



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 05:03 PM EDT

PDB ID : 5L59  
Title : Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P2(1)  
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.  
Deposited on : 2016-05-28  
Resolution : 6.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

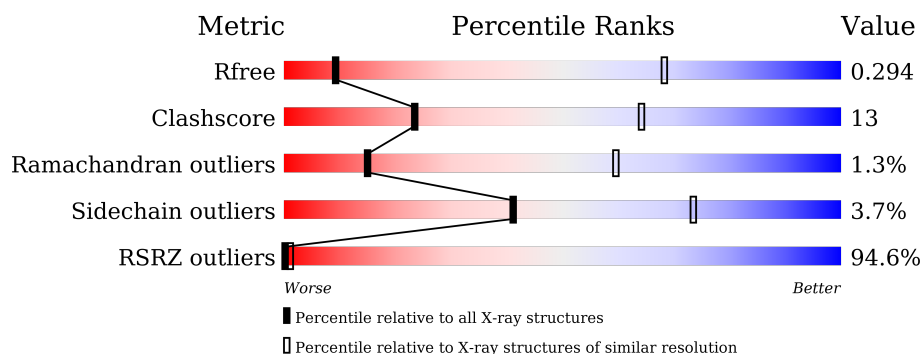
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 6.00 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 91344                       | 1002 (8.30-3.66)                                      |
| Clashscore            | 102246                      | 1050 (8.30-3.70)                                      |
| Ramachandran outliers | 100387                      | 1023 (8.30-3.66)                                      |
| Sidechain outliers    | 100360                      | 1012 (8.30-3.64)                                      |
| RSRZ outliers         | 91569                       | 1001 (8.30-3.66)                                      |

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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   | A     | 1212   | <div> <div>91%</div> <div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div> |
| 1   | B     | 1212   | <div> <div>92%</div> <div> <div>70%</div> <div>24%</div> <div>..</div> </div> </div> |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res  | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 2   | NAG  | A     | 1301 | -         | -        | -       | X                |
| 2   | NAG  | A     | 1305 | -         | -        | -       | X                |
| 2   | NAG  | A     | 1314 | -         | -        | -       | X                |
| 2   | NAG  | A     | 1329 | -         | -        | -       | X                |
| 2   | NAG  | A     | 1334 | X         | -        | -       | -                |
| 2   | NAG  | B     | 1301 | -         | -        | -       | X                |
| 2   | NAG  | B     | 1305 | -         | -        | -       | X                |
| 2   | NAG  | B     | 1315 | -         | -        | -       | X                |
| 2   | NAG  | B     | 1331 | -         | -        | -       | X                |
| 2   | NAG  | B     | 1337 | X         | -        | -       | -                |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19191 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 Plexin-A1.

| Mol | Chain | Residues | Atoms |      |      |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|---------|-------|
| 1   | A     | 1171     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9085  | 5719 | 1593 | 1715 | 58 |         |         |       |
| 1   | B     | 1171     | Total | C    | N    | O    | S  | 0       | 0       | 0     |
|     |       |          | 9085  | 5719 | 1593 | 1715 | 58 |         |         |       |

There are 24 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 34      | GLU      | -      | expression tag | UNP P70206 |
| A     | 35      | THR      | -      | expression tag | UNP P70206 |
| A     | 36      | GLY      | -      | expression tag | UNP P70206 |
| A     | 1237    | ARG      | -      | expression tag | UNP P70206 |
| A     | 1238    | THR      | -      | expression tag | UNP P70206 |
| A     | 1239    | LYS      | -      | expression tag | UNP P70206 |
| A     | 1240    | HIS      | -      | expression tag | UNP P70206 |
| A     | 1241    | HIS      | -      | expression tag | UNP P70206 |
| A     | 1242    | HIS      | -      | expression tag | UNP P70206 |
| A     | 1243    | HIS      | -      | expression tag | UNP P70206 |
| A     | 1244    | HIS      | -      | expression tag | UNP P70206 |
| A     | 1245    | HIS      | -      | expression tag | UNP P70206 |
| B     | 34      | GLU      | -      | expression tag | UNP P70206 |
| B     | 35      | THR      | -      | expression tag | UNP P70206 |
| B     | 36      | GLY      | -      | expression tag | UNP P70206 |
| B     | 1237    | ARG      | -      | expression tag | UNP P70206 |
| B     | 1238    | THR      | -      | expression tag | UNP P70206 |
| B     | 1239    | LYS      | -      | expression tag | UNP P70206 |
| B     | 1240    | HIS      | -      | expression tag | UNP P70206 |
| B     | 1241    | HIS      | -      | expression tag | UNP P70206 |
| B     | 1242    | HIS      | -      | expression tag | UNP P70206 |
| B     | 1243    | HIS      | -      | expression tag | UNP P70206 |
| B     | 1244    | HIS      | -      | expression tag | UNP P70206 |
| B     | 1245    | HIS      | -      | expression tag | UNP P70206 |

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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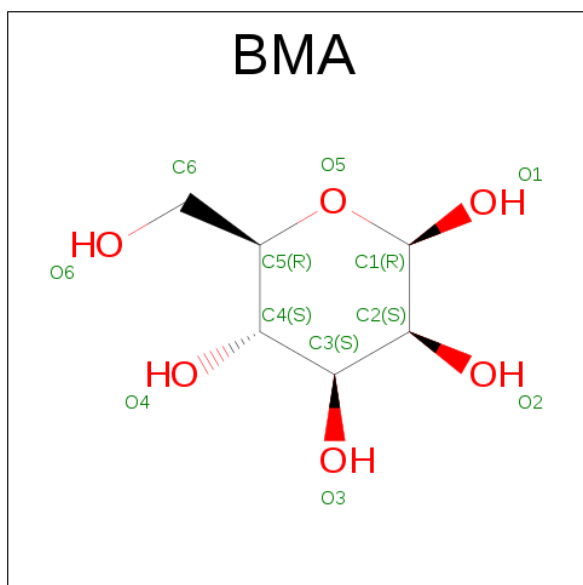
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 2   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



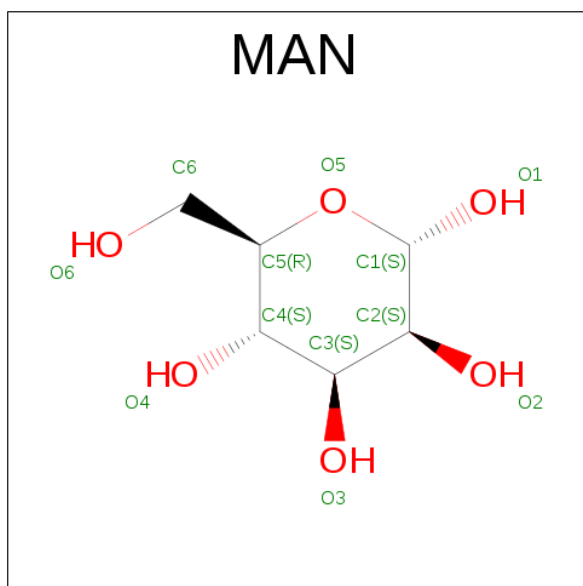
| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 3   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | A     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

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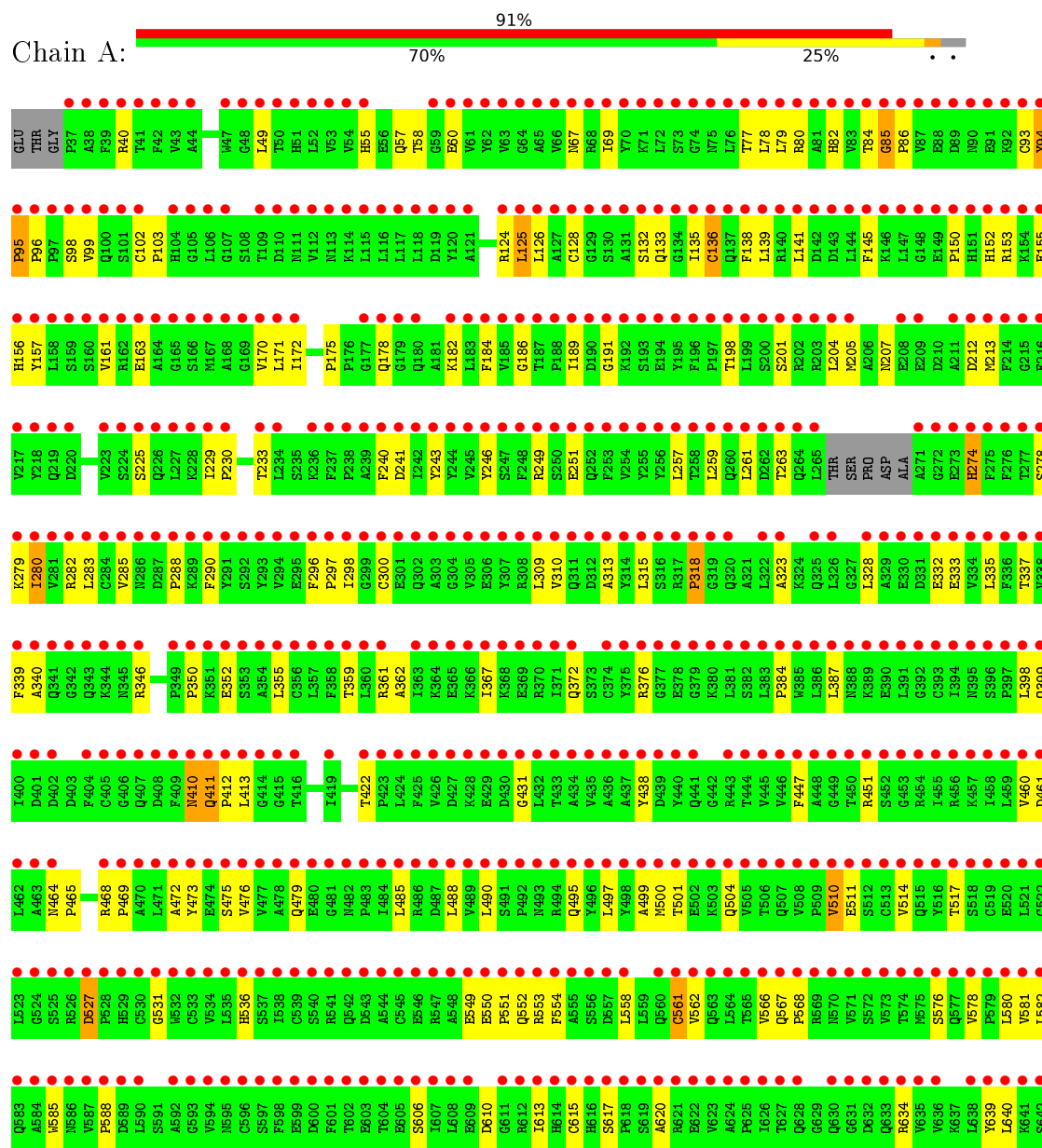
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| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |
| 4   | B     | 1        | Total | C | O | 0       | 0       |
|     |       |          | 11    | 6 | 5 |         |         |

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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: Plexin-A1





