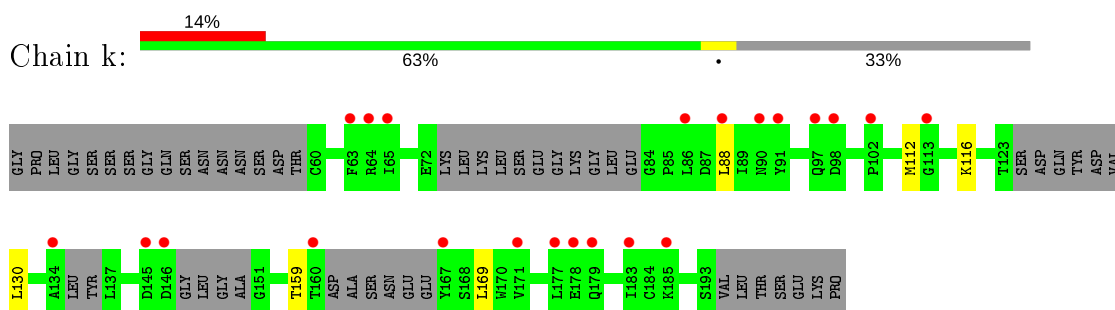
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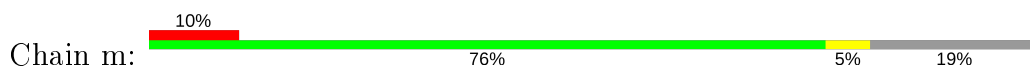
- Molecule 1: Integrin beta-1-binding protein 1

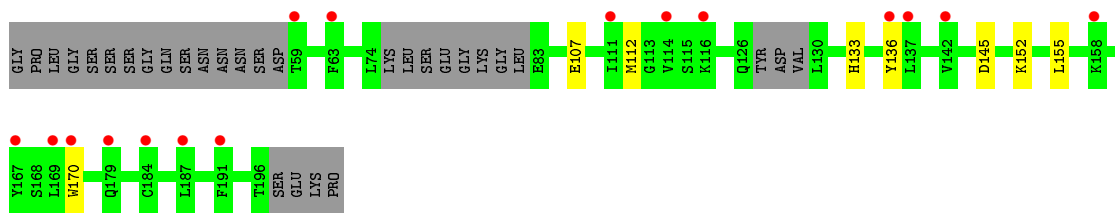


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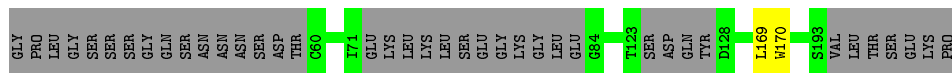


- Molecule 1: Integrin beta-1-binding protein 1

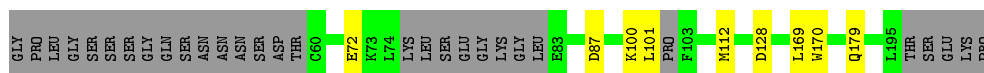




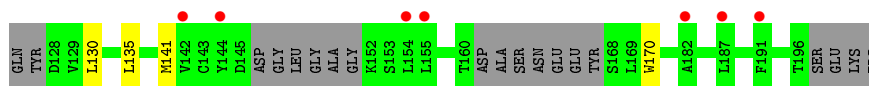
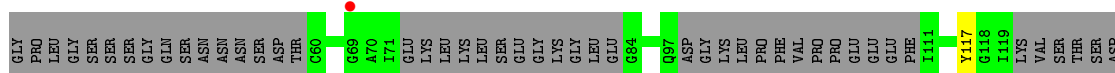
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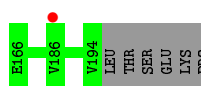
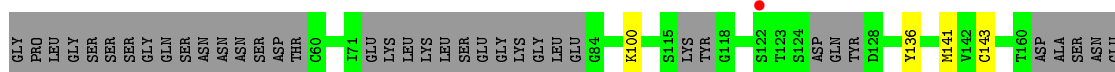
● Molecule 1: Integrin beta-1-binding protein 1



● Molecule 1: Integrin beta-1-binding protein 1

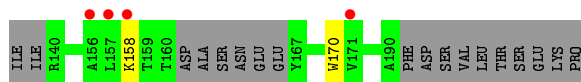


● Molecule 1: Integrin beta-1-binding protein 1



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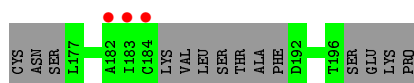
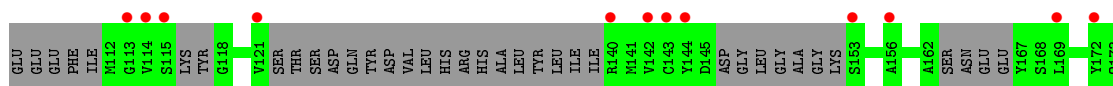
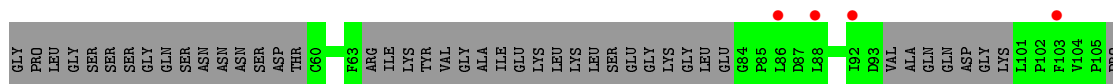




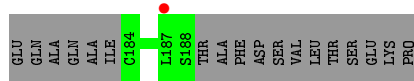
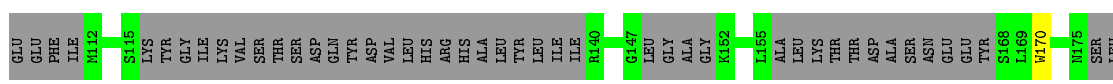
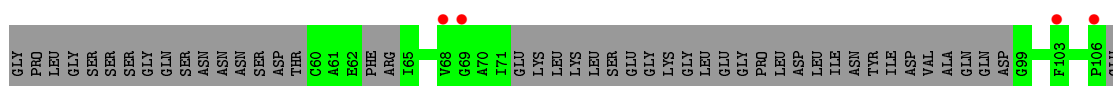
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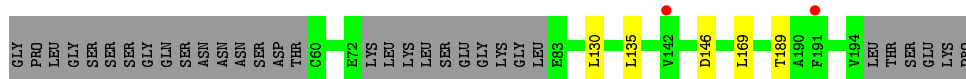
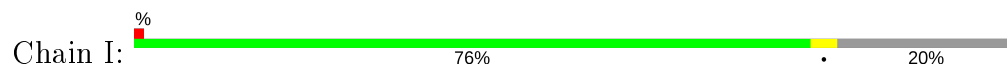
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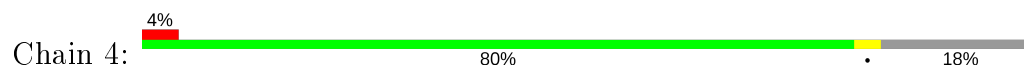
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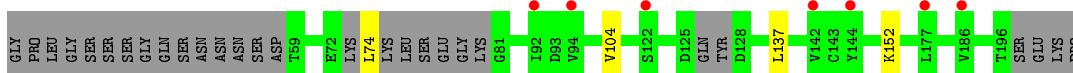


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- Molecule 1: Integrin beta-1-binding protein 1