|       |       |       |       |      |      |      |      |      |      |      |      |      |      |      |
|-------|-------|-------|-------|------|------|------|------|------|------|------|------|------|------|------|
| I1124 | I1064 | I1004 | I0944 | G884 | F824 | L763 | S701 | K641 | P579 | C519 | I458 | L398 | T337 | T277 |
| G125  | T1065 | H1005 | H945  | E885 | E825 | Q764 | E702 | S642 | L580 | B520 | L459 | Q399 | Y338 | S278 |
| F1126 | V1066 | S1006 | T946  | M886 | C826 | C765 | D703 | K643 | V581 | K643 | V460 | D401 | F339 | I280 |
| I1127 | T1067 | R947  | R947  | M887 | G827 | Q766 | C704 | E644 | L582 | C522 | D461 | I401 | A340 |      |
| M1128 | G1068 | E1008 | A948  | G888 | W828 | H767 | P705 | T645 | Q583 | L523 | L462 | D402 | Q341 | R281 |
| M129  | T1069 | I1009 | I949  | L889 | C829 | S768 | Q706 | G646 | A584 | G524 | A463 | D403 | G342 | R282 |
| N1130 | N1070 | R1010 | S950  | R890 | R830 | S769 | T707 | K647 | K585 | S525 | N464 | F404 | Q343 | L283 |
| V1131 | L1071 | C1011 | P951  | F891 | A831 | Y770 | L708 | K648 | K586 | R526 | P465 | C405 | K344 | C284 |
| T1132 | L1072 | K952  | R952  | E892 | E832 | S771 | P709 | K649 | V587 | D527 |      | G406 | R345 | V285 |
| T1133 | T1073 | R1013 | R953  | F893 | R833 | Y772 | S710 | A850 | P588 | P528 | R468 | Q407 | R346 | N286 |
| T1134 | T1074 | P1014 | F954  | V894 | R834 | Y773 | S711 | S651 | D589 | H529 | P469 | D408 |      | N287 |
| L1135 | R1075 | P1015 | T955  | R895 | C835 | G774 | H712 | D652 | L590 | C530 | A470 | F409 | P349 | P288 |
| L1136 | P1076 | G1016 | F956  | L896 | S836 | H775 | I713 | D653 | S591 | G531 | L471 | N410 | P350 | V289 |
| L1137 | P1077 | H1017 | V857  | G897 | L837 | D776 | T714 | F654 | A582 | N632 | A472 | Q411 | K351 | F290 |
| M1138 | R1078 | T958  | P959  | V898 | R838 | Y777 | T715 | F655 | G593 | C533 | Y473 | P412 | E352 |      |
| M1139 | I1079 | H899  | P959  | H899 | H839 | S778 | P716 | F656 | H594 | V534 | E474 | L413 | E353 | Y291 |
| S1140 | R1080 | G1020 | T960  | V900 | H840 | D779 | G717 | N595 | N595 | L535 | S475 | G414 | A354 | Y293 |
| S1141 | A1081 | S1021 | F961  | Q901 | C941 | L780 | V718 | N658 | C596 | H536 | V476 | G415 | A355 | Y294 |
| L1142 | K1082 | A1022 | Y962  | K902 | P842 | S781 | T719 | C659 | S597 | S537 | V477 | T416 | L355 | E295 |
| L1143 | Y1083 | P1023 | R963  | V903 | A843 | H782 | T720 | S660 | F588 | I538 | Q478 | T417 | L357 | F296 |
| L1144 | G1084 | V1025 | V964  | L904 | D844 | H783 | K721 | E599 | E599 | C539 | Q479 | T418 | F358 | P297 |
| Y1145 | G1085 | V1026 | S965  | C905 | S845 | L784 | P722 | H662 | F601 | S540 | G481 | I419 | T359 | I298 |
| P1146 | I1086 | P1026 | P966  | S906 | P846 | Q663 | H723 | Q663 | F601 | H541 | G481 | E420 | L360 | G299 |
| P1147 | E1087 | N1027 | S967  | P907 | A847 | S664 | T724 | S664 | T602 | D542 | N482 | G421 | R361 | C300 |
| P1148 | R1088 | I1028 | R968  | V908 | S848 | H787 | L725 | C665 | E603 | D543 | P483 | T422 | A362 | E301 |
| V1149 | E1089 | N1029 | G969  | E909 | W849 | H788 | A726 | L666 | T604 | A544 | I484 | F423 | L363 | Q302 |
| L1150 | N1090 | R1030 | P970  | S910 | H850 | Y789 | A727 | A667 | E605 | C545 | R485 | F424 | L364 | A303 |
| E1151 | S1091 | A1031 | L971  | E911 | H851 | G790 | K728 | S606 | S606 | E545 | E365 | F425 | E365 | G304 |
| P1152 | C1092 | Q1032 | S972  | Y912 | A852 | H791 | N729 | V669 | I607 | H547 | D487 | V426 | K366 | V305 |
| L1153 | M1093 | L1033 | G973  | I913 | H853 | F792 | L730 | N670 | I607 | A548 | L488 | D427 | I367 | V307 |
|       | V1094 | S1034 | G974  | S914 | H854 | V793 | P731 | G671 | P609 | P549 | V489 | K428 | K368 |      |
| PRO   | Y1095 | N1035 | T975  | A915 | G855 | S794 | Q732 | S672 | D610 | E560 | L490 | E429 | E389 | R308 |
| THR   | M1096 | P1036 | H976  | E916 | S856 | F673 | P733 | F673 | G611 | P551 | S491 | D430 | R370 | L309 |
| GLY   | D1097 | E1037 | I977  | Q917 | S857 | P874 | Q734 | P874 | I613 | Q552 | P492 | G431 | I371 | V310 |
| LEU   | T1098 | Y1038 | G978  | I918 | R858 | C675 |      | C675 | I613 | H553 | J493 | L432 | Q372 | Q311 |
| LEU   | M1099 | K1039 | I979  | V919 | C859 | H676 | Q737 | H677 | C615 | A565 | R494 | T433 | S373 | D312 |
| GLU   | T1100 | Y1040 | E980  | C920 | T860 | C677 | R738 | C678 | H614 | A566 | Q495 | A434 | C374 | A313 |
| LEU   | V1101 | N1041 | G981  | E921 | D861 | Q801 | G739 | E679 | E616 | S566 | Y496 | V435 | Y375 | Y314 |
| LYS   | C1102 | Y1042 | S982  | I922 | P862 | A802 | E740 | K679 | S617 | D657 | L497 | A437 | R376 | L315 |
| PRO   | R1103 | T1043 | H983  | G923 | K863 | H803 | E741 | Y680 | P618 | L558 | Y498 | Y438 | G377 | S316 |
| S1164 | A1104 | E1044 | L984  | D924 | L864 | L804 | C742 | R681 | S619 | L559 | A499 | D439 | E378 | R317 |
| S1165 | P1105 | D1045 | N985  | A925 | L865 | Y805 | L743 | H682 | A620 | O560 | M500 | Y440 | C379 | P318 |
| P1166 | S1106 | P1046 | A986  | S926 | K866 | K806 | F744 | V683 | R621 | C561 | T501 | Q441 | K380 | G319 |
| L1167 | L1107 | T1047 | G987  | T927 | L867 | C807 | H745 | C584 | E622 | V662 | E502 | G442 | L381 | Q320 |
| L1168 | D1108 | I1048 | S988  | L928 | S868 | T885 | I746 | T885 | E623 | Q503 | Q504 | R443 | S382 | A321 |
| L1169 | M1109 | L1049 | D989  | R929 | P869 | A809 | P747 | M686 | P625 | T565 | V505 | T444 | P384 | L322 |
| K1170 | P1110 | R1050 | V990  | A930 | E870 | L810 | G748 | N687 | A624 | L564 | V506 | V445 | V385 | A323 |
| G1171 | K1111 | I1051 | A991  | H931 | T871 | R811 | S749 | A688 | I626 | V566 | Q507 | V446 | L386 | Q325 |
| R1172 | R1112 | D1052 | V992  | D932 | G872 | Q812 | P750 | A689 | T627 | D567 | L387 | F447 | L387 | L326 |
| M1173 | S1113 | P1063 | S993  | A933 | P873 | S813 | A751 | D690 | Q628 | P568 | V508 | A448 | N388 | G327 |
| L1174 | P1114 | E1064 | I994  | L934 | Q874 | C814 | R752 | C691 | G629 | H569 | P509 | A449 | N389 | L328 |
| L1175 | E1115 | W1055 | G995  | V935 | Q875 | G815 | V753 | A692 | Q630 | N570 | V510 | G449 | K390 | L329 |
| P1176 | P1176 | S1056 | G996  | E936 | G876 | L816 | T754 | F693 | G631 | H571 | E511 | T450 | E390 | A329 |
| P1177 | I1107 | N1057 | R997  | V937 | G877 | C817 | A755 | L694 | D632 | S572 | S512 | R451 | L391 | E330 |
| A1178 | H1058 | L1058 | P998  | C938 | T878 | K818 | L756 | E695 | Q633 | V573 | C513 | S452 | G392 | D331 |
| P1179 | E1119 | S1059 | C999  | V939 | R879 | K819 | R757 | G596 | R634 | T574 | V514 | G453 | C393 | E332 |
| G1180 | R1120 | G1060 | S1000 | R940 | L880 | R897 | F758 | G597 | L638 | H575 | Q515 | R454 | I394 | E333 |
| S1181 | P1121 | T1062 | F1001 | D941 | T881 | D821 | N759 | V698 | L640 | S576 | T517 | I455 | N395 | S334 |
| E1182 | D1122 | G1062 | S1002 | C942 | I882 | R822 | S760 | M699 |      | Q577 | L516 | R456 | S396 | L335 |
| R1183 | E1123 | L1063 | W1003 | S943 | R883 | R823 |      | M700 |      | V578 | S518 | K457 | P397 | F336 |

[illegible]

## 4 Data and refinement statistics

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 1 21 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 139.99Å 196.45Å 144.94Å<br>90.00° 94.57° 90.00°             | Depositor        |
| Resolution (Å)  | 58.22 – 6.00<br>58.22 – 6.00                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 94.3 (58.22-6.00)<br>76.2 (58.22-6.00)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | (Not available)   | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.80 (at 6.17Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.2_1309)                          | Depositor        |
| R, $R_{free}$   | 0.274 , 0.299<br>0.273 , 0.294                              | Depositor<br>DCC |
| $R_{free}$ test set   | 994 reflections (5.13%)                                     | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 291.6   | Xtriage          |
| Anisotropy  | 0.529   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.44 , 436.5  | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$ | Xtriage          |
| Estimated twinning fraction   | 0.077 for l,-k,h  | Xtriage          |
| $F_o, F_c$ correlation  | 0.89  | EDS              |
| Total number of atoms   | 19191   | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 272.0   | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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

| Mol | Chain | Bond lengths |                 | Bond angles |                 |
|-----|-------|--------------|-----------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$     | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.45         | 4/9293 (0.0%)   | 0.60        | 3/12628 (0.0%)  |
| 1   | B     | 0.63         | 7/9296 (0.1%)   | 0.77        | 13/12639 (0.1%) |
| All | All   | 0.55         | 11/18589 (0.1%) | 0.69        | 16/25267 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | A     | 0                   | 8                   |
| 1   | B     | 0                   | 10                  |
| All | All   | 0                   | 18                  |

All (11) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z      | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|--------|-------------|----------|
| 1   | B     | 1147 | ASP  | C-N   | 32.49  | 1.96        | 1.34     |
| 1   | B     | 561  | CYS  | C-N   | 28.65  | 2.00        | 1.34     |
| 1   | A     | 859  | CYS  | C-N   | -19.30 | 0.89        | 1.34     |
| 1   | B     | 859  | CYS  | C-N   | 18.57  | 1.76        | 1.34     |
| 1   | A     | 510  | VAL  | C-N   | 17.80  | 1.75        | 1.34     |
| 1   | B     | 1043 | THR  | C-N   | 13.12  | 1.64        | 1.34     |
| 1   | B     | 957  | VAL  | C-N   | 12.12  | 1.61        | 1.34     |
| 1   | A     | 806  | LYS  | C-N   | 9.09   | 1.54        | 1.34     |
| 1   | B     | 704  | CYS  | C-N   | 8.92   | 1.51        | 1.34     |
| 1   | B     | 510  | VAL  | C-N   | -6.29  | 1.19        | 1.34     |
| 1   | A     | 561  | CYS  | C-N   | -5.90  | 1.20        | 1.34     |

All (16) bond angle outliers are listed below:



| Mol | Chain | Res  | Type | Atoms  | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|--------|--------|-------------|----------|
| 1   | B     | 1043 | THR  | O-C-N  | 31.38  | 172.91      | 122.70   |
| 1   | B     | 1043 | THR  | CA-C-N | -23.75 | 64.96       | 117.20   |
| 1   | B     | 1043 | THR  | C-N-CA | -19.45 | 73.09       | 121.70   |
| 1   | B     | 1147 | ASP  | O-C-N  | -14.82 | 92.94       | 121.10   |
| 1   | B     | 859  | CYS  | O-C-N  | -13.50 | 101.10      | 122.70   |
| 1   | B     | 1147 | ASP  | C-N-CD | -13.32 | 91.30       | 120.60   |
| 1   | B     | 957  | VAL  | CA-C-N | -12.64 | 89.39       | 117.20   |
| 1   | B     | 806  | LYS  | O-C-N  | 9.91   | 138.55      | 122.70   |
| 1   | B     | 704  | CYS  | O-C-N  | -8.65  | 104.67      | 121.10   |
| 1   | A     | 561  | CYS  | O-C-N  | -8.04  | 109.83      | 122.70   |
| 1   | B     | 806  | LYS  | CA-C-N | -7.69  | 100.28      | 117.20   |
| 1   | B     | 704  | CYS  | C-N-CD | -7.13  | 104.91      | 120.60   |
| 1   | B     | 957  | VAL  | C-N-CA | -7.08  | 104.01      | 121.70   |
| 1   | A     | 561  | CYS  | C-N-CA | 5.36   | 135.11      | 121.70   |
| 1   | A     | 561  | CYS  | CA-C-N | 5.26   | 128.77      | 117.20   |
| 1   | B     | 704  | CYS  | CA-C-N | 5.07   | 131.30      | 117.10   |

There are no chirality outliers.

All (18) planarity outliers are listed below:

| Mol | Chain | Res  | Type | Group     |
|-----|-------|------|------|-----------|
| 1   | A     | 1052 | ASP  | Peptide   |
| 1   | A     | 410  | ASN  | Peptide   |
| 1   | A     | 527  | ASP  | Peptide   |
| 1   | A     | 807  | CYS  | Peptide   |
| 1   | A     | 85   | GLY  | Peptide   |
| 1   | A     | 868  | SER  | Peptide   |
| 1   | A     | 94   | TYR  | Peptide   |
| 1   | A     | 965  | SER  | Peptide   |
| 1   | B     | 1052 | ASP  | Peptide   |
| 1   | B     | 410  | ASN  | Peptide   |
| 1   | B     | 527  | ASP  | Peptide   |
| 1   | B     | 704  | CYS  | Mainchain |
| 1   | B     | 807  | CYS  | Peptide   |
| 1   | B     | 85   | GLY  | Peptide   |
| 1   | B     | 868  | SER  | Peptide   |
| 1   | B     | 94   | TYR  | Peptide   |
| 1   | B     | 957  | VAL  | Mainchain |
| 1   | B     | 965  | SER  | Peptide   |

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 9085  | 0        | 8876     | 241     | 22           |
| 1   | B     | 9085  | 0        | 8877     | 280     | 33           |
| 2   | A     | 252   | 0        | 217      | 4       | 0            |
| 2   | B     | 252   | 0        | 217      | 2       | 0            |
| 3   | A     | 88    | 0        | 72       | 0       | 0            |
| 3   | B     | 88    | 0        | 69       | 0       | 0            |
| 4   | A     | 154   | 0        | 134      | 1       | 0            |
| 4   | B     | 187   | 0        | 164      | 1       | 0            |
| All | All   | 19191 | 0        | 18626    | 504     | 35           |

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 13.

All (504) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:A:855:GLY:HA3 | 1:A:890:ARG:NH2  | 1.22                     | 1.48              |
| 1:B:1116:GLU:O  | 1:B:1177:PRO:CD  | 1.68                     | 1.42              |
| 1:A:510:VAL:C   | 1:A:511:GLU:N    | 1.75                     | 1.40              |
| 1:B:859:CYS:C   | 1:B:860:THR:N    | 1.76                     | 1.39              |
| 1:B:813:SER:HB2 | 1:B:886:ASN:OD1  | 1.22                     | 1.36              |
| 1:A:855:GLY:CA  | 1:A:890:ARG:NH2  | 1.88                     | 1.35              |
| 1:B:813:SER:HB2 | 1:B:886:ASN:CG   | 1.48                     | 1.33              |
| 1:B:858:ARG:HB3 | 1:B:940:ARG:NH2  | 1.43                     | 1.30              |
| 1:B:813:SER:CB  | 1:B:886:ASN:OD1  | 1.80                     | 1.29              |
| 1:B:1147:ASP:C  | 1:B:1148:PRO:N   | 1.96                     | 1.19              |
| 1:A:98:SER:C    | 1:B:756:LEU:HD21 | 1.58                     | 1.19              |
| 1:B:561:CYS:C   | 1:B:562:VAL:N    | 1.99                     | 1.14              |
| 1:A:855:GLY:CA  | 1:A:890:ARG:HH22 | 1.52                     | 1.12              |
| 1:A:877:GLY:HA3 | 1:A:1030:ARG:HG3 | 1.16                     | 1.12              |
| 1:A:658:ASN:C   | 1:A:659:CYS:N    | 2.04                     | 1.10              |
| 1:B:813:SER:HB2 | 1:B:886:ASN:ND2  | 1.64                     | 1.10              |
| 1:A:99:VAL:O    | 1:B:766:GLN:NE2  | 1.83                     | 1.10              |
| 1:A:99:VAL:HA   | 1:B:756:LEU:HD11 | 1.17                     | 1.10              |
| 1:B:411:GLN:HG2 | 1:B:412:PRO:HD2  | 1.35                     | 1.09              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:855:GLY:C    | 1:B:890:ARG:HH22 | 1.56                     | 1.08              |
| 1:A:704:CYS:C    | 1:A:705:PRO:N    | 2.07                     | 1.08              |
| 1:B:1116:GLU:O   | 1:B:1177:PRO:HD2 | 0.92                     | 1.08              |
| 1:A:411:GLN:HG2  | 1:A:412:PRO:HD2  | 1.35                     | 1.05              |
| 1:B:860:THR:HA   | 1:B:946:TYR:CE1  | 1.93                     | 1.04              |
| 1:A:860:THR:HA   | 1:A:946:TYR:CE1  | 1.93                     | 1.02              |
| 1:B:658:ASN:C    | 1:B:659:CYS:N    | 2.12                     | 1.02              |
| 1:B:860:THR:HA   | 1:B:946:TYR:HE1  | 1.28                     | 0.98              |
| 1:B:855:GLY:CA   | 1:B:890:ARG:HH22 | 1.75                     | 0.97              |
| 1:B:855:GLY:HA3  | 1:B:890:ARG:NH2  | 1.79                     | 0.96              |
| 1:A:855:GLY:C    | 1:A:890:ARG:NH2  | 2.19                     | 0.96              |
| 1:B:855:GLY:C    | 1:B:890:ARG:NH2  | 2.19                     | 0.96              |
| 1:B:859:CYS:O    | 1:B:946:TYR:CE1  | 2.20                     | 0.95              |
| 1:B:858:ARG:HB3  | 1:B:940:ARG:HH22 | 1.19                     | 0.94              |
| 1:A:860:THR:HA   | 1:A:946:TYR:HE1  | 1.29                     | 0.94              |
| 1:A:1043:THR:C   | 1:A:1044:GLU:N   | 2.21                     | 0.93              |
| 1:A:468:ARG:HG2  | 1:A:469:PRO:HD2  | 1.51                     | 0.92              |
| 1:A:189:ILE:HD12 | 1:A:198:THR:HG23 | 1.52                     | 0.91              |
| 1:B:189:ILE:HD12 | 1:B:198:THR:HG23 | 1.52                     | 0.91              |
| 1:A:98:SER:O     | 1:B:756:LEU:HD21 | 1.70                     | 0.91              |
| 1:B:855:GLY:CA   | 1:B:890:ARG:NH2  | 2.33                     | 0.91              |
| 1:B:468:ARG:HG2  | 1:B:469:PRO:HD2  | 1.51                     | 0.89              |
| 1:B:813:SER:OG   | 1:B:886:ASN:OD1  | 1.91                     | 0.89              |
| 1:B:94:TYR:CD2   | 1:B:95:PRO:HD3   | 2.08                     | 0.89              |
| 1:A:973:GLY:O    | 1:A:1129:ASP:HB3 | 1.72                     | 0.89              |
| 1:A:94:TYR:CD2   | 1:A:95:PRO:HD3   | 2.08                     | 0.88              |
| 1:B:855:GLY:O    | 1:B:890:ARG:NH2  | 2.07                     | 0.88              |
| 1:B:459:LEU:HD21 | 1:B:528:PRO:HG3  | 1.56                     | 0.88              |
| 1:B:819:LYS:NZ   | 1:B:914:SER:O    | 2.07                     | 0.87              |
| 1:A:98:SER:CA    | 1:B:756:LEU:HD21 | 2.05                     | 0.87              |
| 1:A:808:PRO:HD2  | 1:A:835:CYS:O    | 1.76                     | 0.86              |
| 1:A:99:VAL:HA    | 1:B:756:LEU:CD1  | 2.06                     | 0.85              |
| 1:B:1116:GLU:O   | 1:B:1177:PRO:CG  | 2.25                     | 0.84              |
| 1:B:808:PRO:HD2  | 1:B:835:CYS:O    | 1.76                     | 0.84              |
| 1:B:859:CYS:C    | 1:B:946:TYR:CE1  | 2.51                     | 0.83              |
| 1:B:859:CYS:C    | 1:B:946:TYR:HE1  | 1.83                     | 0.82              |
| 1:B:567:GLN:HB3  | 1:B:568:PRO:HD3  | 1.61                     | 0.81              |
| 1:B:1147:ASP:C   | 1:B:1148:PRO:CD  | 2.48                     | 0.81              |
| 1:A:98:SER:CB    | 1:B:756:LEU:CD2  | 2.59                     | 0.81              |
| 1:B:818:LEU:HB3  | 1:B:852:ALA:HB2  | 1.62                     | 0.81              |
| 1:B:813:SER:HB2  | 1:B:886:ASN:HD21 | 1.46                     | 0.81              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:98:SER:CB     | 1:B:756:LEU:HD21 | 2.11                     | 0.81              |
| 1:B:553:ARG:HD2   | 1:B:588:PRO:HG3  | 1.63                     | 0.81              |
| 1:A:818:LEU:HB3   | 1:A:852:ALA:HB2  | 1.63                     | 0.80              |
| 1:A:567:GLN:HB3   | 1:A:568:PRO:HD3  | 1.62                     | 0.80              |
| 1:A:855:GLY:CA    | 1:A:890:ARG:HH21 | 1.75                     | 0.80              |
| 1:A:280:ILE:HB    | 1:A:298:ILE:HD12 | 1.64                     | 0.79              |
| 1:A:876:GLY:O     | 1:A:1030:ARG:HB2 | 1.82                     | 0.79              |
| 1:B:789:ASN:HD22  | 1:B:792:PHE:HE2  | 1.31                     | 0.79              |
| 1:A:789:ASN:HD22  | 1:A:792:PHE:HE2  | 1.31                     | 0.79              |
| 1:B:153:ARG:H     | 1:B:156:HIS:HD2  | 1.30                     | 0.78              |
| 1:A:411:GLN:CG    | 1:A:412:PRO:HD2  | 2.14                     | 0.78              |
| 1:A:153:ARG:H     | 1:A:156:HIS:HD2  | 1.30                     | 0.78              |
| 1:A:855:GLY:HA3   | 1:A:890:ARG:HH21 | 0.97                     | 0.78              |
| 1:B:259:LEU:HD23  | 1:B:346:ARG:HG3  | 1.66                     | 0.77              |
| 1:B:858:ARG:HB3   | 1:B:940:ARG:HH21 | 1.47                     | 0.77              |
| 1:B:411:GLN:CG    | 1:B:412:PRO:HD2  | 2.14                     | 0.77              |
| 1:A:877:GLY:HA3   | 1:A:1030:ARG:CG  | 2.06                     | 0.76              |
| 1:A:895:ARG:O     | 1:A:896:LEU:HB2  | 1.85                     | 0.76              |
| 1:B:280:ILE:HB    | 1:B:298:ILE:HD12 | 1.64                     | 0.76              |
| 1:A:98:SER:HB2    | 1:B:756:LEU:CD2  | 2.14                     | 0.76              |
| 1:A:259:LEU:HD23  | 1:A:346:ARG:HG3  | 1.66                     | 0.75              |
| 1:B:230:PRO:O     | 1:B:233:THR:HG22 | 1.86                     | 0.75              |
| 1:B:895:ARG:O     | 1:B:896:LEU:HB2  | 1.85                     | 0.75              |
| 1:A:230:PRO:O     | 1:A:233:THR:HG22 | 1.86                     | 0.74              |
| 1:A:743:LEU:HD22  | 1:A:752:ARG:HG2  | 1.70                     | 0.73              |
| 1:A:877:GLY:CA    | 1:A:1030:ARG:HG3 | 2.09                     | 0.73              |
| 1:A:171:LEU:HD22  | 1:A:204:LEU:HD11 | 1.72                     | 0.72              |
| 1:B:1145:TYR:OH   | 1:B:1179:PRO:HD2 | 1.90                     | 0.72              |
| 1:B:743:LEU:HD22  | 1:B:752:ARG:HG2  | 1.70                     | 0.72              |
| 1:B:82:HIS:HD2    | 1:B:84:THR:HG22  | 1.55                     | 0.72              |
| 1:A:82:HIS:HD2    | 1:A:84:THR:HG22  | 1.55                     | 0.71              |
| 1:B:553:ARG:HD2   | 1:B:588:PRO:CG   | 2.20                     | 0.71              |
| 1:B:171:LEU:HD22  | 1:B:204:LEU:HD11 | 1.72                     | 0.71              |
| 1:A:805:TYR:CG    | 1:A:824:PHE:CD1  | 2.79                     | 0.71              |
| 1:B:472:ALA:HB3   | 1:B:527:ASP:OD1  | 1.91                     | 0.71              |
| 1:B:852:ALA:HA    | 1:B:857:SER:OG   | 1.90                     | 0.70              |
| 1:B:1079:ILE:HD11 | 1:B:1102:CYS:HB3 | 1.73                     | 0.70              |
| 1:B:1116:GLU:HG2  | 1:B:1177:PRO:HD3 | 1.74                     | 0.70              |
| 1:B:663:GLN:NE2   | 4:B:1321:MAN:O6  | 2.24                     | 0.70              |
| 1:A:852:ALA:HA    | 1:A:857:SER:OG   | 1.91                     | 0.70              |
| 1:B:974:GLY:HA3   | 1:B:1130:ASN:HB2 | 1.73                     | 0.70              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:A:606:SER:HB3   | 1:A:615:CYS:HB3  | 1.74                     | 0.70              |
| 1:A:860:THR:CA    | 1:A:946:TYR:HE1  | 2.03                     | 0.70              |
| 1:B:860:THR:CA    | 1:B:946:TYR:HE1  | 2.03                     | 0.69              |
| 1:A:55:HIS:HE2    | 1:A:141:LEU:HD21 | 1.57                     | 0.69              |
| 1:B:310:VAL:HG22  | 1:B:339:PHE:CE1  | 2.28                     | 0.69              |
| 1:B:606:SER:HB3   | 1:B:615:CYS:HB3  | 1.74                     | 0.69              |
| 1:B:55:HIS:HE2    | 1:B:141:LEU:HD21 | 1.57                     | 0.69              |
| 1:A:310:VAL:HG22  | 1:A:339:PHE:CE1  | 2.28                     | 0.69              |
| 1:B:813:SER:CB    | 1:B:886:ASN:CG   | 2.42                     | 0.68              |
| 1:A:1079:ILE:HD11 | 1:A:1102:CYS:HB3 | 1.73                     | 0.68              |
| 1:A:468:ARG:CG    | 1:A:469:PRO:HD2  | 2.24                     | 0.68              |
| 1:A:566:VAL:HG22  | 1:A:582:LEU:HD23 | 1.76                     | 0.67              |
| 1:B:813:SER:CB    | 1:B:886:ASN:ND2  | 2.51                     | 0.67              |
| 1:A:175:PRO:HG2   | 1:A:178:GLN:HG3  | 1.77                     | 0.67              |
| 1:A:746:ILE:HB    | 1:A:749:SER:O    | 1.95                     | 0.67              |
| 1:B:895:ARG:HA    | 1:B:907:PRO:HG2  | 1.76                     | 0.67              |
| 1:B:468:ARG:CG    | 1:B:469:PRO:HD2  | 2.24                     | 0.67              |
| 1:B:746:ILE:HB    | 1:B:749:SER:O    | 1.95                     | 0.67              |
| 1:B:859:CYS:O     | 1:B:946:TYR:HE1  | 1.75                     | 0.67              |
| 1:B:973:GLY:O     | 1:B:1130:ASN:HB3 | 1.95                     | 0.67              |
| 1:A:98:SER:O      | 1:B:756:LEU:CD2  | 2.40                     | 0.66              |
| 1:A:895:ARG:HA    | 1:A:907:PRO:HG2  | 1.76                     | 0.66              |
| 1:B:813:SER:CB    | 1:B:886:ASN:HD21 | 2.09                     | 0.66              |
| 1:B:566:VAL:HG22  | 1:B:582:LEU:HD23 | 1.76                     | 0.66              |
| 1:A:472:ALA:HB3   | 1:A:527:ASP:OD1  | 1.95                     | 0.66              |
| 1:B:315:LEU:HD11  | 1:B:333:GLU:HB3  | 1.78                     | 0.66              |
| 1:B:973:GLY:O     | 1:B:1130:ASN:CB  | 2.44                     | 0.65              |
| 1:A:69:ILE:HD12   | 1:A:84:THR:HG21  | 1.79                     | 0.65              |
| 1:B:175:PRO:HG2   | 1:B:178:GLN:HG3  | 1.77                     | 0.65              |
| 1:A:99:VAL:CA     | 1:B:756:LEU:HD11 | 2.10                     | 0.65              |
| 1:A:1057:ILE:HD12 | 1:A:1147:ASP:OD1 | 1.96                     | 0.65              |
| 1:B:1057:ILE:HD12 | 1:B:1147:ASP:OD1 | 1.97                     | 0.65              |
| 1:A:855:GLY:N     | 1:A:890:ARG:HH22 | 1.93                     | 0.65              |
| 1:B:858:ARG:CB    | 1:B:940:ARG:HH22 | 2.04                     | 0.64              |
| 1:A:315:LEU:HD11  | 1:A:333:GLU:HB3  | 1.78                     | 0.64              |
| 1:B:553:ARG:HD2   | 1:B:588:PRO:CB   | 2.28                     | 0.64              |
| 1:B:69:ILE:HD12   | 1:B:84:THR:HG21  | 1.79                     | 0.64              |
| 1:B:472:ALA:CB    | 1:B:527:ASP:OD1  | 2.46                     | 0.64              |
| 1:A:550:GLU:HB3   | 1:A:551:PRO:HD2  | 1.80                     | 0.63              |
| 1:B:550:GLU:HB3   | 1:B:551:PRO:HD2  | 1.80                     | 0.63              |
| 1:B:887:LEU:HB2   | 1:B:915:ALA:HA   | 1.80                     | 0.63              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:536:HIS:HA   | 1:A:645:THR:HG21 | 1.80                     | 0.63              |
| 1:A:58:THR:OG1   | 1:A:60:GLU:HG2   | 1.99                     | 0.62              |
| 1:A:887:LEU:HB2  | 1:A:915:ALA:HA   | 1.80                     | 0.62              |
| 1:B:560:GLN:O    | 1:B:586:ASN:HB3  | 2.00                     | 0.62              |
| 1:A:939:VAL:HG22 | 1:A:946:TYR:HB3  | 1.82                     | 0.62              |
| 1:A:871:THR:OG1  | 1:A:986:ALA:HA   | 1.99                     | 0.62              |
| 1:B:58:THR:OG1   | 1:B:60:GLU:HG2   | 1.99                     | 0.62              |
| 1:B:939:VAL:HG22 | 1:B:946:TYR:HB3  | 1.82                     | 0.61              |
| 1:A:732:GLN:HG2  | 1:A:757:ARG:HH22 | 1.66                     | 0.61              |
| 1:A:855:GLY:C    | 1:A:890:ARG:HH22 | 1.94                     | 0.61              |
| 1:B:858:ARG:CB   | 1:B:940:ARG:NH2  | 2.39                     | 0.61              |
| 1:A:259:LEU:HD23 | 1:A:346:ARG:CG   | 2.31                     | 0.61              |
| 1:A:639:TYR:CD2  | 1:A:648:LYS:HD2  | 2.36                     | 0.61              |
| 1:A:740:TYR:CD1  | 1:A:788:TRP:HB3  | 2.36                     | 0.61              |
| 1:B:1145:TYR:OH  | 1:B:1179:PRO:CD  | 2.49                     | 0.61              |
| 1:B:578:VAL:H    | 1:B:617:SER:HB3  | 1.66                     | 0.61              |
| 1:B:740:TYR:CD1  | 1:B:788:TRP:HB3  | 2.36                     | 0.61              |
| 1:B:732:GLN:HG2  | 1:B:757:ARG:HH22 | 1.66                     | 0.61              |
| 1:A:663:GLN:NE2  | 4:A:1320:MAN:O6  | 2.34                     | 0.60              |
| 1:B:1147:ASP:C   | 1:B:1148:PRO:HD3 | 2.21                     | 0.60              |
| 1:A:661:VAL:HG13 | 2:A:1314:NAG:O6  | 2.01                     | 0.60              |
| 1:B:259:LEU:HD23 | 1:B:346:ARG:CG   | 2.31                     | 0.60              |
| 1:A:578:VAL:H    | 1:A:617:SER:HB3  | 1.66                     | 0.60              |
| 1:B:639:TYR:CD2  | 1:B:648:LYS:HD2  | 2.36                     | 0.60              |
| 1:B:878:THR:HG23 | 1:B:987:GLY:HA2  | 1.84                     | 0.60              |