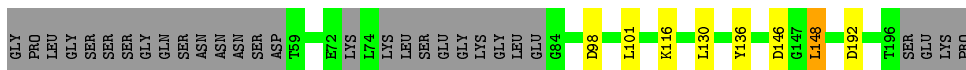




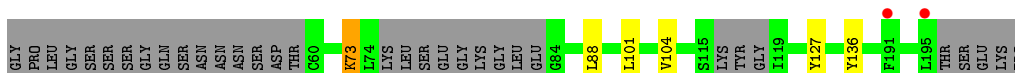
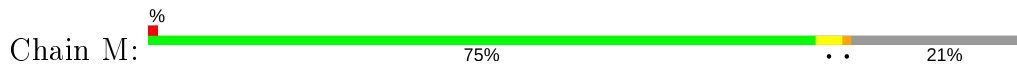
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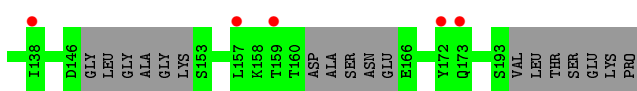
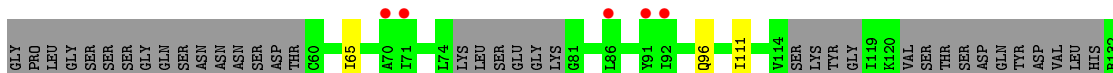
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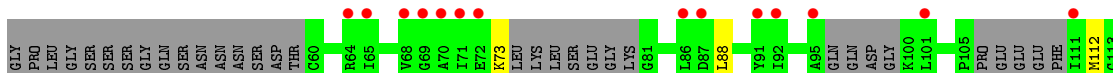
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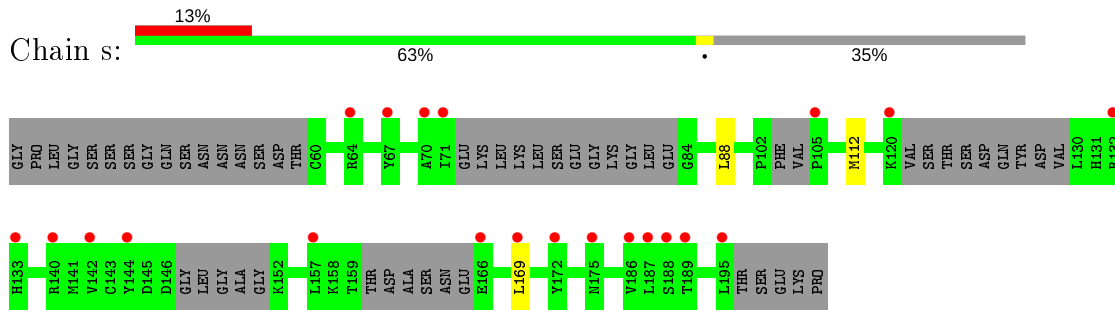
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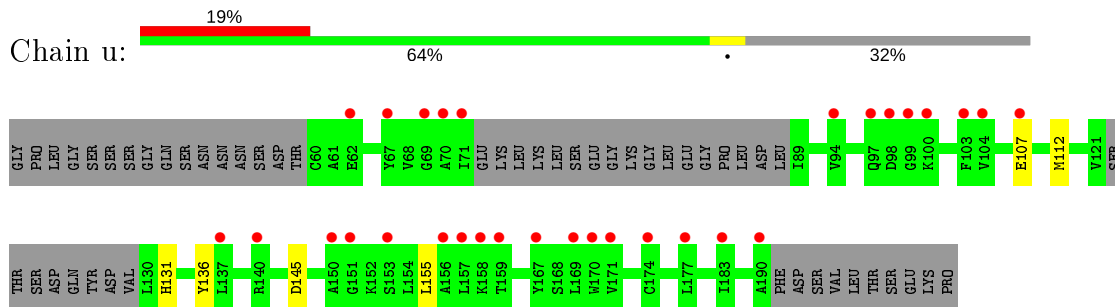
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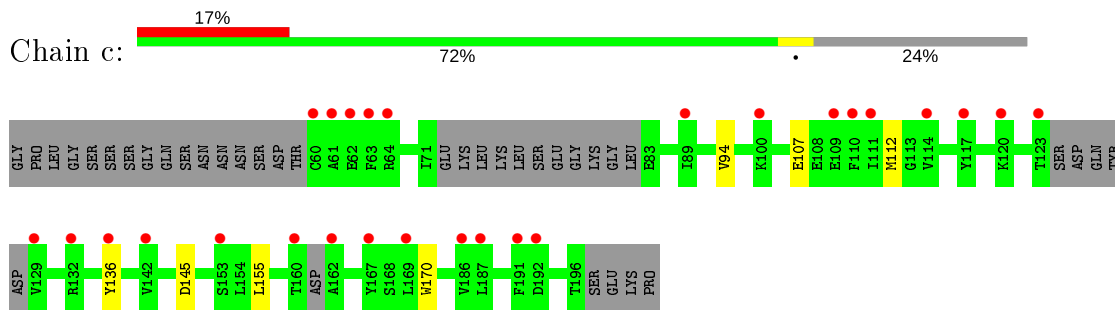
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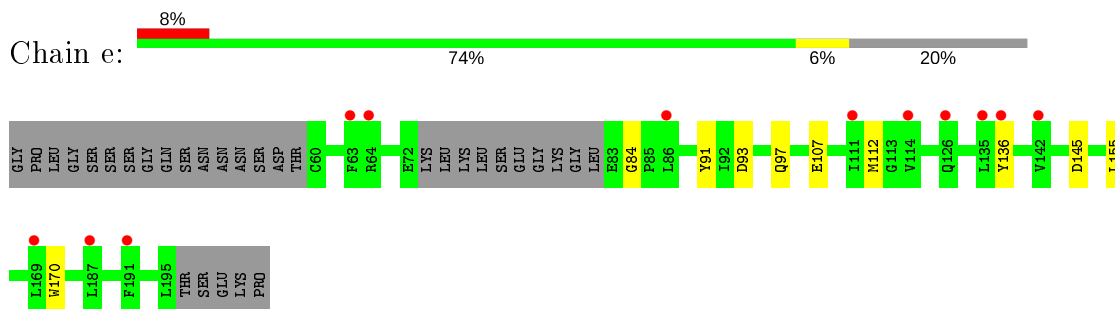
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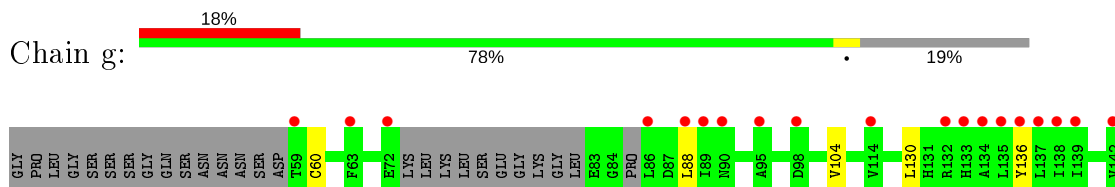
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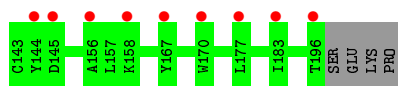


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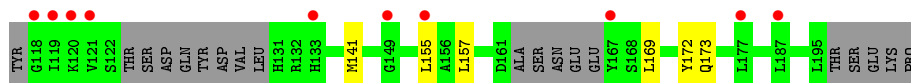
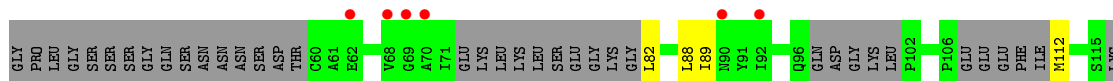


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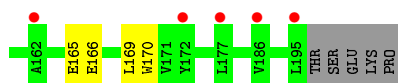
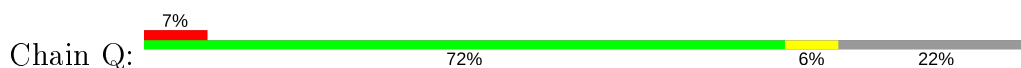




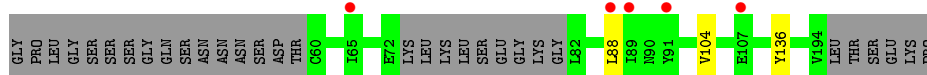
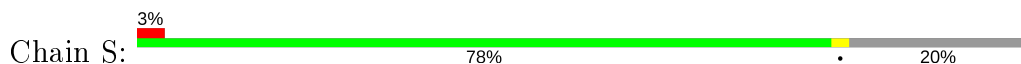
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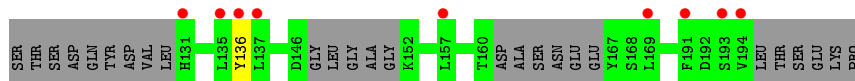
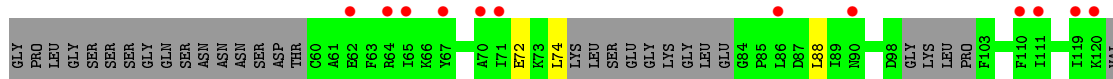
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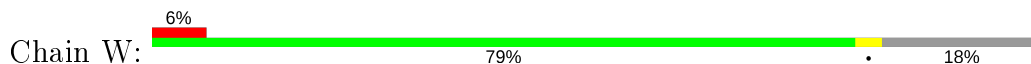
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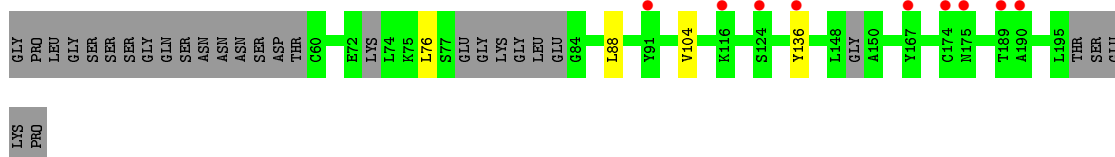


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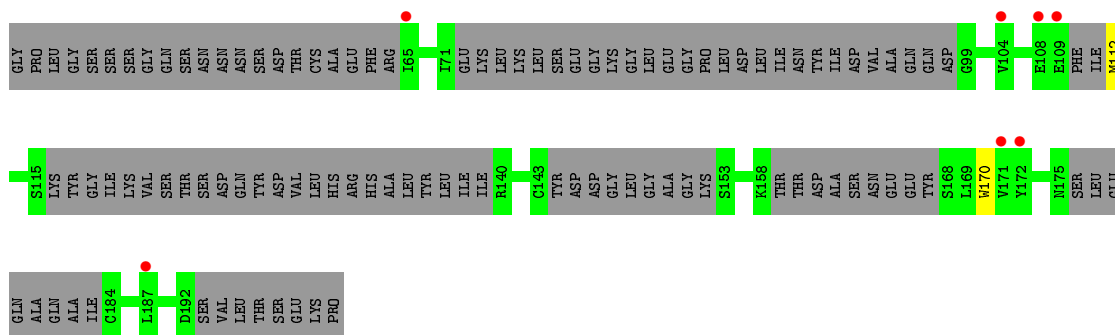


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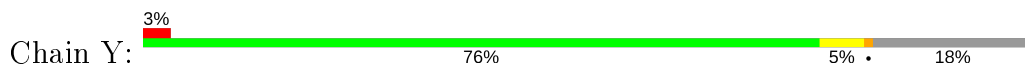




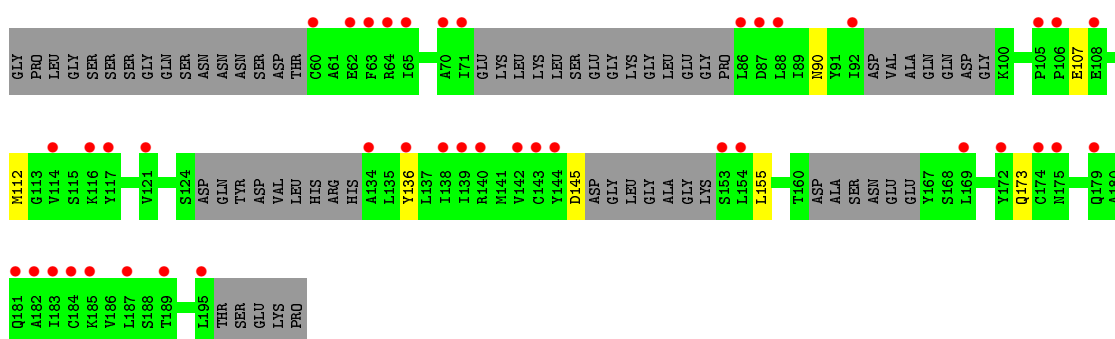
- Molecule 1: Integrin beta-1-binding protein 1