| 1:A:55:HIS:NE2   | 1:A:141:LEU:HD21 | 2.17                     | 0.60              |
| 1:B:879:ARG:HB2  | 1:B:988:SER:OG   | 2.02                     | 0.59              |
| 1:A:878:THR:HB   | 1:A:922:ILE:HD12 | 1.84                     | 0.59              |
| 1:B:55:HIS:NE2   | 1:B:141:LEU:HD21 | 2.17                     | 0.59              |
| 1:B:859:CYS:SG   | 1:B:860:THR:N    | 2.75                     | 0.59              |
| 1:B:878:THR:HB   | 1:B:922:ILE:HD12 | 1.84                     | 0.59              |
| 1:B:153:ARG:N    | 1:B:156:HIS:HD2  | 1.99                     | 0.59              |
| 1:A:153:ARG:N    | 1:A:156:HIS:HD2  | 1.99                     | 0.59              |
| 1:B:957:VAL:C    | 1:B:958:THR:OG1  | 2.41                     | 0.59              |
| 1:B:859:CYS:O    | 1:B:860:THR:N    | 2.33                     | 0.58              |
| 1:A:485:LEU:HD12 | 1:A:500:MET:HG2  | 1.86                     | 0.58              |
| 1:B:153:ARG:H    | 1:B:156:HIS:CD2  | 2.18                     | 0.58              |
| 1:A:246:TYR:CD2  | 1:A:313:ALA:HB3  | 2.39                     | 0.58              |
| 1:B:485:LEU:HD12 | 1:B:500:MET:HG2  | 1.86                     | 0.58              |
| 1:A:447:PHE:HZ   | 1:A:510:VAL:HG23 | 1.69                     | 0.57              |
| 1:B:719:VAL:HG21 | 1:B:837:LEU:CD1  | 2.33                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:1116:GLU:O   | 1:B:1177:PRO:HG2 | 2.05                     | 0.57              |
| 1:A:732:GLN:HG2  | 1:A:757:ARG:NH2  | 2.20                     | 0.57              |
| 1:B:132:SER:HB2  | 1:B:135:ILE:HG12 | 1.87                     | 0.57              |
| 1:B:337:THR:O    | 1:B:355:LEU:HD12 | 2.05                     | 0.57              |
| 1:B:447:PHE:HZ   | 1:B:510:VAL:HG23 | 1.69                     | 0.57              |
| 1:B:970:PRO:CB   | 1:B:1131:VAL:CG2 | 2.83                     | 0.57              |
| 1:B:246:TYR:CD2  | 1:B:313:ALA:HB3  | 2.39                     | 0.57              |
| 1:B:531:GLY:HA3  | 1:B:554:PHE:CZ   | 2.40                     | 0.57              |
| 1:A:808:PRO:HG3  | 1:A:835:CYS:HB3  | 1.87                     | 0.57              |
| 1:A:132:SER:HB2  | 1:A:135:ILE:HG12 | 1.87                     | 0.56              |
| 1:B:172:ILE:HG22 | 1:B:249:ARG:HD2  | 1.87                     | 0.56              |
| 1:A:531:GLY:HA3  | 1:A:554:PHE:CZ   | 2.40                     | 0.56              |
| 1:A:661:VAL:HG22 | 2:A:1314:NAG:O5  | 2.05                     | 0.56              |
| 1:B:732:GLN:HG2  | 1:B:757:ARG:NH2  | 2.20                     | 0.56              |
| 1:B:1147:ASP:O   | 1:B:1148:PRO:N   | 2.37                     | 0.56              |
| 1:A:1055:TRP:CE2 | 1:A:1178:ALA:HB1 | 2.40                     | 0.56              |
| 1:A:789:ASN:HB3  | 1:A:792:PHE:CD2  | 2.41                     | 0.56              |
| 1:B:296:PHE:CE1  | 1:B:367:ILE:HG12 | 2.41                     | 0.56              |
| 1:A:337:THR:O    | 1:A:355:LEU:HD12 | 2.05                     | 0.56              |
| 1:B:560:GLN:C    | 1:B:586:ASN:HD22 | 2.09                     | 0.56              |
| 1:B:789:ASN:HB3  | 1:B:792:PHE:CD2  | 2.41                     | 0.56              |
| 1:B:808:PRO:HG3  | 1:B:835:CYS:HB3  | 1.87                     | 0.56              |
| 1:A:172:ILE:HG22 | 1:A:249:ARG:HD2  | 1.87                     | 0.56              |
| 1:A:567:GLN:HB2  | 1:A:581:VAL:HG22 | 1.87                     | 0.56              |
| 1:B:567:GLN:HB2  | 1:B:581:VAL:HG22 | 1.87                     | 0.55              |
| 1:A:566:VAL:HG22 | 1:A:582:LEU:CD2  | 2.37                     | 0.55              |
| 1:A:98:SER:O     | 1:B:756:LEU:CG   | 2.54                     | 0.55              |
| 1:B:1116:GLU:HG2 | 1:B:1177:PRO:CD  | 2.36                     | 0.55              |
| 1:B:738:ARG:HB2  | 1:B:789:ASN:HA   | 1.89                     | 0.55              |
| 1:A:296:PHE:CE1  | 1:A:367:ILE:HG12 | 2.41                     | 0.55              |
| 1:B:566:VAL:HG22 | 1:B:582:LEU:CD2  | 2.37                     | 0.55              |
| 1:B:737:GLN:HG2  | 1:B:789:ASN:ND2  | 2.22                     | 0.55              |
| 1:A:98:SER:HB2   | 1:B:756:LEU:HD23 | 1.89                     | 0.55              |
| 1:B:318:PRO:HG2  | 1:B:323:ALA:HB2  | 1.89                     | 0.55              |
| 1:A:318:PRO:HG2  | 1:A:323:ALA:HB2  | 1.89                     | 0.55              |
| 1:A:93:CYS:O     | 1:A:133:GLN:NE2  | 2.40                     | 0.55              |
| 1:B:282:ARG:HG3  | 1:B:283:LEU:N    | 2.22                     | 0.55              |
| 1:B:552:GLN:O    | 1:B:588:PRO:HD3  | 2.06                     | 0.55              |
| 1:B:93:CYS:O     | 1:B:133:GLN:NE2  | 2.40                     | 0.55              |
| 1:B:279:LYS:HG2  | 1:B:297:PRO:HA   | 1.87                     | 0.55              |
| 1:A:279:LYS:HG2  | 1:A:297:PRO:HA   | 1.87                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:282:ARG:HG3  | 1:A:283:LEU:N    | 2.22                     | 0.54              |
| 1:A:738:ARG:HB2  | 1:A:789:ASN:HA   | 1.89                     | 0.54              |
| 1:A:98:SER:C     | 1:B:756:LEU:CD2  | 2.54                     | 0.54              |
| 1:A:488:LEU:HD12 | 1:A:499:ALA:HA   | 1.89                     | 0.54              |
| 1:A:679:LYS:HE2  | 1:A:729:ASN:HB3  | 1.89                     | 0.54              |
| 1:B:1055:TRP:CZ2 | 1:B:1182:SER:HB2 | 2.43                     | 0.54              |
| 1:B:1116:GLU:C   | 1:B:1177:PRO:HG2 | 2.27                     | 0.54              |
| 1:A:970:PRO:CG   | 1:A:1129:ASP:OD2 | 2.56                     | 0.54              |
| 1:B:1116:GLU:HG2 | 1:B:1177:PRO:CG  | 2.38                     | 0.54              |
| 1:A:737:GLN:HG2  | 1:A:789:ASN:ND2  | 2.22                     | 0.54              |
| 1:B:205:MET:HG3  | 1:B:212:ASP:HB3  | 1.90                     | 0.53              |
| 1:B:789:ASN:HB3  | 1:B:792:PHE:HD2  | 1.73                     | 0.53              |
| 1:A:789:ASN:HB3  | 1:A:792:PHE:HD2  | 1.73                     | 0.53              |
| 1:A:332:GLU:OE2  | 1:A:361:ARG:NH2  | 2.41                     | 0.53              |
| 1:A:805:TYR:CD1  | 1:A:824:PHE:HD1  | 2.26                     | 0.53              |
| 1:B:488:LEU:HD12 | 1:B:499:ALA:HA   | 1.89                     | 0.53              |
| 1:A:124:ARG:HD2  | 1:A:138:PHE:HD2  | 1.74                     | 0.53              |
| 1:A:640:LEU:HD12 | 1:A:650:ALA:HB3  | 1.91                     | 0.53              |
| 1:A:126:LEU:HD11 | 1:A:136:CYS:SG   | 2.49                     | 0.53              |
| 1:A:170:VAL:HG11 | 1:A:249:ARG:HB2  | 1.91                     | 0.53              |
| 1:A:205:MET:HG3  | 1:A:212:ASP:HB3  | 1.90                     | 0.53              |
| 1:A:278:SER:HB3  | 1:A:310:VAL:HG23 | 1.91                     | 0.53              |
| 1:A:310:VAL:HG22 | 1:A:339:PHE:HE1  | 1.72                     | 0.53              |
| 1:B:278:SER:HB3  | 1:B:310:VAL:HG23 | 1.91                     | 0.53              |
| 1:A:58:THR:CB    | 1:A:60:GLU:HG2   | 2.39                     | 0.52              |
| 1:B:126:LEU:HD11 | 1:B:136:CYS:SG   | 2.49                     | 0.52              |
| 1:B:332:GLU:OE2  | 1:B:361:ARG:NH2  | 2.41                     | 0.52              |
| 1:B:58:THR:CB    | 1:B:60:GLU:HG2   | 2.40                     | 0.52              |
| 1:B:973:GLY:C    | 1:B:1130:ASN:HB3 | 2.30                     | 0.52              |
| 1:A:153:ARG:H    | 1:A:156:HIS:CD2  | 2.18                     | 0.52              |
| 1:B:677:TRP:HB3  | 1:B:698:VAL:HB   | 1.92                     | 0.52              |
| 1:A:447:PHE:CZ   | 1:A:510:VAL:HG23 | 2.45                     | 0.52              |
| 1:A:869:PRO:HG3  | 1:A:988:SER:OG   | 2.10                     | 0.52              |
| 1:B:821:ASP:HB2  | 1:B:824:PHE:CD2  | 2.45                     | 0.52              |
| 1:A:461:ASP:HA   | 1:A:464:ASN:HB3  | 1.92                     | 0.52              |
| 1:B:1116:GLU:C   | 1:B:1177:PRO:CD  | 2.66                     | 0.52              |
| 1:B:124:ARG:HD2  | 1:B:138:PHE:HD2  | 1.74                     | 0.52              |
| 1:B:640:LEU:HD12 | 1:B:650:ALA:HB3  | 1.91                     | 0.51              |
| 1:A:438:TYR:CE1  | 1:A:510:VAL:HG21 | 2.46                     | 0.51              |
| 1:A:821:ASP:HB2  | 1:A:824:PHE:CD2  | 2.44                     | 0.51              |
| 1:B:447:PHE:CZ   | 1:B:510:VAL:HG23 | 2.45                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:438:TYR:CE1  | 1:B:510:VAL:HG21 | 2.46                     | 0.51              |
| 1:B:170:VAL:HG11 | 1:B:249:ARG:HB2  | 1.91                     | 0.51              |
| 1:B:461:ASP:HA   | 1:B:464:ASN:HB3  | 1.92                     | 0.51              |
| 1:A:153:ARG:NH2  | 1:A:212:ASP:HA   | 2.26                     | 0.51              |
| 1:B:153:ARG:NH2  | 1:B:212:ASP:HA   | 2.26                     | 0.51              |
| 1:A:229:ILE:HD12 | 1:A:240:PHE:HE2  | 1.76                     | 0.51              |
| 1:B:805:TYR:OH   | 1:B:824:PHE:O    | 2.16                     | 0.51              |
| 1:A:431:GLY:HA3  | 1:A:451:ARG:HD2  | 1.93                     | 0.51              |
| 1:B:229:ILE:HD12 | 1:B:240:PHE:HE2  | 1.76                     | 0.51              |
| 1:A:337:THR:HG1  | 1:A:339:PHE:HE2  | 1.60                     | 0.51              |
| 1:B:55:HIS:CE1   | 1:B:57:GLN:HB2   | 2.46                     | 0.51              |
| 1:B:971:LEU:N    | 1:B:1045:ASP:OD1 | 2.41                     | 0.51              |
| 1:B:859:CYS:O    | 1:B:946:TYR:CD1  | 2.64                     | 0.50              |
| 1:B:970:PRO:HB2  | 1:B:1131:VAL:CG2 | 2.42                     | 0.50              |
| 1:A:472:ALA:CB   | 1:A:527:ASP:OD1  | 2.59                     | 0.50              |
| 1:A:677:TRP:HB3  | 1:A:698:VAL:HB   | 1.92                     | 0.50              |
| 1:A:55:HIS:CE1   | 1:A:57:GLN:HB2   | 2.46                     | 0.50              |
| 2:A:1314:NAG:H61 | 2:A:1315:NAG:HN2 | 1.76                     | 0.50              |
| 1:A:805:TYR:HB3  | 1:A:824:PHE:CE1  | 2.47                     | 0.50              |
| 1:A:186:GLY:HA2  | 1:A:198:THR:O    | 2.12                     | 0.50              |
| 1:B:310:VAL:HG22 | 1:B:339:PHE:HE1  | 1.72                     | 0.50              |
| 1:B:553:ARG:HG2  | 1:B:588:PRO:HB3  | 1.92                     | 0.50              |
| 2:B:1315:NAG:H61 | 2:B:1316:NAG:HN2 | 1.77                     | 0.50              |
| 1:B:186:GLY:HA2  | 1:B:198:THR:O    | 2.12                     | 0.50              |
| 1:B:875:GLN:O    | 1:B:1030:ARG:NH1 | 2.45                     | 0.50              |
| 1:A:323:ALA:HA   | 1:A:328:LEU:HD12 | 1.94                     | 0.50              |
| 1:A:708:LEU:H    | 1:A:727:ALA:HA   | 1.77                     | 0.50              |
| 1:B:323:ALA:HA   | 1:B:328:LEU:HD12 | 1.93                     | 0.50              |
| 1:B:464:ASN:CG   | 1:B:465:PRO:HD2  | 2.32                     | 0.50              |
| 1:B:172:ILE:HD11 | 1:B:184:PHE:HE2  | 1.77                     | 0.49              |
| 1:B:431:GLY:HA3  | 1:B:451:ARG:HD2  | 1.94                     | 0.49              |
| 1:A:145:PHE:HD1  | 1:B:734:GLN:OE1  | 1.96                     | 0.49              |
| 1:A:172:ILE:HD11 | 1:A:184:PHE:HE2  | 1.77                     | 0.49              |
| 1:B:708:LEU:H    | 1:B:727:ALA:HA   | 1.77                     | 0.49              |
| 1:B:1116:GLU:CG  | 1:B:1177:PRO:HD3 | 2.42                     | 0.49              |
| 1:A:464:ASN:CG   | 1:A:465:PRO:HD2  | 2.32                     | 0.49              |
| 1:A:495:GLN:O    | 1:A:510:VAL:HG12 | 2.13                     | 0.49              |
| 1:B:153:ARG:HB2  | 1:B:156:HIS:CD2  | 2.48                     | 0.49              |
| 1:A:1027:ASN:HB3 | 1:A:1032:GLN:HG3 | 1.95                     | 0.48              |
| 1:B:495:GLN:O    | 1:B:510:VAL:HG12 | 2.13                     | 0.48              |
| 1:B:1147:ASP:HB3 | 1:B:1148:PRO:CD  | 2.43                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:460:VAL:HA   | 1:A:469:PRO:HB3   | 1.95                     | 0.48              |
| 1:B:40:ARG:NH2   | 2:B:1301:NAG:O3   | 2.47                     | 0.48              |
| 1:B:501:THR:OG1  | 1:B:504:GLN:N     | 2.44                     | 0.48              |
| 1:A:145:PHE:HE1  | 1:B:734:GLN:NE2   | 2.12                     | 0.48              |
| 1:B:96:PRO:HD2   | 1:B:157:TYR:CZ    | 2.48                     | 0.48              |
| 1:A:40:ARG:NH2   | 2:A:1301:NAG:O3   | 2.47                     | 0.48              |
| 1:B:719:VAL:HG21 | 1:B:837:LEU:HD13  | 1.95                     | 0.48              |
| 1:B:970:PRO:HB2  | 1:B:1131:VAL:HG22 | 1.94                     | 0.48              |
| 1:A:96:PRO:HD2   | 1:A:157:TYR:CZ    | 2.48                     | 0.48              |
| 1:A:939:VAL:CG2  | 1:A:946:TYR:HB3   | 2.42                     | 0.48              |
| 1:A:98:SER:O     | 1:B:756:LEU:HD11  | 2.14                     | 0.48              |
| 1:B:1027:ASN:HB3 | 1:B:1032:GLN:HG3  | 1.95                     | 0.47              |
| 1:A:153:ARG:HB2  | 1:A:156:HIS:CD2   | 2.48                     | 0.47              |
| 1:B:460:VAL:HA   | 1:B:469:PRO:HB3   | 1.96                     | 0.47              |
| 1:B:907:PRO:HA   | 1:B:920:CYS:HA    | 1.96                     | 0.47              |
| 1:B:567:GLN:CB   | 1:B:581:VAL:HG22  | 2.44                     | 0.47              |
| 1:B:821:ASP:HB2  | 1:B:824:PHE:CE2   | 2.50                     | 0.47              |
| 1:A:821:ASP:HB2  | 1:A:824:PHE:CE2   | 2.49                     | 0.47              |
| 1:A:372:GLN:O    | 1:A:376:ARG:HD3   | 2.15                     | 0.47              |
| 1:A:447:PHE:CD2  | 1:A:497:LEU:HD22  | 2.50                     | 0.47              |
| 1:B:172:ILE:HD13 | 1:B:285:VAL:HG13  | 1.97                     | 0.47              |
| 1:B:939:VAL:CG2  | 1:B:946:TYR:HB3   | 2.42                     | 0.47              |
| 1:A:934:LEU:HD23 | 1:A:953:ARG:HB3   | 1.97                     | 0.47              |
| 1:B:372:GLN:O    | 1:B:376:ARG:HD3   | 2.15                     | 0.47              |
| 1:A:907:PRO:HA   | 1:A:920:CYS:HA    | 1.96                     | 0.47              |
| 1:B:934:LEU:HD23 | 1:B:953:ARG:HB3   | 1.97                     | 0.47              |
| 1:A:567:GLN:CB   | 1:A:581:VAL:HG22  | 2.44                     | 0.47              |
| 1:A:854:HIS:C    | 1:A:890:ARG:HH22  | 2.18                     | 0.47              |
| 1:B:337:THR:HG1  | 1:B:339:PHE:HE2   | 1.60                     | 0.47              |