- Molecule 1: Integrin beta-1-binding protein 1



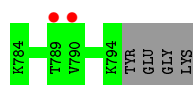
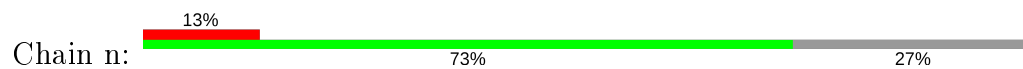
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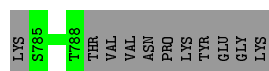
- Molecule 2: Integrin beta-1



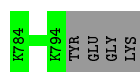
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- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



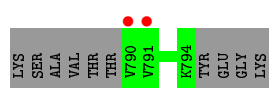
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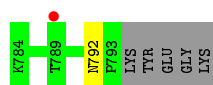
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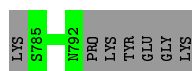
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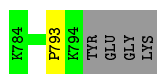
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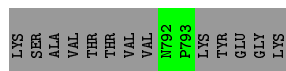
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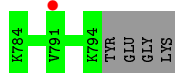
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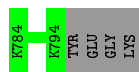
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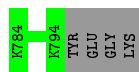
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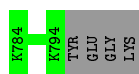
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



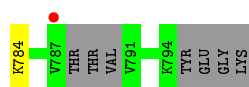
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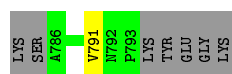
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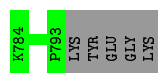
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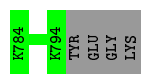
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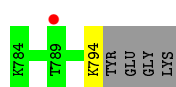
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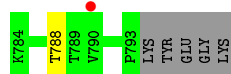
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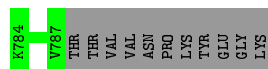
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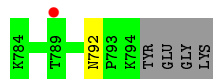
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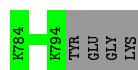
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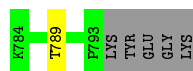
- Molecule 2: Integrin beta-1



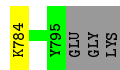
- Molecule 2: Integrin beta-1



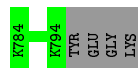
- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1



- Molecule 2: Integrin beta-1

Chain z:  33% 67%

| | |
|------|-----|
| LYS | LYS |
| SER | TYR |
| ALA | GLU |
| VAL | GLY |
| THR | LYS |
| T789 | |
| F793 | |

4 Data and refinement statistics

| Property | Value | Source |
|---|--|------------------|
| Space group | P 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 75.62Å 122.21Å 135.27Å 89.97° 89.99° 108.11° | Depositor |
| Resolution (Å) | 50.01 – 2.99 49.28 – 2.79 | Depositor EDS |
| % Data completeness (in resolution range) | 98.2 (50.01-2.99) 97.1 (49.28-2.79) | Depositor EDS |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | 0.13 | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 1.32 (at 2.77Å) | Xtrriage |
| Refinement program | REFMAC 5.6.0117 | Depositor |
| R, R_{free} | 0.251 , 0.312 0.251 , 0.311 | Depositor DCC |
| R_{free} test set | 5828 reflections (5.22%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 67.0 | Xtrriage |
| Anisotropy | 0.392 | Xtrriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 34.5 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$ | Xtrriage |
| Estimated twinning fraction | 0.458 for h,-h-k,-l 0.458 for -h,-k,l 0.458 for -h,h+k,-l | Xtrriage |
| Reported twinning fraction | 0.273 for H, K, L 0.239 for -h,-k,l 0.248 for h,-h-k,-l 0.239 for -H, H+K, -L | Depositor |
| Outliers | 0 of 111606 reflections | Xtrriage |
| F_o, F_c correlation | 0.90 | EDS |
| Total number of atoms | 29306 | wwPDB-VP |
| Average B, all atoms (Å ²) | 90.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 0 | 0.40 | 1/869 (0.1%) | 0.48 | 0/1168 |
| 1 | 1 | 0.39 | 0/933 | 0.47 | 0/1258 |
| 1 | 2 | 0.41 | 1/721 (0.1%) | 0.45 | 0/966 |
| 1 | 3 | 0.40 | 1/820 (0.1%) | 0.46 | 0/1100 |
| 1 | 4 | 0.38 | 0/1013 | 0.50 | 0/1366 |
| 1 | 5 | 0.39 | 0/1015 | 0.50 | 0/1371 |
| 1 | A | 0.40 | 1/856 (0.1%) | 0.44 | 0/1149 |
| 1 | C | 0.42 | 1/1011 (0.1%) | 0.54 | 0/1362 |
| 1 | E | 0.39 | 0/886 | 0.47 | 0/1192 |
| 1 | G | 0.38 | 0/1011 | 0.47 | 0/1366 |
| 1 | I | 0.40 | 0/995 | 0.50 | 0/1344 |
| 1 | K | 0.39 | 0/918 | 0.47 | 0/1236 |
| 1 | M | 0.40 | 0/984 | 0.50 | 1/1328 (0.1%) |
| 1 | O | 0.38 | 0/821 | 0.51 | 0/1101 |
| 1 | Q | 0.38 | 1/956 (0.1%) | 0.48 | 0/1287 |
| 1 | S | 0.37 | 0/1003 | 0.45 | 0/1355 |
| 1 | U | 0.55 | 1/821 (0.1%) | 0.47 | 0/1100 |
| 1 | W | 0.38 | 0/1019 | 0.45 | 0/1373 |
| 1 | Y | 1.06 | 2/1029 (0.2%) | 0.59 | 4/1388 (0.3%) |
| 1 | a | 0.38 | 1/784 (0.1%) | 0.46 | 0/1046 |
| 1 | c | 0.40 | 1/947 (0.1%) | 0.46 | 0/1276 |
| 1 | e | 0.38 | 1/1003 (0.1%) | 0.45 | 0/1355 |
| 1 | g | 0.38 | 0/1008 | 0.46 | 0/1360 |
| 1 | i | 0.40 | 0/788 | 0.49 | 0/1058 |
| 1 | k | 0.39 | 0/837 | 0.47 | 0/1122 |
| 1 | m | 0.38 | 1/1005 (0.1%) | 0.47 | 0/1355 |
| 1 | o | 0.40 | 0/489 | 0.45 | 0/651 |
| 1 | q | 0.45 | 1/359 (0.3%) | 0.46 | 0/472 |
| 1 | s | 0.39 | 0/823 | 0.45 | 0/1102 |
| 1 | u | 0.39 | 0/843 | 0.45 | 0/1134 |
| 1 | w | 0.45 | 1/379 (0.3%) | 0.47 | 0/501 |
| 1 | y | 0.53 | 2/746 (0.3%) | 0.45 | 0/1001 |
| 2 | 6 | 0.33 | 0/79 | 0.47 | 0/107 |
| 2 | 7 | 0.35 | 0/79 | 0.50 | 0/107 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | 8 | 0.35 | 0/54 | 0.50 | 0/73 |
| 2 | 9 | 0.36 | 0/53 | 0.45 | 0/73 |
| 2 | B | 0.37 | 0/70 | 0.53 | 0/96 |
| 2 | D | 0.35 | 0/79 | 0.45 | 0/107 |
| 2 | F | 0.34 | 0/79 | 0.52 | 0/107 |
| 2 | H | 0.32 | 0/79 | 0.52 | 0/107 |
| 2 | J | 0.31 | 0/79 | 0.52 | 0/107 |
| 2 | L | 0.36 | 0/79 | 0.55 | 0/107 |
| 2 | N | 0.32 | 0/79 | 0.44 | 0/107 |
| 2 | P | 0.32 | 0/79 | 0.53 | 0/107 |
| 2 | R | 0.34 | 0/79 | 0.49 | 0/107 |
| 2 | T | 0.32 | 0/79 | 0.46 | 0/107 |
| 2 | V | 0.31 | 0/70 | 0.48 | 0/96 |
| 2 | X | 0.33 | 0/92 | 0.50 | 0/125 |
| 2 | Z | 0.32 | 0/79 | 0.45 | 0/107 |
| 2 | b | 0.33 | 0/70 | 0.43 | 0/96 |
| 2 | d | 0.31 | 0/79 | 0.50 | 0/107 |
| 2 | f | 0.32 | 0/79 | 0.47 | 0/107 |
| 2 | h | 0.35 | 0/70 | 0.46 | 0/96 |
| 2 | j | 0.38 | 0/26 | 0.37 | 0/33 |
| 2 | l | 0.32 | 0/48 | 0.40 | 0/63 |
| 2 | n | 0.31 | 0/79 | 0.48 | 0/107 |
| 2 | p | 0.37 | 0/38 | 0.44 | 0/51 |
| 2 | r | 0.48 | 0/15 | 0.40 | 0/20 |
| 2 | t | 0.36 | 0/57 | 0.54 | 0/74 |
| 2 | v | 0.34 | 0/55 | 0.48 | 0/77 |
| 2 | x | 0.48 | 0/24 | 0.45 | 0/32 |
| 2 | z | 0.42 | 0/36 | 0.41 | 0/50 |
| All | All | 0.44 | 17/29655 (0.1%) | 0.48 | 5/39903 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | Y | 0 | 1 |