| 1:A:461:ASP:CA   | 1:A:464:ASN:HB3   | 2.45                     | 0.47              |
| 1:A:805:TYR:CE2  | 1:A:824:PHE:HB3   | 2.50                     | 0.47              |
| 1:A:818:LEU:HD22 | 1:A:852:ALA:H     | 1.80                     | 0.46              |
| 1:B:566:VAL:CG2  | 1:B:652:VAL:HG21  | 2.45                     | 0.46              |
| 1:B:952:LYS:HD2  | 1:B:952:LYS:HA    | 1.70                     | 0.46              |
| 1:A:145:PHE:CE1  | 1:B:734:GLN:NE2   | 2.84                     | 0.46              |
| 1:B:818:LEU:HD22 | 1:B:852:ALA:H     | 1.80                     | 0.46              |
| 1:A:566:VAL:CG2  | 1:A:652:VAL:HG21  | 2.45                     | 0.46              |
| 1:A:805:TYR:CZ   | 1:A:824:PHE:O     | 2.68                     | 0.46              |
| 1:A:860:THR:HG22 | 1:A:946:TYR:OH    | 2.16                     | 0.46              |
| 1:B:447:PHE:CD2  | 1:B:497:LEU:HD22  | 2.50                     | 0.46              |
| 1:B:805:TYR:CE2  | 1:B:824:PHE:HB3   | 2.51                     | 0.46              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:A:553:ARG:HD2   | 1:A:588:PRO:HG3   | 1.98                     | 0.46              |
| 1:B:859:CYS:C     | 1:B:860:THR:CA    | 2.76                     | 0.46              |
| 1:A:877:GLY:HA2   | 1:A:1030:ARG:NE   | 2.31                     | 0.46              |
| 1:B:461:ASP:CA    | 1:B:464:ASN:HB3   | 2.45                     | 0.46              |
| 1:A:805:TYR:CE2   | 1:A:824:PHE:O     | 2.69                     | 0.46              |
| 1:B:1055:TRP:HZ2  | 1:B:1182:SER:HB2  | 1.81                     | 0.46              |
| 1:B:558:LEU:HD12  | 1:B:561:CYS:SG    | 2.56                     | 0.45              |
| 1:A:79:LEU:O      | 1:A:80:ARG:HG3    | 2.16                     | 0.45              |
| 1:B:1043:THR:HG21 | 1:B:1073:THR:HG21 | 1.98                     | 0.45              |
| 1:B:201:SER:HB2   | 1:B:290:PHE:HE1   | 1.81                     | 0.45              |
| 1:B:937:VAL:HG23  | 1:B:948:ALA:HB3   | 1.98                     | 0.45              |
| 1:A:501:THR:OG1   | 1:A:504:GLN:N     | 2.44                     | 0.45              |
| 1:A:510:VAL:C     | 1:A:511:GLU:CA    | 2.77                     | 0.45              |
| 1:A:558:LEU:HD12  | 1:A:561:CYS:SG    | 2.56                     | 0.45              |
| 1:A:566:VAL:HG23  | 1:A:652:VAL:HG21  | 1.98                     | 0.45              |
| 1:B:125:LEU:HD23  | 1:B:139:LEU:HB2   | 1.99                     | 0.45              |
| 1:B:887:LEU:HD23  | 1:B:918:ILE:HD11  | 1.98                     | 0.45              |
| 1:A:887:LEU:HD23  | 1:A:918:ILE:HD11  | 1.98                     | 0.45              |
| 1:B:860:THR:HG22  | 1:B:946:TYR:OH    | 2.16                     | 0.45              |
| 1:B:79:LEU:O      | 1:B:80:ARG:HG3    | 2.17                     | 0.45              |
| 1:B:815:GLY:O     | 1:B:819:LYS:HB2   | 2.17                     | 0.45              |
| 1:A:172:ILE:HD13  | 1:A:285:VAL:HG13  | 1.97                     | 0.45              |
| 1:A:858:ARG:HE    | 1:A:946:TYR:HE2   | 1.64                     | 0.45              |
| 1:B:932:ASP:OD1   | 1:B:932:ASP:N     | 2.50                     | 0.45              |
| 1:A:132:SER:CB    | 1:A:135:ILE:HG12  | 2.47                     | 0.45              |
| 1:A:98:SER:OG     | 1:B:756:LEU:CD2   | 2.64                     | 0.45              |
| 1:A:937:VAL:HG23  | 1:A:948:ALA:HB3   | 1.98                     | 0.45              |
| 1:A:102:CYS:HA    | 1:A:103:PRO:HD3   | 1.87                     | 0.44              |
| 1:B:1088:ARG:HD2  | 1:B:1106:SER:O    | 2.18                     | 0.44              |
| 1:B:1145:TYR:OH   | 1:B:1178:ALA:HA   | 2.17                     | 0.44              |
| 1:A:201:SER:HB2   | 1:A:290:PHE:HE1   | 1.81                     | 0.44              |
| 1:A:278:SER:HG    | 1:A:309:LEU:HA    | 1.82                     | 0.44              |
| 1:A:932:ASP:N     | 1:A:932:ASP:OD1   | 2.50                     | 0.44              |
| 1:B:132:SER:CB    | 1:B:135:ILE:HG12  | 2.47                     | 0.44              |
| 1:A:1088:ARG:HD2  | 1:A:1106:SER:O    | 2.18                     | 0.44              |
| 1:A:1078:ARG:HG3  | 1:A:1127:ILE:HB   | 1.99                     | 0.44              |
| 1:A:125:LEU:HD23  | 1:A:139:LEU:HB2   | 1.99                     | 0.44              |
| 1:B:566:VAL:HG23  | 1:B:652:VAL:HG21  | 1.98                     | 0.44              |
| 1:A:952:LYS:HD2   | 1:A:952:LYS:HA    | 1.70                     | 0.44              |
| 1:B:894:VAL:HG11  | 1:B:918:ILE:HD13  | 1.99                     | 0.44              |
| 1:A:550:GLU:HB2   | 1:A:553:ARG:HG3   | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:359:THR:HG23 | 1:B:362:ALA:CB   | 2.48                     | 0.44              |
| 1:B:789:ASN:ND2  | 1:B:792:PHE:HE2  | 2.09                     | 0.44              |
| 1:B:67:ASN:CB    | 1:B:85:GLY:HA3   | 2.48                     | 0.44              |
| 1:A:815:GLY:O    | 1:A:819:LYS:HB2  | 2.17                     | 0.44              |
| 1:B:808:PRO:HB2  | 1:B:811:ARG:H    | 1.82                     | 0.44              |
| 1:A:860:THR:CA   | 1:A:946:TYR:CE1  | 2.81                     | 0.44              |
| 1:A:805:TYR:CD1  | 1:A:824:PHE:CD1  | 3.06                     | 0.43              |
| 1:A:805:TYR:CG   | 1:A:824:PHE:HD1  | 2.29                     | 0.43              |
| 1:B:138:PHE:CZ   | 1:B:213:MET:HE2  | 2.52                     | 0.43              |
| 1:A:138:PHE:CZ   | 1:A:213:MET:HE2  | 2.54                     | 0.43              |
| 1:A:740:TYR:HE1  | 1:A:794:ILE:HD11 | 1.83                     | 0.43              |
| 1:A:808:PRO:HB2  | 1:A:811:ARG:H    | 1.82                     | 0.43              |
| 1:B:155:GLU:OE1  | 1:B:155:GLU:N    | 2.51                     | 0.43              |
| 1:B:818:LEU:HB3  | 1:B:852:ALA:CB   | 2.41                     | 0.43              |
| 1:B:161:VAL:HG12 | 1:B:163:GLU:H    | 1.84                     | 0.43              |
| 1:A:67:ASN:CB    | 1:A:85:GLY:HA3   | 2.48                     | 0.43              |
| 1:B:740:TYR:HE1  | 1:B:794:ILE:HD11 | 1.83                     | 0.43              |
| 1:B:973:GLY:O    | 1:B:1130:ASN:N   | 2.51                     | 0.43              |
| 1:A:359:THR:HG23 | 1:A:362:ALA:CB   | 2.48                     | 0.43              |
| 1:A:576:SER:OG   | 1:A:620:ALA:N    | 2.51                     | 0.43              |
| 1:A:838:ARG:NH1  | 1:A:841:CYS:O    | 2.51                     | 0.43              |
| 1:B:261:LEU:HD11 | 1:B:274:HIS:CB   | 2.48                     | 0.43              |
| 1:B:559:LEU:O    | 1:B:586:ASN:ND2  | 2.50                     | 0.43              |
| 1:B:706:GLN:O    | 1:B:727:ALA:HB1  | 2.19                     | 0.43              |
| 1:B:838:ARG:NH1  | 1:B:841:CYS:O    | 2.51                     | 0.43              |
| 1:A:161:VAL:HG12 | 1:A:163:GLU:H    | 1.83                     | 0.43              |
| 1:A:639:TYR:HD2  | 1:A:648:LYS:HD2  | 1.84                     | 0.43              |
| 1:A:818:LEU:HB3  | 1:A:852:ALA:CB   | 2.41                     | 0.43              |
| 1:B:150:PRO:HB2  | 1:B:156:HIS:ND1  | 2.34                     | 0.43              |
| 1:A:155:GLU:N    | 1:A:155:GLU:OE1  | 2.51                     | 0.43              |
| 1:A:261:LEU:HD11 | 1:A:274:HIS:CB   | 2.48                     | 0.43              |
| 1:A:894:VAL:HG11 | 1:A:918:ILE:HD13 | 1.99                     | 0.43              |
| 1:B:476:VAL:HB   | 1:B:479:GLN:HG2  | 2.01                     | 0.43              |
| 1:B:553:ARG:CD   | 1:B:588:PRO:CB   | 2.96                     | 0.43              |
| 1:A:58:THR:HB    | 1:A:60:GLU:HG2   | 2.01                     | 0.43              |
| 1:B:1078:ARG:HG3 | 1:B:1127:ILE:HB  | 1.99                     | 0.43              |
| 1:B:58:THR:HB    | 1:B:60:GLU:HG2   | 2.01                     | 0.43              |
| 1:A:150:PRO:HB2  | 1:A:156:HIS:ND1  | 2.34                     | 0.43              |
| 1:A:789:ASN:ND2  | 1:A:792:PHE:HE2  | 2.09                     | 0.43              |
| 1:B:550:GLU:HB2  | 1:B:553:ARG:HG3  | 2.00                     | 0.43              |
| 1:A:468:ARG:HG2  | 1:A:469:PRO:CD   | 2.36                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:805:TYR:OH   | 1:A:824:PHE:O    | 2.27                     | 0.43              |
| 1:B:606:SER:CB   | 1:B:615:CYS:HB3  | 2.47                     | 0.43              |
| 1:A:410:ASN:O    | 1:A:411:GLN:O    | 2.37                     | 0.42              |
| 1:A:787:VAL:HG22 | 1:A:793:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:818:LEU:HD22 | 1:A:852:ALA:N    | 2.34                     | 0.42              |
| 1:B:576:SER:OG   | 1:B:620:ALA:N    | 2.51                     | 0.42              |
| 1:B:410:ASN:O    | 1:B:411:GLN:O    | 2.37                     | 0.42              |
| 1:B:818:LEU:HD22 | 1:B:852:ALA:N    | 2.34                     | 0.42              |
| 1:B:959:PRO:HA   | 1:B:983:HIS:HB2  | 2.01                     | 0.42              |
| 1:A:309:LEU:O    | 1:A:339:PHE:HA   | 2.19                     | 0.42              |
| 1:A:706:GLN:O    | 1:A:727:ALA:HB1  | 2.19                     | 0.42              |
| 1:A:69:ILE:CD1   | 1:A:84:THR:HG21  | 2.48                     | 0.42              |
| 1:B:973:GLY:C    | 1:B:1130:ASN:CB  | 2.88                     | 0.42              |
| 1:A:972:SER:HB3  | 1:A:1130:ASN:HB3 | 2.02                     | 0.42              |
| 1:A:476:VAL:HB   | 1:A:479:GLN:HG2  | 2.01                     | 0.42              |
| 1:B:309:LEU:O    | 1:B:339:PHE:HA   | 2.19                     | 0.42              |
| 1:B:263:THR:HB   | 1:B:384:PRO:HB2  | 2.02                     | 0.42              |
| 1:B:787:VAL:HG22 | 1:B:793:VAL:HG22 | 2.01                     | 0.42              |
| 1:A:340:ALA:HB1  | 1:A:350:PRO:HG2  | 2.02                     | 0.42              |
| 1:A:263:THR:HB   | 1:A:384:PRO:HB2  | 2.01                     | 0.42              |
| 1:A:1169:LEU:HB2 | 1:A:1204:LEU:HB2 | 2.02                     | 0.42              |
| 1:A:959:PRO:HA   | 1:A:983:HIS:HB2  | 2.01                     | 0.42              |
| 1:B:340:ALA:HB1  | 1:B:350:PRO:HG2  | 2.02                     | 0.42              |
| 1:B:49:LEU:HD13  | 1:B:500:MET:HE2  | 2.01                     | 0.42              |
| 1:B:1001:PHE:HZ  | 1:B:1004:ARG:HB2 | 1.85                     | 0.42              |
| 1:B:568:PRO:HG2  | 1:B:580:LEU:HD23 | 2.01                     | 0.42              |
| 1:B:970:PRO:HB3  | 1:B:1131:VAL:CG2 | 2.48                     | 0.42              |
| 1:B:468:ARG:HG2  | 1:B:469:PRO:CD   | 2.36                     | 0.41              |
| 1:B:1116:GLU:HG2 | 1:B:1177:PRO:HG3 | 2.02                     | 0.41              |
| 1:A:1001:PHE:HZ  | 1:A:1004:ARG:HB2 | 1.85                     | 0.41              |
| 1:A:552:GLN:O    | 1:A:588:PRO:HD3  | 2.20                     | 0.41              |
| 1:A:582:LEU:HB2  | 1:A:613:ILE:HB   | 2.02                     | 0.41              |
| 1:B:150:PRO:O    | 1:B:156:HIS:HB3  | 2.21                     | 0.41              |
| 1:B:906:SER:HA   | 1:B:907:PRO:HD3  | 1.77                     | 0.41              |
| 1:A:568:PRO:HG2  | 1:A:580:LEU:HD23 | 2.01                     | 0.41              |
| 1:B:189:ILE:HG22 | 1:B:191:GLY:H    | 1.85                     | 0.41              |
| 1:A:871:THR:HG22 | 1:A:955:THR:HB   | 2.02                     | 0.41              |
| 1:B:488:LEU:HG   | 1:B:497:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:461:ASP:CB   | 1:B:464:ASN:HB3  | 2.50                     | 0.41              |
| 1:A:138:PHE:CZ   | 1:A:213:MET:CE   | 3.04                     | 0.41              |
| 1:A:313:ALA:HB1  | 1:A:335:LEU:HD11 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:136:CYS:HB3  | 1:B:214:PHE:CZ   | 2.56                     | 0.41              |
| 1:B:459:LEU:HD23 | 1:B:459:LEU:HA   | 1.95                     | 0.41              |
| 1:B:582:LEU:HB2  | 1:B:613:ILE:HB   | 2.02                     | 0.41              |
| 1:B:69:ILE:CD1   | 1:B:84:THR:HG21  | 2.48                     | 0.41              |
| 1:A:1104:ALA:HA  | 1:A:1105:PRO:HD3 | 1.89                     | 0.41              |
| 1:A:261:LEU:HD11 | 1:A:274:HIS:HB3  | 2.03                     | 0.41              |
| 1:A:944:LEU:H    | 1:A:944:LEU:HD12 | 1.85                     | 0.41              |
| 1:B:1147:ASP:CA  | 1:B:1148:PRO:HD3 | 2.51                     | 0.41              |
| 1:B:313:ALA:HB1  | 1:B:335:LEU:HD11 | 2.03                     | 0.41              |
| 1:B:944:LEU:HD12 | 1:B:944:LEU:H    | 1.85                     | 0.41              |
| 1:A:461:ASP:CB   | 1:A:464:ASN:HB3  | 2.50                     | 0.41              |
| 1:A:488:LEU:HG   | 1:A:497:LEU:HD11 | 2.02                     | 0.41              |
| 1:B:138:PHE:CZ   | 1:B:213:MET:CE   | 3.04                     | 0.41              |
| 1:B:473:TYR:CE2  | 1:B:475:SER:HB2  | 2.56                     | 0.41              |
| 1:A:150:PRO:O    | 1:A:156:HIS:HB3  | 2.21                     | 0.41              |
| 1:A:189:ILE:HG22 | 1:A:191:GLY:H    | 1.86                     | 0.41              |
| 1:A:241:ASP:HB3  | 1:A:243:TYR:CZ   | 2.56                     | 0.41              |
| 1:A:473:TYR:CE2  | 1:A:475:SER:HB2  | 2.56                     | 0.41              |
| 1:A:734:GLN:O    | 1:A:737:GLN:HB2  | 2.21                     | 0.41              |
| 1:A:225:SER:HB3  | 1:A:288:PRO:O    | 2.20                     | 0.40              |
| 1:A:49:LEU:HD13  | 1:A:500:MET:HE2  | 2.02                     | 0.40              |
| 1:B:1169:LEU:HB2 | 1:B:1204:LEU:HB2 | 2.02                     | 0.40              |
| 1:B:855:GLY:HA3  | 1:B:890:ARG:HH22 | 1.43                     | 0.40              |
| 1:B:873:PRO:HD2  | 1:B:878:THR:OG1  | 2.21                     | 0.40              |
| 1:A:668:CYS:O    | 1:A:675:CYS:HB2  | 2.22                     | 0.40              |
| 1:B:205:MET:N    | 1:B:213:MET:SD   | 2.93                     | 0.40              |
| 1:A:490:LEU:HD23 | 1:A:497:LEU:HB2  | 2.03                     | 0.40              |
| 1:A:836:SER:O    | 1:A:849:TRP:NE1  | 2.54                     | 0.40              |
| 1:A:906:SER:HA   | 1:A:907:PRO:HD3  | 1.77                     | 0.40              |
| 1:B:189:ILE:CD1  | 1:B:198:THR:HG23 | 2.37                     | 0.40              |
| 1:B:225:SER:HB3  | 1:B:288:PRO:O    | 2.21                     | 0.40              |
| 1:B:860:THR:CA   | 1:B:946:TYR:CE1  | 2.81                     | 0.40              |
| 1:A:1043:THR:OG1 | 1:A:1073:THR:HB  | 2.21                     | 0.40              |
| 1:B:69:ILE:HD13  | 1:B:127:ALA:HB1  | 2.04                     | 0.40              |