All (17) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | Y | 72 | GLU | CD-OE2 | 30.35 | 1.59 | 1.25 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | U | 72 | GLU | CD-OE1 | 10.66 | 1.37 | 1.25 |
| 1 | Y | 72 | GLU | C-O | -8.52 | 1.07 | 1.23 |
| 1 | y | 173 | GLN | CD-NE2 | -7.73 | 1.13 | 1.32 |
| 1 | y | 173 | GLN | CD-OE1 | -7.25 | 1.07 | 1.24 |
| 1 | C | 170 | TRP | CD2-CE2 | 5.08 | 1.47 | 1.41 |
| 1 | q | 170 | TRP | CD2-CE2 | 5.06 | 1.47 | 1.41 |
| 1 | a | 170 | TRP | CD2-CE2 | 5.06 | 1.47 | 1.41 |
| 1 | A | 170 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 1 | 3 | 170 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 1 | Q | 170 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | m | 170 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | 2 | 170 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | w | 170 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | 0 | 170 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |
| 1 | c | 170 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |
| 1 | e | 170 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |

All (5) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | Y | 72 | GLU | OE1-CD-OE2 | -6.96 | 114.95 | 123.30 |
| 1 | Y | 72 | GLU | CA-C-N | 6.70 | 131.94 | 117.20 |
| 1 | Y | 72 | GLU | O-C-N | -6.16 | 112.84 | 122.70 |
| 1 | Y | 72 | GLU | C-N-CA | -6.00 | 106.69 | 121.70 |
| 1 | M | 73 | LYS | N-CA-C | 5.61 | 126.14 | 111.00 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | Y | 72 | GLU | Sidechain |

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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 | 0 | 100/157 (64%) | 92 (92%) | 7 (7%) | 1 (1%) | 15 | 53 |
| 1 | 1 | 112/157 (71%) | 105 (94%) | 7 (6%) | 0 | 100 | 100 |
| 1 | 2 | 79/157 (50%) | 74 (94%) | 5 (6%) | 0 | 100 | 100 |
| 1 | 3 | 94/157 (60%) | 88 (94%) | 6 (6%) | 0 | 100 | 100 |
| 1 | 4 | 122/157 (78%) | 107 (88%) | 15 (12%) | 0 | 100 | 100 |
| 1 | 5 | 123/157 (78%) | 115 (94%) | 7 (6%) | 1 (1%) | 19 | 57 |
| 1 | A | 96/157 (61%) | 88 (92%) | 7 (7%) | 1 (1%) | 15 | 53 |
| 1 | C | 121/157 (77%) | 103 (85%) | 18 (15%) | 0 | 100 | 100 |
| 1 | E | 103/157 (66%) | 98 (95%) | 5 (5%) | 0 | 100 | 100 |
| 1 | G | 123/157 (78%) | 115 (94%) | 8 (6%) | 0 | 100 | 100 |
| 1 | I | 121/157 (77%) | 110 (91%) | 11 (9%) | 0 | 100 | 100 |
| 1 | K | 108/157 (69%) | 95 (88%) | 12 (11%) | 1 (1%) | 17 | 55 |
| 1 | M | 118/157 (75%) | 113 (96%) | 5 (4%) | 0 | 100 | 100 |
| 1 | O | 90/157 (57%) | 84 (93%) | 6 (7%) | 0 | 100 | 100 |
| 1 | Q | 113/157 (72%) | 105 (93%) | 6 (5%) | 2 (2%) | 8 | 37 |
| 1 | S | 122/157 (78%) | 119 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | U | 89/157 (57%) | 88 (99%) | 1 (1%) | 0 | 100 | 100 |
| 1 | W | 120/157 (76%) | 116 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | Y | 125/157 (80%) | 120 (96%) | 4 (3%) | 1 (1%) | 19 | 57 |
| 1 | a | 85/157 (54%) | 85 (100%) | 0 | 0 | 100 | 100 |
| 1 | c | 112/157 (71%) | 105 (94%) | 7 (6%) | 0 | 100 | 100 |
| 1 | e | 122/157 (78%) | 114 (93%) | 7 (6%) | 1 (1%) | 19 | 57 |
| 1 | g | 121/157 (77%) | 117 (97%) | 4 (3%) | 0 | 100 | 100 |
| 1 | i | 87/157 (55%) | 77 (88%) | 10 (12%) | 0 | 100 | 100 |
| 1 | k | 93/157 (59%) | 92 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | m | 121/157 (77%) | 110 (91%) | 11 (9%) | 0 | 100 | 100 |
| 1 | o | 43/157 (27%) | 41 (95%) | 2 (5%) | 0 | 100 | 100 |
| 1 | q | 31/157 (20%) | 29 (94%) | 2 (6%) | 0 | 100 | 100 |
| 1 | s | 90/157 (57%) | 86 (96%) | 4 (4%) | 0 | 100 | 100 |
| 1 | u | 100/157 (64%) | 93 (93%) | 7 (7%) | 0 | 100 | 100 |
| 1 | w | 35/157 (22%) | 31 (89%) | 4 (11%) | 0 | 100 | 100 |
| 1 | y | 81/157 (52%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 2 | 6 | 9/15 (60%) | 9 (100%) | 0 | 0 | 100 | 100 |
| 2 | 7 | 9/15 (60%) | 7 (78%) | 2 (22%) | 0 | 100 | 100 |
| 2 | 8 | 6/15 (40%) | 6 (100%) | 0 | 0 | 100 | 100 |
| 2 | 9 | 6/15 (40%) | 5 (83%) | 1 (17%) | 0 | 100 | 100 |
| 2 | B | 8/15 (53%) | 7 (88%) | 1 (12%) | 0 | 100 | 100 |
| 2 | D | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | F | 9/15 (60%) | 8 (89%) | 0 | 1 (11%) | 0 | 2 |
| 2 | H | 9/15 (60%) | 7 (78%) | 1 (11%) | 1 (11%) | 0 | 2 |
| 2 | J | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | L | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | N | 9/15 (60%) | 9 (100%) | 0 | 0 | 100 | 100 |
| 2 | P | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | R | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | T | 9/15 (60%) | 7 (78%) | 2 (22%) | 0 | 100 | 100 |
| 2 | V | 8/15 (53%) | 8 (100%) | 0 | 0 | 100 | 100 |
| 2 | X | 10/15 (67%) | 9 (90%) | 1 (10%) | 0 | 100 | 100 |
| 2 | Z | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | b | 8/15 (53%) | 8 (100%) | 0 | 0 | 100 | 100 |
| 2 | d | 9/15 (60%) | 7 (78%) | 2 (22%) | 0 | 100 | 100 |
| 2 | f | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |
| 2 | h | 8/15 (53%) | 8 (100%) | 0 | 0 | 100 | 100 |
| 2 | j | 2/15 (13%) | 2 (100%) | 0 | 0 | 100 | 100 |
| 2 | l | 3/15 (20%) | 3 (100%) | 0 | 0 | 100 | 100 |
| 2 | n | 9/15 (60%) | 8 (89%) | 1 (11%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 2 | p | 3/15 (20%) | 3 (100%) | 0 | 0 | 100 | 100 |
| 2 | t | 4/15 (27%) | 3 (75%) | 1 (25%) | 0 | 100 | 100 |
| 2 | v | 6/15 (40%) | 6 (100%) | 0 | 0 | 100 | 100 |
| 2 | x | 2/15 (13%) | 1 (50%) | 1 (50%) | 0 | 100 | 100 |
| 2 | z | 3/15 (20%) | 2 (67%) | 1 (33%) | 0 | 100 | 100 |
| All | All | 3412/5459 (62%) | 3183 (93%) | 219 (6%) | 10 (0%) | 41 | 76 |

All (10) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 151 | GLY |
| 1 | K | 107 | GLU |
| 1 | 5 | 116 | LYS |
| 1 | Y | 126 | GLN |
| 1 | A | 103 | PHE |
| 1 | 0 | 68 | VAL |
| 1 | Q | 98 | ASP |
| 2 | H | 793 | PRO |
| 1 | e | 84 | GLY |
| 2 | F | 793 | PRO |