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1        | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|-------------------------|--------------------------|-------------------|
| 1:A:399:GLN:N | 1:B:1007:ARG:NH2[2_445] | 0.67                     | 1.53              |

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| Atom-1          | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|-------------------------|--------------------------|-------------------|
| 1:A:398:LEU:C   | 1:B:1007:ARG:NH2[2_445] | 0.78                     | 1.42              |
| 1:A:962:TYR:OH  | 1:B:361:ARG:NH1[1_656]  | 1.02                     | 1.18              |
| 1:A:398:LEU:O   | 1:B:1007:ARG:NH1[2_445] | 1.61                     | 0.59              |
| 1:A:962:TYR:CZ  | 1:B:361:ARG:NH1[1_656]  | 1.69                     | 0.51              |
| 1:A:398:LEU:O   | 1:B:1007:ARG:NH2[2_445] | 1.73                     | 0.47              |
| 1:B:219:GLN:C   | 1:B:944:LEU:CD1[1_554]  | 1.76                     | 0.44              |
| 1:A:399:GLN:NE2 | 1:B:1007:ARG:CB[2_445]  | 1.80                     | 0.40              |
| 1:A:399:GLN:CA  | 1:B:1007:ARG:NH2[2_445] | 1.80                     | 0.40              |
| 1:B:177:GLY:C   | 1:B:847:ALA:CB[1_554]   | 1.82                     | 0.38              |
| 1:A:398:LEU:C   | 1:B:1007:ARG:NH1[2_445] | 1.82                     | 0.38              |
| 1:A:399:GLN:CD  | 1:B:1007:ARG:CG[2_445]  | 1.82                     | 0.38              |
| 1:B:219:GLN:CB  | 1:B:944:LEU:CD2[1_554]  | 1.84                     | 0.36              |
| 1:A:399:GLN:N   | 1:B:1007:ARG:NE[2_445]  | 1.84                     | 0.36              |
| 1:A:398:LEU:O   | 1:B:1007:ARG:CZ[2_445]  | 1.86                     | 0.34              |
| 1:B:219:GLN:CA  | 1:B:944:LEU:CD1[1_554]  | 1.87                     | 0.33              |
| 1:B:176:PRO:O   | 1:B:847:ALA:N[1_554]    | 1.89                     | 0.31              |
| 1:A:962:TYR:OH  | 1:B:361:ARG:CZ[1_656]   | 1.97                     | 0.23              |
| 1:B:176:PRO:CG  | 1:B:846:PRO:CG[1_554]   | 1.99                     | 0.21              |
| 1:A:399:GLN:CG  | 1:B:1007:ARG:CG[2_445]  | 2.00                     | 0.20              |
| 1:A:398:LEU:CA  | 1:B:1007:ARG:NH2[2_445] | 2.01                     | 0.19              |
| 1:B:176:PRO:CA  | 1:B:845:SER:OG[1_554]   | 2.01                     | 0.19              |
| 1:B:176:PRO:CB  | 1:B:845:SER:OG[1_554]   | 2.03                     | 0.17              |
| 1:A:962:TYR:CE2 | 1:B:361:ARG:NH1[1_656]  | 2.04                     | 0.16              |
| 1:B:177:GLY:CA  | 1:B:847:ALA:CA[1_554]   | 2.04                     | 0.16              |
| 1:B:219:GLN:O   | 1:B:944:LEU:CG[1_554]   | 2.04                     | 0.16              |
| 1:B:219:GLN:N   | 1:B:944:LEU:CD1[1_554]  | 2.07                     | 0.13              |
| 1:B:176:PRO:O   | 1:B:846:PRO:CG[1_554]   | 2.07                     | 0.13              |
| 1:B:176:PRO:CD  | 1:B:846:PRO:CG[1_554]   | 2.11                     | 0.09              |
| 1:A:399:GLN:CA  | 1:B:1007:ARG:CZ[2_445]  | 2.12                     | 0.08              |
| 1:A:399:GLN:CG  | 1:B:1007:ARG:NE[2_445]  | 2.13                     | 0.07              |
| 1:A:182:LYS:CE  | 1:A:844:ASP:OD1[1_455]  | 2.15                     | 0.05              |
| 1:A:1093:MET:CE | 1:B:376:ARG:O[1_656]    | 2.17                     | 0.03              |
| 1:A:399:GLN:NE2 | 1:B:1007:ARG:CA[2_445]  | 2.19                     | 0.01              |
| 1:A:549:GLU:O   | 1:A:1207:GLU:OE2[2_545] | 2.19                     | 0.01              |