5.3.2 Protein sidechains [i](#)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|----|
| 1 | 0 | 94/132 (71%) | 92 (98%) | 2 (2%) | 53 | 82 |
| 1 | 1 | 100/132 (76%) | 98 (98%) | 2 (2%) | 55 | 83 |
| 1 | 2 | 79/132 (60%) | 75 (95%) | 4 (5%) | 24 | 60 |
| 1 | 3 | 88/132 (67%) | 85 (97%) | 3 (3%) | 37 | 72 |
| 1 | 4 | 110/132 (83%) | 106 (96%) | 4 (4%) | 35 | 70 |
| 1 | 5 | 110/132 (83%) | 103 (94%) | 7 (6%) | 17 | 51 |
| 1 | A | 92/132 (70%) | 88 (96%) | 4 (4%) | 29 | 66 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|---------------|-----------|----------|-------------|-----|
| 1 | C | 109/132 (83%) | 101 (93%) | 8 (7%) | 14 | 44 |
| 1 | E | 96/132 (73%) | 92 (96%) | 4 (4%) | 30 | 66 |
| 1 | G | 109/132 (83%) | 106 (97%) | 3 (3%) | 43 | 77 |
| 1 | I | 107/132 (81%) | 102 (95%) | 5 (5%) | 26 | 63 |
| 1 | K | 98/132 (74%) | 92 (94%) | 6 (6%) | 18 | 53 |
| 1 | M | 107/132 (81%) | 101 (94%) | 6 (6%) | 21 | 56 |
| 1 | O | 89/132 (67%) | 86 (97%) | 3 (3%) | 37 | 72 |
| 1 | Q | 104/132 (79%) | 98 (94%) | 6 (6%) | 20 | 55 |
| 1 | S | 108/132 (82%) | 105 (97%) | 3 (3%) | 43 | 77 |
| 1 | U | 89/132 (67%) | 86 (97%) | 3 (3%) | 37 | 72 |
| 1 | W | 111/132 (84%) | 107 (96%) | 4 (4%) | 35 | 70 |
| 1 | Y | 111/132 (84%) | 105 (95%) | 6 (5%) | 22 | 57 |
| 1 | a | 84/132 (64%) | 77 (92%) | 7 (8%) | 11 | 39 |
| 1 | c | 102/132 (77%) | 96 (94%) | 6 (6%) | 19 | 54 |
| 1 | e | 108/132 (82%) | 100 (93%) | 8 (7%) | 13 | 44 |
| 1 | g | 109/132 (83%) | 104 (95%) | 5 (5%) | 27 | 64 |
| 1 | i | 85/132 (64%) | 75 (88%) | 10 (12%) | 5 | 22 |
| 1 | k | 91/132 (69%) | 85 (93%) | 6 (7%) | 16 | 49 |
| 1 | m | 109/132 (83%) | 102 (94%) | 7 (6%) | 17 | 51 |
| 1 | o | 55/132 (42%) | 55 (100%) | 0 | 100 | 100 |
| 1 | q | 41/132 (31%) | 41 (100%) | 0 | 100 | 100 |
| 1 | s | 89/132 (67%) | 86 (97%) | 3 (3%) | 37 | 72 |
| 1 | u | 89/132 (67%) | 83 (93%) | 6 (7%) | 16 | 49 |
| 1 | w | 43/132 (33%) | 42 (98%) | 1 (2%) | 50 | 80 |
| 1 | y | 83/132 (63%) | 77 (93%) | 6 (7%) | 14 | 45 |
| 2 | 6 | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | 7 | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | 8 | 7/13 (54%) | 6 (86%) | 1 (14%) | 3 | 15 |
| 2 | 9 | 7/13 (54%) | 7 (100%) | 0 | 100 | 100 |
| 2 | B | 9/13 (69%) | 8 (89%) | 1 (11%) | 6 | 25 |
| 2 | D | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 2 | F | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | H | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | J | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | L | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | N | 10/13 (77%) | 8 (80%) | 2 (20%) | 1 | 7 |
| 2 | P | 10/13 (77%) | 8 (80%) | 2 (20%) | 1 | 7 |
| 2 | R | 10/13 (77%) | 9 (90%) | 1 (10%) | 7 | 29 |
| 2 | T | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | V | 9/13 (69%) | 8 (89%) | 1 (11%) | 6 | 25 |
| 2 | X | 11/13 (85%) | 10 (91%) | 1 (9%) | 9 | 34 |
| 2 | Z | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | b | 9/13 (69%) | 9 (100%) | 0 | 100 | 100 |
| 2 | d | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | f | 10/13 (77%) | 9 (90%) | 1 (10%) | 7 | 29 |
| 2 | h | 9/13 (69%) | 8 (89%) | 1 (11%) | 6 | 25 |
| 2 | j | 3/13 (23%) | 3 (100%) | 0 | 100 | 100 |
| 2 | l | 6/13 (46%) | 6 (100%) | 0 | 100 | 100 |
| 2 | n | 10/13 (77%) | 10 (100%) | 0 | 100 | 100 |
| 2 | p | 5/13 (38%) | 5 (100%) | 0 | 100 | 100 |
| 2 | r | 2/13 (15%) | 2 (100%) | 0 | 100 | 100 |
| 2 | t | 7/13 (54%) | 6 (86%) | 1 (14%) | 3 | 15 |
| 2 | v | 7/13 (54%) | 6 (86%) | 1 (14%) | 3 | 15 |
| 2 | x | 3/13 (23%) | 3 (100%) | 0 | 100 | 100 |
| 2 | z | 5/13 (38%) | 5 (100%) | 0 | 100 | 100 |
| All | All | 3248/4614 (70%) | 3087 (95%) | 161 (5%) | 24 | 60 |

All (161) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 141 | MSE |
| 1 | A | 155 | LEU |
| 1 | A | 169 | LEU |
| 1 | A | 179 | GLN |
| 1 | 0 | 112 | MSE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 0 | 148 | LEU |
| 1 | k | 88 | LEU |
| 1 | k | 112 | MSE |
| 1 | k | 116 | LYS |
| 1 | k | 130 | LEU |
| 1 | k | 159 | THR |
| 1 | k | 169 | LEU |
| 1 | m | 107 | GLU |
| 1 | m | 112 | MSE |
| 1 | m | 133 | HIS |
| 1 | m | 136 | TYR |
| 1 | m | 145 | ASP |
| 1 | m | 152 | LYS |
| 1 | m | 155 | LEU |
| 1 | 1 | 169 | LEU |
| 1 | 1 | 170 | TRP |
| 1 | C | 72 | GLU |
| 1 | C | 87 | ASP |
| 1 | C | 100 | LYS |
| 1 | C | 101 | LEU |
| 1 | C | 112 | MSE |
| 1 | C | 128 | ASP |
| 1 | C | 169 | LEU |
| 1 | C | 179 | GLN |
| 1 | 2 | 117 | TYR |
| 1 | 2 | 130 | LEU |
| 1 | 2 | 135 | LEU |
| 1 | 2 | 141 | MSE |
| 1 | E | 100 | LYS |
| 1 | E | 136 | TYR |
| 1 | E | 141 | MSE |
| 1 | E | 143 | CYS |
| 1 | 3 | 112 | MSE |
| 1 | 3 | 119 | ILE |
| 1 | 3 | 158 | LYS |
| 1 | G | 82 | LEU |
| 1 | G | 135 | LEU |
| 1 | G | 188 | SER |
| 2 | 8 | 788 | THR |
| 2 | B | 792 | ASN |
| 1 | I | 130 | LEU |
| 1 | I | 135 | LEU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | I | 146 | ASP |
| 1 | I | 169 | LEU |
| 1 | I | 189 | THR |
| 1 | 4 | 74 | LEU |
| 1 | 4 | 104 | VAL |
| 1 | 4 | 137 | LEU |
| 1 | 4 | 152 | LYS |
| 1 | K | 98 | ASP |
| 1 | K | 112 | MSE |
| 1 | K | 140 | ARG |
| 1 | K | 141 | MSE |
| 1 | K | 155 | LEU |
| 1 | K | 157 | LEU |
| 1 | 5 | 98 | ASP |
| 1 | 5 | 101 | LEU |
| 1 | 5 | 130 | LEU |
| 1 | 5 | 136 | TYR |
| 1 | 5 | 146 | ASP |
| 1 | 5 | 148 | LEU |
| 1 | 5 | 192 | ASP |
| 1 | M | 73 | LYS |
| 1 | M | 88 | LEU |
| 1 | M | 101 | LEU |
| 1 | M | 104 | VAL |
| 1 | M | 127 | TYR |
| 1 | M | 136 | TYR |
| 2 | N | 784 | LYS |
| 2 | N | 794 | LYS |
| 1 | O | 65 | ILE |
| 1 | O | 96 | GLN |
| 1 | O | 111 | ILE |
| 2 | P | 791 | VAL |
| 2 | P | 792 | ASN |
| 1 | a | 73 | LYS |
| 1 | a | 88 | LEU |
| 1 | a | 112 | MSE |
| 1 | a | 117 | TYR |
| 1 | a | 135 | LEU |
| 1 | a | 152 | LYS |
| 1 | a | 169 | LEU |
| 1 | s | 88 | LEU |
| 1 | s | 112 | MSE |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | s | 169 | LEU |
| 2 | t | 784 | LYS |
| 1 | u | 107 | GLU |
| 1 | u | 112 | MSE |
| 1 | u | 131 | HIS |
| 1 | u | 136 | TYR |
| 1 | u | 145 | ASP |
| 1 | u | 155 | LEU |
| 2 | v | 791 | VAL |
| 1 | c | 94 | VAL |
| 1 | c | 107 | GLU |
| 1 | c | 112 | MSE |
| 1 | c | 136 | TYR |
| 1 | c | 145 | ASP |
| 1 | c | 155 | LEU |
| 1 | e | 91 | TYR |
| 1 | e | 93 | ASP |
| 1 | e | 97 | GLN |
| 1 | e | 107 | GLU |
| 1 | e | 112 | MSE |
| 1 | e | 136 | TYR |
| 1 | e | 145 | ASP |
| 1 | e | 155 | LEU |
| 2 | f | 794 | LYS |
| 1 | g | 60 | CYS |
| 1 | g | 88 | LEU |
| 1 | g | 104 | VAL |
| 1 | g | 130 | LEU |
| 1 | g | 136 | TYR |
| 2 | h | 788 | THR |
| 1 | i | 82 | LEU |
| 1 | i | 88 | LEU |
| 1 | i | 89 | ILE |
| 1 | i | 112 | MSE |
| 1 | i | 141 | MSE |
| 1 | i | 155 | LEU |
| 1 | i | 157 | LEU |
| 1 | i | 169 | LEU |
| 1 | i | 172 | TYR |
| 1 | i | 173 | GLN |
| 1 | Q | 74 | LEU |
| 1 | Q | 88 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | Q | 112 | MSE |
| 1 | Q | 165 | GLU |
| 1 | Q | 166 | GLU |
| 1 | Q | 169 | LEU |
| 2 | R | 792 | ASN |
| 1 | S | 88 | LEU |
| 1 | S | 104 | VAL |
| 1 | S | 136 | TYR |
| 1 | U | 74 | LEU |
| 1 | U | 88 | LEU |
| 1 | U | 136 | TYR |
| 2 | V | 789 | THR |
| 1 | W | 76 | LEU |
| 1 | W | 88 | LEU |
| 1 | W | 104 | VAL |
| 1 | W | 136 | TYR |
| 1 | w | 112 | MSE |
| 2 | X | 784 | LYS |
| 1 | Y | 74 | LEU |
| 1 | Y | 83 | GLU |
| 1 | Y | 88 | LEU |
| 1 | Y | 104 | VAL |
| 1 | Y | 130 | LEU |
| 1 | Y | 136 | TYR |
| 1 | y | 90 | ASN |
| 1 | y | 107 | GLU |
| 1 | y | 112 | MSE |
| 1 | y | 136 | TYR |
| 1 | y | 145 | ASP |
| 1 | y | 155 | LEU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 131 | HIS |
| 1 | A | 133 | HIS |
| 1 | C | 90 | ASN |
| 1 | 4 | 173 | GLN |
| 1 | U | 181 | GLN |
| 1 | Y | 181 | GLN |