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1   | A     | 1155/1212 (95%) | 1049 (91%) | 92 (8%)  | 14 (1%)  | 16          | 61 |
| 1   | B     | 1161/1212 (96%) | 1048 (90%) | 96 (8%)  | 17 (2%)  | 13          | 57 |
| All | All   | 2316/2424 (96%) | 2097 (90%) | 188 (8%) | 31 (1%)  | 15          | 59 |

All (31) Ramachandran outliers are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 86   | PRO  |
| 1   | A     | 95   | PRO  |
| 1   | A     | 411  | GLN  |
| 1   | A     | 869  | PRO  |
| 1   | A     | 915  | ALA  |
| 1   | A     | 1192 | SER  |
| 1   | B     | 86   | PRO  |
| 1   | B     | 95   | PRO  |
| 1   | B     | 411  | GLN  |
| 1   | B     | 869  | PRO  |
| 1   | B     | 915  | ALA  |
| 1   | B     | 1147 | ASP  |
| 1   | B     | 1148 | PRO  |
| 1   | B     | 1192 | SER  |
| 1   | A     | 251  | GLU  |
| 1   | A     | 1053 | PRO  |
| 1   | A     | 1182 | SER  |
| 1   | B     | 251  | GLU  |
| 1   | B     | 1053 | PRO  |
| 1   | B     | 1182 | SER  |
| 1   | A     | 694  | LEU  |
| 1   | B     | 694  | LEU  |
| 1   | A     | 966  | PRO  |
| 1   | B     | 966  | PRO  |
| 1   | A     | 318  | PRO  |
| 1   | A     | 1108 | ASP  |
| 1   | B     | 318  | PRO  |
| 1   | B     | 1108 | ASP  |
| 1   | B     | 957  | VAL  |
| 1   | A     | 774  | GLY  |
| 1   | B     | 774  | GLY  |



### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 1015/1051 (97%) | 977 (96%)  | 38 (4%)  | 41          | 73 |
| 1   | B     | 1015/1051 (97%) | 977 (96%)  | 38 (4%)  | 41          | 73 |
| All | All   | 2030/2102 (97%) | 1954 (96%) | 76 (4%)  | 41          | 73 |

All (76) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 77  | THR  |
| 1   | A     | 78  | LEU  |
| 1   | A     | 125 | LEU  |
| 1   | A     | 128 | CYS  |
| 1   | A     | 136 | CYS  |
| 1   | A     | 152 | HIS  |
| 1   | A     | 207 | ASN  |
| 1   | A     | 257 | LEU  |
| 1   | A     | 274 | HIS  |
| 1   | A     | 280 | ILE  |
| 1   | A     | 300 | CYS  |
| 1   | A     | 352 | GLU  |
| 1   | A     | 387 | LEU  |
| 1   | A     | 413 | LEU  |
| 1   | A     | 422 | THR  |
| 1   | A     | 514 | VAL  |
| 1   | A     | 517 | THR  |
| 1   | A     | 562 | VAL  |
| 1   | A     | 585 | TRP  |
| 1   | A     | 610 | ASP  |
| 1   | A     | 634 | ARG  |
| 1   | A     | 652 | VAL  |
| 1   | A     | 693 | PHE  |
| 1   | A     | 812 | GLN  |
| 1   | A     | 814 | CYS  |
| 1   | A     | 821 | ASP  |
| 1   | A     | 837 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 882  | ILE  |
| 1   | A     | 929  | ARG  |
| 1   | A     | 937  | VAL  |
| 1   | A     | 977  | ILE  |
| 1   | A     | 982  | SER  |
| 1   | A     | 1018 | THR  |
| 1   | A     | 1030 | ARG  |
| 1   | A     | 1033 | LEU  |
| 1   | A     | 1075 | ARG  |
| 1   | A     | 1079 | ILE  |
| 1   | A     | 1197 | LEU  |
| 1   | B     | 77   | THR  |
| 1   | B     | 78   | LEU  |
| 1   | B     | 125  | LEU  |
| 1   | B     | 128  | CYS  |
| 1   | B     | 136  | CYS  |
| 1   | B     | 152  | HIS  |
| 1   | B     | 207  | ASN  |
| 1   | B     | 257  | LEU  |
| 1   | B     | 274  | HIS  |
| 1   | B     | 280  | ILE  |
| 1   | B     | 300  | CYS  |
| 1   | B     | 352  | GLU  |
| 1   | B     | 387  | LEU  |
| 1   | B     | 413  | LEU  |
| 1   | B     | 422  | THR  |
| 1   | B     | 514  | VAL  |
| 1   | B     | 517  | THR  |
| 1   | B     | 562  | VAL  |
| 1   | B     | 585  | TRP  |
| 1   | B     | 610  | ASP  |
| 1   | B     | 634  | ARG  |
| 1   | B     | 652  | VAL  |
| 1   | B     | 693  | PHE  |
| 1   | B     | 812  | GLN  |
| 1   | B     | 814  | CYS  |
| 1   | B     | 821  | ASP  |
| 1   | B     | 837  | LEU  |
| 1   | B     | 882  | ILE  |
| 1   | B     | 929  | ARG  |
| 1   | B     | 937  | VAL  |
| 1   | B     | 977  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 982  | SER  |
| 1   | B     | 1018 | THR  |
| 1   | B     | 1030 | ARG  |
| 1   | B     | 1033 | LEU  |
| 1   | B     | 1075 | ARG  |
| 1   | B     | 1079 | ILE  |
| 1   | B     | 1197 | LEU  |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 156 | HIS  |
| 1   | A     | 663 | GLN  |
| 1   | A     | 706 | GLN  |
| 1   | A     | 729 | ASN  |
| 1   | A     | 764 | GLN  |
| 1   | A     | 899 | HIS  |
| 1   | B     | 156 | HIS  |
| 1   | B     | 586 | ASN  |
| 1   | B     | 663 | GLN  |
| 1   | B     | 706 | GLN  |
| 1   | B     | 729 | ASN  |
| 1   | B     | 764 | GLN  |
| 1   | B     | 766 | GLN  |
| 1   | B     | 899 | HIS  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