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 | 0 | 108/157 (68%) | 0.26 | 5 (4%) 32 12 | 65, 77, 88, 97 | 0 |
| 1 | 1 | 116/157 (73%) | 0.20 | 0 100 100 | 66, 72, 83, 91 | 0 |
| 1 | 2 | 89/157 (56%) | 0.69 | 8 (8%) 9 3 | 76, 85, 94, 97 | 0 |
| 1 | 3 | 102/157 (64%) | 0.58 | 12 (11%) 4 1 | 75, 91, 105, 110 | 0 |
| 1 | 4 | 127/157 (80%) | 0.50 | 7 (5%) 25 9 | 58, 76, 87, 90 | 0 |
| 1 | 5 | 126/157 (80%) | 0.29 | 0 100 100 | 55, 72, 82, 86 | 0 |
| 1 | A | 104/157 (66%) | 0.26 | 4 (3%) 40 16 | 64, 77, 85, 90 | 0 |
| 1 | C | 125/157 (79%) | -0.07 | 0 100 100 | 46, 50, 56, 67 | 0 |
| 1 | E | 111/157 (70%) | 0.18 | 2 (1%) 68 40 | 60, 73, 86, 95 | 0 |
| 1 | G | 125/157 (79%) | 0.11 | 0 100 100 | 58, 67, 79, 91 | 0 |
| 1 | I | 123/157 (78%) | 0.05 | 2 (1%) 72 44 | 49, 57, 66, 77 | 0 |
| 1 | K | 114/157 (72%) | 0.11 | 1 (0%) 84 63 | 55, 70, 82, 85 | 0 |
| 1 | M | 122/157 (77%) | 0.44 | 2 (1%) 72 44 | 64, 78, 92, 105 | 0 |
| 1 | O | 100/157 (63%) | 0.66 | 10 (10%) 7 2 | 73, 97, 116, 124 | 0 |
| 1 | Q | 120/157 (76%) | 0.56 | 11 (9%) 9 3 | 72, 94, 106, 113 | 0 |
| 1 | S | 124/157 (78%) | 0.46 | 5 (4%) 38 15 | 71, 87, 101, 110 | 0 |
| 1 | U | 99/157 (63%) | 1.21 | 21 (21%) 0 0 | 82, 116, 134, 149 | 0 |
| 1 | W | 126/157 (80%) | 0.76 | 9 (7%) 16 5 | 67, 89, 106, 115 | 0 |
| 1 | Y | 127/157 (80%) | 0.62 | 5 (3%) 39 15 | 67, 85, 107, 123 | 0 |
| 1 | a | 97/157 (61%) | 1.36 | 27 (27%) 0 0 | 101, 119, 153, 158 | 0 |
| 1 | c | 118/157 (75%) | 1.55 | 27 (22%) 0 0 | 91, 116, 149, 159 | 0 |
| 1 | e | 124/157 (78%) | 0.72 | 12 (9%) 7 2 | 68, 92, 108, 116 | 0 |
| 1 | g | 125/157 (79%) | 1.13 | 28 (22%) 0 0 | 87, 106, 120, 134 | 0 |
| 1 | i | 99/157 (63%) | 0.73 | 16 (16%) 1 0 | 79, 105, 118, 128 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|---------------|--------|--------------|-----------------------|-------|
| 1 | k | 103/157 (65%) | 1.07 | 22 (21%) 0 0 | 90, 110, 125, 131 | 0 |
| 1 | m | 125/157 (79%) | 0.80 | 16 (12%) 3 1 | 75, 98, 110, 120 | 0 |
| 1 | o | 61/157 (38%) | 1.58 | 19 (31%) 0 0 | 64, 112, 132, 147 | 0 |
| 1 | q | 45/157 (28%) | 0.83 | 5 (11%) 5 1 | 73, 107, 121, 127 | 0 |
| 1 | s | 100/157 (63%) | 1.26 | 21 (21%) 1 0 | 89, 112, 129, 134 | 0 |
| 1 | u | 104/157 (66%) | 1.32 | 30 (28%) 0 0 | 88, 116, 139, 147 | 0 |
| 1 | w | 47/157 (29%) | 0.91 | 7 (14%) 2 1 | 77, 107, 133, 139 | 0 |
| 1 | y | 91/157 (57%) | 2.14 | 41 (45%) 0 0 | 106, 134, 155, 168 | 0 |
| 2 | 6 | 11/15 (73%) | 0.03 | 0 100 100 | 72, 77, 82, 90 | 0 |
| 2 | 7 | 11/15 (73%) | -0.28 | 0 100 100 | 66, 72, 75, 75 | 0 |
| 2 | 8 | 8/15 (53%) | 0.31 | 1 (12%) 3 1 | 68, 73, 79, 80 | 0 |
| 2 | 9 | 8/15 (53%) | 0.04 | 0 100 100 | 64, 70, 78, 79 | 0 |
| 2 | B | 10/15 (66%) | 0.63 | 1 (10%) 7 2 | 54, 69, 74, 75 | 0 |
| 2 | D | 11/15 (73%) | 0.02 | 0 100 100 | 36, 38, 64, 71 | 0 |
| 2 | F | 11/15 (73%) | 0.28 | 0 100 100 | 44, 65, 79, 80 | 0 |
| 2 | H | 11/15 (73%) | 0.02 | 0 100 100 | 46, 54, 63, 63 | 0 |
| 2 | J | 11/15 (73%) | 0.69 | 1 (9%) 9 3 | 78, 83, 104, 112 | 0 |
| 2 | L | 11/15 (73%) | -0.04 | 0 100 100 | 59, 64, 70, 72 | 0 |
| 2 | N | 11/15 (73%) | 0.40 | 0 100 100 | 61, 66, 75, 80 | 0 |
| 2 | P | 11/15 (73%) | 0.22 | 0 100 100 | 45, 70, 90, 92 | 0 |
| 2 | R | 11/15 (73%) | 0.70 | 1 (9%) 9 3 | 75, 85, 102, 104 | 0 |
| 2 | T | 11/15 (73%) | 0.13 | 0 100 100 | 80, 84, 87, 87 | 0 |
| 2 | V | 10/15 (66%) | 0.47 | 0 100 100 | 67, 71, 92, 93 | 0 |
| 2 | X | 12/15 (80%) | 0.33 | 0 100 100 | 64, 73, 80, 81 | 0 |
| 2 | Z | 11/15 (73%) | 0.78 | 0 100 100 | 87, 90, 92, 93 | 0 |
| 2 | b | 10/15 (66%) | 0.57 | 0 100 100 | 88, 100, 116, 117 | 0 |
| 2 | d | 11/15 (73%) | 0.46 | 0 100 100 | 65, 90, 99, 101 | 0 |
| 2 | f | 11/15 (73%) | 0.44 | 1 (9%) 9 3 | 73, 78, 81, 83 | 0 |
| 2 | h | 10/15 (66%) | 0.80 | 1 (10%) 7 2 | 78, 88, 93, 94 | 0 |
| 2 | j | 4/15 (26%) | -0.01 | 0 100 100 | 90, 92, 92, 95 | 0 |
| 2 | l | 7/15 (46%) | 0.03 | 0 100 100 | 72, 80, 99, 101 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 2 | n | 11/15 (73%) | 0.65 | 2 (18%) 1 0 | 89, 92, 94, 95 | 0 |
| 2 | p | 5/15 (33%) | 1.11 | 2 (40%) 0 0 | 111, 117, 118, 121 | 0 |
| 2 | r | 2/15 (13%) | -0.09 | 0 100 100 | 76, 76, 76, 82 | 0 |
| 2 | t | 8/15 (53%) | 0.04 | 1 (12%) 3 1 | 53, 57, 92, 94 | 0 |
| 2 | v | 8/15 (53%) | 0.46 | 0 100 100 | 80, 88, 104, 104 | 0 |
| 2 | x | 4/15 (26%) | 0.46 | 0 100 100 | 74, 78, 80, 83 | 0 |
| 2 | z | 5/15 (33%) | 0.58 | 0 100 100 | 99, 102, 108, 109 | 0 |
| All | All | 3703/5474 (67%) | 0.66 | 386 (10%) 6 2 | 36, 87, 129, 168 | 0 |

All (386) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | c | 60 | CYS | 22.8 |
| 1 | a | 70 | ALA | 12.6 |
| 1 | y | 70 | ALA | 11.6 |
| 1 | y | 169 | LEU | 11.3 |
| 1 | c | 109 | GLU | 9.5 |
| 1 | c | 110 | PHE | 8.8 |
| 1 | u | 70 | ALA | 8.5 |
| 1 | U | 194 | VAL | 8.5 |
| 1 | o | 142 | VAL | 8.5 |
| 1 | c | 132 | ARG | 8.4 |
| 1 | y | 92 | ILE | 7.8 |
| 1 | k | 178 | GLU | 7.3 |
| 1 | 4 | 142 | VAL | 7.1 |
| 1 | o | 121 | VAL | 7.1 |
| 1 | M | 195 | LEU | 7.0 |
| 1 | u | 100 | LYS | 6.8 |
| 1 | k | 91 | TYR | 6.7 |
| 1 | U | 70 | ALA | 6.4 |
| 1 | m | 142 | VAL | 6.4 |
| 1 | W | 167 | TYR | 6.3 |
| 1 | c | 117 | TYR | 6.0 |
| 1 | y | 62 | GLU | 5.9 |
| 1 | g | 139 | ILE | 5.9 |
| 1 | y | 142 | VAL | 5.9 |
| 1 | s | 187 | LEU | 5.8 |
| 1 | i | 69 | GLY | 5.7 |
| 1 | s | 188 | SER | 5.7 |
| 1 | Y | 195 | LEU | 5.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | s | 70 | ALA | 5.6 |
| 1 | u | 170 | TRP | 5.6 |
| 1 | y | 105 | PRO | 5.6 |
| 1 | a | 86 | LEU | 5.6 |
| 1 | W | 136 | TYR | 5.6 |
| 1 | y | 88 | LEU | 5.4 |
| 1 | m | 167 | TYR | 5.4 |
| 1 | g | 138 | ILE | 5.4 |
| 1 | U | 120 | LYS | 5.3 |
| 1 | q | 68 | VAL | 5.3 |
| 1 | w | 187 | LEU | 5.2 |
| 1 | c | 111 | ILE | 5.2 |
| 1 | W | 91 | TYR | 5.1 |
| 1 | o | 144 | TYR | 5.1 |
| 1 | u | 103 | PHE | 5.1 |
| 1 | c | 61 | ALA | 5.0 |
| 1 | w | 104 | VAL | 5.0 |
| 1 | o | 114 | VAL | 4.9 |
| 1 | a | 175 | ASN | 4.9 |
| 1 | a | 111 | ILE | 4.8 |
| 1 | o | 140 | ARG | 4.8 |
| 1 | i | 120 | LYS | 4.8 |
| 1 | s | 133 | HIS | 4.8 |
| 1 | a | 65 | ILE | 4.7 |
| 1 | k | 64 | ARG | 4.7 |
| 1 | y | 136 | TYR | 4.7 |
| 1 | 0 | 111 | ILE | 4.7 |
| 1 | 3 | 100 | LYS | 4.6 |
| 1 | u | 157 | LEU | 4.6 |
| 1 | g | 144 | TYR | 4.6 |
| 1 | s | 142 | VAL | 4.6 |
| 1 | 3 | 99 | GLY | 4.6 |
| 1 | g | 134 | ALA | 4.6 |
| 1 | c | 64 | ARG | 4.6 |
| 1 | 2 | 69 | GLY | 4.6 |
| 1 | W | 174 | CYS | 4.5 |
| 1 | 2 | 142 | VAL | 4.5 |
| 1 | k | 179 | GLN | 4.5 |
| 1 | o | 184 | CYS | 4.5 |
| 1 | a | 92 | ILE | 4.4 |
| 1 | 2 | 191 | PHE | 4.4 |
| 1 | s | 195 | LEU | 4.4 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | W | 124 | SER | 4.3 |
| 1 | i | 177 | LEU | 4.3 |
| 1 | y | 71 | ILE | 4.3 |
| 1 | w | 109 | GLU | 4.3 |
| 1 | o | 92 | ILE | 4.3 |
| 1 | o | 143 | CYS | 4.2 |
| 1 | y | 64 | ARG | 4.2 |
| 1 | y | 106 | PRO | 4.2 |
| 1 | g | 135 | LEU | 4.2 |
| 1 | g | 167 | TYR | 4.2 |
| 1 | a | 167 | TYR | 4.1 |
| 1 | u | 177 | LEU | 4.1 |
| 1 | u | 69 | GLY | 4.1 |
| 2 | R | 789 | THR | 4.1 |
| 1 | o | 183 | ILE | 4.1 |
| 1 | u | 153 | SER | 4.1 |
| 1 | u | 158 | LYS | 4.1 |
| 1 | i | 149 | GLY | 4.0 |
| 1 | 2 | 187 | LEU | 4.0 |
| 1 | g | 59 | THR | 4.0 |
| 1 | U | 193 | SER | 4.0 |
| 1 | Q | 135 | LEU | 4.0 |
| 1 | g | 89 | ILE | 3.9 |
| 1 | a | 71 | ILE | 3.9 |
| 1 | a | 72 | GLU | 3.9 |
| 1 | m | 137 | LEU | 3.9 |
| 1 | y | 154 | LEU | 3.9 |
| 1 | g | 158 | LYS | 3.9 |
| 1 | g | 133 | HIS | 3.9 |
| 1 | i | 133 | HIS | 3.9 |
| 1 | u | 97 | GLN | 3.9 |
| 1 | k | 134 | ALA | 3.9 |
| 1 | y | 108 | GLU | 3.9 |
| 1 | k | 167 | TYR | 3.8 |
| 1 | o | 169 | LEU | 3.8 |
| 1 | O | 159 | THR | 3.8 |
| 1 | a | 91 | TYR | 3.8 |
| 1 | a | 120 | LYS | 3.8 |
| 1 | y | 187 | LEU | 3.8 |
| 1 | O | 172 | TYR | 3.7 |
| 2 | B | 789 | THR | 3.7 |
| 1 | Q | 89 | ILE | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | y | 139 | ILE | 3.7 |
| 1 | g | 170 | TRP | 3.7 |
| 1 | c | 191 | PHE | 3.7 |
| 1 | e | 136 | TYR | 3.7 |
| 1 | m | 116 | LYS | 3.6 |
| 1 | u | 171 | VAL | 3.6 |
| 1 | U | 65 | ILE | 3.6 |
| 1 | k | 63 | PHE | 3.6 |
| 1 | y | 116 | LYS | 3.6 |
| 1 | u | 62 | GLU | 3.6 |
| 1 | s | 67 | TYR | 3.6 |
| 1 | 2 | 155 | LEU | 3.6 |
| 1 | 3 | 156 | ALA | 3.6 |
| 1 | k | 113 | GLY | 3.6 |
| 1 | u | 151 | GLY | 3.6 |
| 1 | c | 136 | TYR | 3.6 |
| 1 | s | 71 | ILE | 3.5 |
| 1 | a | 173 | GLN | 3.5 |
| 1 | s | 132 | ARG | 3.5 |
| 1 | O | 138 | ILE | 3.5 |
| 1 | w | 108 | GLU | 3.5 |
| 1 | O | 92 | ILE | 3.5 |
| 1 | g | 142 | VAL | 3.5 |
| 1 | e | 111 | ILE | 3.5 |
| 1 | y | 63 | PHE | 3.5 |
| 1 | k | 65 | ILE | 3.5 |
| 1 | i | 70 | ALA | 3.5 |
| 1 | o | 172 | TYR | 3.4 |
| 1 | Q | 162 | ALA | 3.4 |
| 1 | U | 135 | LEU | 3.4 |
| 1 | c | 63 | PHE | 3.4 |
| 1 | W | 175 | ASN | 3.4 |
| 1 | a | 133 | HIS | 3.4 |
| 1 | i | 121 | VAL | 3.4 |
| 1 | y | 140 | ARG | 3.4 |
| 1 | y | 134 | ALA | 3.4 |
| 1 | c | 129 | VAL | 3.4 |
| 1 | u | 67 | TYR | 3.4 |
| 1 | a | 68 | VAL | 3.3 |
| 1 | s | 64 | ARG | 3.3 |
| 1 | u | 104 | VAL | 3.3 |
| 1 | g | 196 | THR | 3.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | a | 95 | ALA | 3.3 |
| 1 | m | 136 | TYR | 3.3 |
| 1 | U | 136 | TYR | 3.3 |
| 1 | y | 189 | THR | 3.3 |
| 1 | Q | 195 | LEU | 3.3 |
| 1 | y | 153 | SER | 3.3 |
| 1 | y | 172 | TYR | 3.3 |
| 1 | y | 174 | CYS | 3.3 |
| 1 | y | 65 | ILE | 3.3 |
| 1 | U | 67 | TYR | 3.2 |
| 1 | 2 | 182 | ALA | 3.2 |
| 1 | s | 144 | TYR | 3.2 |
| 1 | e | 63 | PHE | 3.2 |
| 1 | 4 | 94 | VAL | 3.2 |
| 1 | g | 136 | TYR | 3.2 |
| 1 | u | 174 | CYS | 3.1 |
| 1 | i | 155 | LEU | 3.1 |
| 1 | m | 111 | ILE | 3.1 |
| 1 | y | 121 | VAL | 3.1 |
| 1 | k | 160 | THR | 3.1 |
| 1 | c | 167 | TYR | 3.1 |
| 1 | c | 162 | ALA | 3.1 |
| 1 | c | 120 | LYS | 3.1 |
| 1 | g | 183 | ILE | 3.1 |
| 1 | m | 114 | VAL | 3.1 |
| 1 | 4 | 177 | LEU | 3.1 |
| 1 | y | 143 | CYS | 3.1 |
| 1 | O | 71 | ILE | 3.1 |
| 1 | m | 63 | PHE | 3.1 |
| 1 | g | 63 | PHE | 3.1 |
| 1 | 3 | 92 | ILE | 3.0 |
| 1 | i | 119 | ILE | 3.0 |
| 1 | y | 86 | LEU | 3.0 |
| 1 | a | 170 | TRP | 3.0 |
| 1 | g | 137 | LEU | 3.0 |
| 1 | U | 71 | ILE | 3.0 |
| 1 | Q | 172 | TYR | 3.0 |
| 1 | 3 | 129 | VAL | 3.0 |
| 1 | g | 114 | VAL | 3.0 |
| 1 | a | 101 | LEU | 3.0 |
| 1 | w | 65 | ILE | 3.0 |
| 1 | k | 88 | LEU | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | o | 86 | LEU | 2.9 |
| 1 | m | 59 | THR | 2.9 |
| 1 | a | 177 | LEU | 2.9 |
| 1 | e | 187 | LEU | 2.9 |
| 1 | U | 119 | ILE | 2.9 |
| 1 | a | 114 | VAL | 2.9 |
| 1 | c | 123 | THR | 2.9 |
| 1 | e | 114 | VAL | 2.9 |
| 1 | o | 88 | LEU | 2.9 |
| 1 | O | 86 | LEU | 2.9 |
| 1 | 4 | 92 | ILE | 2.9 |
| 1 | w | 171 | VAL | 2.9 |
| 1 | o | 115 | SER | 2.9 |
| 1 | Y | 85 | PRO | 2.8 |
| 1 | 3 | 94 | VAL | 2.8 |
| 1 | s | 186 | VAL | 2.8 |
| 1 | q | 106 | PRO | 2.8 |
| 1 | O | 173 | GLN | 2.8 |
| 1 | U | 131 | HIS | 2.8 |
| 1 | u | 137 | LEU | 2.8 |
| 1 | S | 91 | TYR | 2.8 |
| 1 | m | 179 | GLN | 2.8 |
| 1 | g | 132 | ARG | 2.8 |
| 1 | a | 172 | TYR | 2.8 |
| 1 | s | 120 | LYS | 2.8 |
| 1 | e | 191 | PHE | 2.8 |
| 2 | p | 791 | VAL | 2.8 |
| 1 | U | 191 | PHE | 2.8 |
| 1 | q | 69 | GLY | 2.7 |
| 1 | O | 70 | ALA | 2.7 |
| 1 | g | 156 | ALA | 2.7 |
| 1 | g | 90 | ASN | 2.7 |
| 1 | m | 184 | CYS | 2.7 |
| 1 | u | 156 | ALA | 2.7 |
| 1 | s | 157 | LEU | 2.7 |
| 1 | o | 153 | SER | 2.7 |
| 1 | 3 | 97 | GLN | 2.6 |
| 1 | e | 86 | LEU | 2.6 |
| 1 | Q | 120 | LYS | 2.6 |
| 1 | S | 107 | GLU | 2.6 |
| 1 | c | 114 | VAL | 2.6 |
| 1 | c | 62 | GLU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | U | 62 | GLU | 2.6 |
| 1 | i | 167 | TYR | 2.6 |
| 1 | c | 192 | ASP | 2.6 |
| 1 | e | 142 | VAL | 2.6 |
| 1 | e | 126 | GLN | 2.6 |
| 1 | S | 89 | ILE | 2.6 |
| 1 | Q | 64 | ARG | 2.6 |
| 1 | g | 98 | ASP | 2.6 |
| 1 | E | 122 | SER | 2.6 |
| 2 | n | 790 | VAL | 2.6 |
| 2 | p | 790 | VAL | 2.6 |
| 1 | Q | 110 | PHE | 2.6 |
| 1 | u | 169 | LEU | 2.6 |
| 1 | c | 187 | LEU | 2.6 |
| 1 | S | 88 | LEU | 2.6 |
| 1 | A | 157 | LEU | 2.6 |
| 1 | m | 169 | LEU | 2.6 |
| 1 | u | 94 | VAL | 2.6 |
| 1 | 2 | 144 | TYR | 2.6 |
| 1 | a | 64 | ARG | 2.6 |
| 1 | u | 159 | THR | 2.5 |
| 1 | U | 137 | LEU | 2.5 |
| 1 | a | 116 | LYS | 2.5 |
| 1 | k | 86 | LEU | 2.5 |
| 1 | A | 120 | LYS | 2.5 |
| 2 | J | 791 | VAL | 2.5 |
| 1 | c | 153 | SER | 2.5 |
| 1 | k | 185 | LYS | 2.5 |
| 1 | a | 179 | GLN | 2.5 |
| 1 | S | 65 | ILE | 2.5 |
| 1 | U | 90 | ASN | 2.5 |
| 1 | g | 86 | LEU | 2.5 |
| 1 | y | 182 | ALA | 2.5 |
| 1 | a | 69 | GLY | 2.5 |
| 1 | q | 187 | LEU | 2.5 |
| 1 | u | 98 | ASP | 2.5 |
| 1 | c | 160 | THR | 2.5 |
| 1 | i | 118 | GLY | 2.5 |
| 1 | c | 89 | ILE | 2.5 |
| 1 | m | 158 | LYS | 2.5 |
| 1 | o | 182 | ALA | 2.5 |
| 1 | u | 71 | ILE | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | y | 185 | LYS | 2.5 |
| 1 | M | 191 | PHE | 2.5 |
| 1 | o | 113 | GLY | 2.5 |
| 1 | c | 100 | LYS | 2.5 |
| 1 | k | 146 | ASP | 2.5 |
| 1 | y | 87 | ASP | 2.5 |
| 1 | E | 186 | VAL | 2.4 |
| 1 | I | 191 | PHE | 2.4 |
| 1 | A | 194 | VAL | 2.4 |
| 1 | y | 60 | CYS | 2.4 |
| 1 | W | 190 | ALA | 2.4 |
| 1 | U | 86 | LEU | 2.4 |
| 1 | U | 111 | ILE | 2.4 |
| 1 | 3 | 103 | PHE | 2.4 |
| 1 | I | 142 | VAL | 2.4 |
| 1 | s | 175 | ASN | 2.4 |
| 1 | s | 169 | LEU | 2.4 |
| 1 | k | 97 | GLN | 2.4 |
| 1 | o | 156 | ALA | 2.4 |
| 1 | i | 62 | GLU | 2.4 |
| 1 | m | 187 | LEU | 2.4 |
| 1 | U | 169 | LEU | 2.4 |
| 1 | Y | 154 | LEU | 2.4 |
| 1 | s | 166 | GLU | 2.3 |
| 1 | y | 181 | GLN | 2.3 |
| 1 | i | 187 | LEU | 2.3 |
| 1 | q | 103 | PHE | 2.3 |
| 1 | U | 110 | PHE | 2.3 |
| 1 | O | 157 | LEU | 2.3 |
| 1 | Q | 177 | LEU | 2.3 |
| 2 | n | 789 | THR | 2.3 |
| 1 | c | 186 | VAL | 2.3 |
| 1 | k | 98 | ASP | 2.3 |
| 2 | h | 790 | VAL | 2.3 |
| 1 | 0 | 120 | LYS | 2.3 |
| 1 | y | 138 | ILE | 2.3 |
| 1 | U | 64 | ARG | 2.3 |
| 1 | u | 150 | ALA | 2.3 |
| 1 | y | 144 | TYR | 2.3 |
| 1 | Q | 186 | VAL | 2.3 |
| 1 | k | 183 | ILE | 2.3 |
| 1 | s | 172 | TYR | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 1 | k | 171 | VAL | 2.3 |
| 1 | Y | 175 | ASN | 2.3 |
| 1 | 3 | 86 | LEU | 2.3 |
| 1 | c | 169 | LEU | 2.3 |
| 1 | g | 88 | LEU | 2.3 |
| 1 | u | 183 | ILE | 2.3 |
| 1 | 3 | 158 | LYS | 2.2 |
| 1 | Q | 144 | TYR | 2.2 |
| 1 | y | 183 | ILE | 2.2 |
| 1 | m | 170 | TRP | 2.2 |
| 1 | k | 145 | ASP | 2.2 |
| 2 | f | 789 | THR | 2.2 |
| 1 | a | 181 | GLN | 2.2 |
| 1 | 4 | 186 | VAL | 2.2 |
| 1 | 0 | 98 | ASP | 2.2 |
| 1 | a | 87 | ASP | 2.2 |
| 1 | 4 | 122 | SER | 2.2 |
| 1 | y | 179 | GLN | 2.2 |
| 2 | 8 | 787 | VAL | 2.2 |
| 1 | K | 110 | PHE | 2.2 |
| 1 | y | 175 | ASN | 2.2 |
| 1 | i | 92 | ILE | 2.2 |
| 1 | y | 117 | TYR | 2.2 |
| 1 | i | 68 | VAL | 2.2 |
| 1 | 3 | 157 | LEU | 2.1 |
| 1 | k | 90 | ASN | 2.1 |
| 1 | e | 64 | ARG | 2.1 |
| 1 | m | 191 | PHE | 2.1 |
| 1 | s | 140 | ARG | 2.1 |
| 1 | 0 | 102 | PRO | 2.1 |
| 1 | e | 169 | LEU | 2.1 |
| 1 | 0 | 88 | LEU | 2.1 |
| 1 | O | 91 | TYR | 2.1 |
| 1 | g | 177 | LEU | 2.1 |
| 1 | u | 190 | ALA | 2.1 |
| 1 | c | 142 | VAL | 2.1 |
| 1 | y | 195 | LEU | 2.1 |
| 1 | a | 135 | LEU | 2.1 |
| 1 | U | 157 | LEU | 2.1 |
| 2 | t | 787 | VAL | 2.1 |
| 1 | A | 191 | PHE | 2.1 |
| 1 | 2 | 154 | LEU | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | u | 167 | TYR | 2.1 |
| 1 | Y | 135 | LEU | 2.1 |
| 1 | g | 145 | ASP | 2.1 |
| 1 | u | 107 | GLU | 2.1 |
| 1 | k | 177 | LEU | 2.0 |
| 1 | s | 189 | THR | 2.0 |
| 1 | u | 99 | GLY | 2.0 |
| 1 | W | 189 | THR | 2.0 |
| 1 | 3 | 171 | VAL | 2.0 |
| 1 | 4 | 144 | TYR | 2.0 |
| 1 | y | 184 | CYS | 2.0 |
| 1 | o | 103 | PHE | 2.0 |
| 1 | s | 105 | PRO | 2.0 |
| 1 | g | 72 | GLU | 2.0 |
| 1 | w | 172 | TYR | 2.0 |
| 1 | y | 114 | VAL | 2.0 |
| 1 | k | 102 | PRO | 2.0 |
| 1 | g | 95 | ALA | 2.0 |
| 1 | u | 140 | ARG | 2.0 |
| 1 | e | 135 | LEU | 2.0 |
| 1 | W | 116 | LYS | 2.0 |
| 1 | i | 90 | ASN | 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.