83 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res  | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|------|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |      |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | NAG  | A     | 1301 | 1,2  | 14,14,15     | 0.75 | 0           | 15,19,21    | 1.74 | 3 (20%)     |
| 2   | NAG  | A     | 1302 | 3,2  | 14,14,15     | 0.55 | 0           | 15,19,21    | 1.44 | 1 (6%)      |
| 3   | BMA  | A     | 1303 | 2,4  | 11,11,12     | 0.65 | 0           | 15,15,17    | 0.83 | 0           |
| 4   | MAN  | A     | 1304 | 3    | 11,11,12     | 0.64 | 0           | 15,15,17    | 1.00 | 1 (6%)      |
| 2   | NAG  | A     | 1305 | 1,2  | 14,14,15     | 0.64 | 0           | 15,19,21    | 1.22 | 1 (6%)      |
| 2   | NAG  | A     | 1306 | 3,2  | 14,14,15     | 0.47 | 0           | 15,19,21    | 1.19 | 1 (6%)      |
| 3   | BMA  | A     | 1307 | 2,4  | 11,11,12     | 0.55 | 0           | 15,15,17    | 0.65 | 0           |
| 4   | MAN  | A     | 1308 | 3,4  | 11,11,12     | 0.67 | 0           | 15,15,17    | 0.95 | 1 (6%)      |
| 4   | MAN  | A     | 1309 | 4    | 11,11,12     | 0.56 | 0           | 15,15,17    | 1.22 | 2 (13%)     |
| 2   | NAG  | A     | 1310 | 1,2  | 14,14,15     | 0.62 | 0           | 15,19,21    | 1.14 | 1 (6%)      |
| 2   | NAG  | A     | 1311 | 3,2  | 14,14,15     | 0.55 | 0           | 15,19,21    | 1.20 | 2 (13%)     |
| 3   | BMA  | A     | 1312 | 2,4  | 11,11,12     | 0.86 | 1 (9%)      | 15,15,17    | 2.24 | 4 (26%)     |
| 4   | MAN  | A     | 1313 | 3    | 11,11,12     | 0.58 | 0           | 15,15,17    | 1.05 | 2 (13%)     |
| 2   | NAG  | A     | 1314 | 1,2  | 14,14,15     | 0.64 | 0           | 15,19,21    | 1.16 | 1 (6%)      |
| 2   | NAG  | A     | 1315 | 3,2  | 14,14,15     | 0.53 | 0           | 15,19,21    | 1.10 | 1 (6%)      |
| 3   | BMA  | A     | 1316 | 2,4  | 11,11,12     | 0.60 | 0           | 15,15,17    | 1.65 | 3 (20%)     |
| 4   | MAN  | A     | 1317 | 3    | 11,11,12     | 0.59 | 0           | 15,15,17    | 0.88 | 1 (6%)      |
| 4   | MAN  | A     | 1318 | 3,4  | 11,11,12     | 0.60 | 0           | 15,15,17    | 0.91 | 0           |
| 4   | MAN  | A     | 1319 | 4    | 11,11,12     | 0.51 | 0           | 15,15,17    | 1.22 | 1 (6%)      |
| 4   | MAN  | A     | 1320 | 4    | 11,11,12     | 0.57 | 0           | 15,15,17    | 1.32 | 2 (13%)     |
| 2   | NAG  | A     | 1321 | 1    | 14,14,15     | 0.60 | 0           | 15,19,21    | 1.21 | 1 (6%)      |
| 2   | NAG  | A     | 1322 | 1,2  | 14,14,15     | 0.62 | 0           | 15,19,21    | 0.94 | 1 (6%)      |
| 2   | NAG  | A     | 1323 | 3,2  | 14,14,15     | 0.65 | 0           | 15,19,21    | 1.07 | 1 (6%)      |
| 3   | BMA  | A     | 1324 | 2    | 11,11,12     | 0.42 | 0           | 15,15,17    | 1.70 | 2 (13%)     |
| 2   | NAG  | A     | 1325 | 1    | 14,14,15     | 0.51 | 0           | 15,19,21    | 0.98 | 0           |
| 2   | NAG  | A     | 1326 | 1,2  | 14,14,15     | 0.54 | 0           | 15,19,21    | 1.04 | 1 (6%)      |
| 2   | NAG  | A     | 1327 | 3,2  | 14,14,15     | 0.55 | 0           | 15,19,21    | 1.05 | 1 (6%)      |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BMA  | A     | 1328 | 2    | 11,11,12     | 0.48 | 0        | 15,15,17    | 1.15 | 2 (13%)  |
| 2   | NAG  | A     | 1329 | 1,2  | 14,14,15     | 0.56 | 0        | 15,19,21    | 1.05 | 1 (6%)   |
| 2   | NAG  | A     | 1330 | 3,2  | 14,14,15     | 0.55 | 0        | 15,19,21    | 1.19 | 1 (6%)   |
| 3   | BMA  | A     | 1331 | 2,4  | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.26 | 2 (13%)  |
| 4   | MAN  | A     | 1332 | 3,4  | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.34 | 1 (6%)   |
| 4   | MAN  | A     | 1333 | 4    | 11,11,12     | 0.59 | 0        | 15,15,17    | 1.05 | 2 (13%)  |
| 2   | NAG  | A     | 1334 | 1,2  | 14,14,15     | 0.63 | 0        | 15,19,21    | 1.26 | 1 (6%)   |
| 2   | NAG  | A     | 1335 | 3,2  | 14,14,15     | 0.51 | 0        | 15,19,21    | 1.38 | 2 (13%)  |
| 3   | BMA  | A     | 1336 | 2,4  | 11,11,12     | 0.36 | 0        | 15,15,17    | 0.76 | 0        |
| 4   | MAN  | A     | 1337 | 3    | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.11 | 2 (13%)  |
| 4   | MAN  | A     | 1338 | 3,4  | 11,11,12     | 0.62 | 0        | 15,15,17    | 0.93 | 0        |
| 4   | MAN  | A     | 1339 | 4    | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.27 | 1 (6%)   |
| 4   | MAN  | A     | 1340 | 4    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.04 | 1 (6%)   |
| 2   | NAG  | B     | 1301 | 1,2  | 14,14,15     | 0.76 | 0        | 15,19,21    | 1.74 | 3 (20%)  |
| 2   | NAG  | B     | 1302 | 3,2  | 14,14,15     | 0.56 | 0        | 15,19,21    | 1.43 | 1 (6%)   |
| 3   | BMA  | B     | 1303 | 2,4  | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.83 | 0        |
| 4   | MAN  | B     | 1304 | 3    | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.00 | 1 (6%)   |
| 2   | NAG  | B     | 1305 | 1,2  | 14,14,15     | 0.64 | 0        | 15,19,21    | 1.22 | 1 (6%)   |
| 2   | NAG  | B     | 1306 | 3,2  | 14,14,15     | 0.48 | 0        | 15,19,21    | 1.19 | 1 (6%)   |
| 3   | BMA  | B     | 1307 | 2,4  | 11,11,12     | 0.54 | 0        | 15,15,17    | 0.67 | 0        |
| 4   | MAN  | B     | 1308 | 3    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.06 | 2 (13%)  |
| 4   | MAN  | B     | 1309 | 3,4  | 11,11,12     | 0.67 | 0        | 15,15,17    | 0.96 | 1 (6%)   |
| 4   | MAN  | B     | 1310 | 4    | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 2   | NAG  | B     | 1311 | 1,2  | 14,14,15     | 0.61 | 0        | 15,19,21    | 1.13 | 1 (6%)   |
| 2   | NAG  | B     | 1312 | 3,2  | 14,14,15     | 0.53 | 0        | 15,19,21    | 1.21 | 2 (13%)  |
| 3   | BMA  | B     | 1313 | 2,4  | 11,11,12     | 0.86 | 1 (9%)   | 15,15,17    | 2.24 | 4 (26%)  |
| 4   | MAN  | B     | 1314 | 3    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.04 | 2 (13%)  |
| 2   | NAG  | B     | 1315 | 1,2  | 14,14,15     | 0.63 | 0        | 15,19,21    | 1.16 | 1 (6%)   |
| 2   | NAG  | B     | 1316 | 3,2  | 14,14,15     | 0.54 | 0        | 15,19,21    | 1.09 | 1 (6%)   |
| 3   | BMA  | B     | 1317 | 2,4  | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.64 | 3 (20%)  |
| 4   | MAN  | B     | 1318 | 3    | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.87 | 1 (6%)   |
| 4   | MAN  | B     | 1319 | 3,4  | 11,11,12     | 0.62 | 0        | 15,15,17    | 0.91 | 0        |
| 4   | MAN  | B     | 1320 | 4    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.22 | 1 (6%)   |
| 4   | MAN  | B     | 1321 | 4    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.31 | 2 (13%)  |
| 2   | NAG  | B     | 1322 | 1    | 14,14,15     | 0.59 | 0        | 15,19,21    | 1.22 | 1 (6%)   |
| 2   | NAG  | B     | 1323 | 1,2  | 14,14,15     | 0.62 | 0        | 15,19,21    | 0.95 | 1 (6%)   |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | B     | 1324 | 3,2  | 14,14,15     | 0.66 | 0        | 15,19,21    | 1.06 | 1 (6%)   |
| 3   | BMA  | B     | 1325 | 2,4  | 11,11,12     | 0.43 | 0        | 15,15,17    | 1.70 | 2 (13%)  |
| 4   | MAN  | B     | 1326 | 3    | 11,11,12     | 0.54 | 0        | 15,15,17    | 0.88 | 1 (6%)   |
| 2   | NAG  | B     | 1327 | 1    | 14,14,15     | 0.51 | 0        | 15,19,21    | 0.97 | 0        |
| 2   | NAG  | B     | 1328 | 1,2  | 14,14,15     | 0.56 | 0        | 15,19,21    | 1.05 | 1 (6%)   |
| 2   | NAG  | B     | 1329 | 3,2  | 14,14,15     | 0.54 | 0        | 15,19,21    | 1.06 | 1 (6%)   |
| 3   | BMA  | B     | 1330 | 2    | 11,11,12     | 0.48 | 0        | 15,15,17    | 1.16 | 2 (13%)  |
| 2   | NAG  | B     | 1331 | 1,2  | 14,14,15     | 0.58 | 0        | 15,19,21    | 1.05 | 1 (6%)   |
| 2   | NAG  | B     | 1332 | 3,2  | 14,14,15     | 0.56 | 0        | 15,19,21    | 1.20 | 1 (6%)   |
| 3   | BMA  | B     | 1333 | 2,4  | 11,11,12     | 0.55 | 0        | 15,15,17    | 1.25 | 2 (13%)  |
| 4   | MAN  | B     | 1334 | 3    | 11,11,12     | 0.65 | 0        | 15,15,17    | 0.87 | 1 (6%)   |
| 4   | MAN  | B     | 1335 | 3,4  | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.34 | 1 (6%)   |
| 4   | MAN  | B     | 1336 | 4    | 11,11,12     | 0.59 | 0        | 15,15,17    | 1.06 | 2 (13%)  |
| 2   | NAG  | B     | 1337 | 1,2  | 14,14,15     | 0.63 | 0        | 15,19,21    | 1.27 | 2 (13%)  |
| 2   | NAG  | B     | 1338 | 3,2  | 14,14,15     | 0.51 | 0        | 15,19,21    | 1.38 | 2 (13%)  |
| 3   | BMA  | B     | 1339 | 2,4  | 11,11,12     | 0.38 | 0        | 15,15,17    | 0.76 | 0        |
| 4   | MAN  | B     | 1340 | 3    | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.11 | 2 (13%)  |
| 4   | MAN  | B     | 1341 | 3,4  | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.92 | 0        |
| 4   | MAN  | B     | 1342 | 4    | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.28 | 1 (6%)   |
| 4   | MAN  | B     | 1343 | 4    | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.04 | 1 (6%)   |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | NAG  | A     | 1301 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1302 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1303 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1304 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1305 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1306 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1307 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1308 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1309 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1310 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1311 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1312 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 4   | MAN  | A     | 1313 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1314 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1315 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1316 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1317 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1318 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1319 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1320 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1321 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1322 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1323 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1324 | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1325 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1326 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1327 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1328 | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1329 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1330 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1331 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1332 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1333 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | A     | 1334 | 1,2  | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | A     | 1335 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | A     | 1336 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1337 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1338 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1339 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | A     | 1340 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1301 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1302 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1303 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1304 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1305 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1306 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1307 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1308 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1309 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1310 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1311 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1312 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1313 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1314 | 3    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 2   | NAG  | B     | 1315 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1316 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1317 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1318 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1319 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1320 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1321 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1322 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1323 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1324 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1325 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1326 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1327 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1328 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1329 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1330 | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1331 | 1,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1332 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1333 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1334 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1335 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1336 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | B     | 1337 | 1,2  | 1/1/5/7 | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | B     | 1338 | 3,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | B     | 1339 | 2,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1340 | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1341 | 3,4  | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1342 | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 4   | MAN  | B     | 1343 | 4    | -       | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 3   | A     | 1312 | BMA  | C2-C3 | 2.30 | 1.55        | 1.52     |
| 3   | B     | 1313 | BMA  | C2-C3 | 2.31 | 1.55        | 1.52     |

All (107) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | B     | 1332 | NAG  | O5-C5-C4 | -2.42 | 106.13      | 110.13   |
| 2   | A     | 1330 | NAG  | O5-C5-C4 | -2.39 | 106.17      | 110.13   |
| 2   | B     | 1337 | NAG  | O5-C5-C4 | -2.27 | 106.38      | 110.13   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 2   | A     | 1334 | NAG  | O5-C5-C4 | -2.25 | 106.40      | 110.13   |
| 2   | B     | 1337 | NAG  | C4-C3-C2 | 2.03  | 114.49      | 111.34   |
| 3   | A     | 1312 | BMA  | C1-O5-C5 | 2.03  | 115.13      | 112.14   |
| 3   | B     | 1313 | BMA  | C1-O5-C5 | 2.04  | 115.13      | 112.14   |
| 3   | A     | 1331 | BMA  | C2-C3-C4 | 2.04  | 114.60      | 111.05   |
| 4   | B     | 1318 | MAN  | C1-O5-C5 | 2.04  | 115.14      | 112.14   |
| 3   | B     | 1333 | BMA  | C2-C3-C4 | 2.05  | 114.62      | 111.05   |
| 4   | A     | 1317 | MAN  | C1-O5-C5 | 2.07  | 115.18      | 112.14   |
| 4   | A     | 1337 | MAN  | C1-O5-C5 | 2.11  | 115.25      | 112.14   |
| 3   | A     | 1312 | BMA  | O5-C1-C2 | 2.12  | 114.28      | 110.89   |
| 3   | B     | 1313 | BMA  | O5-C1-C2 | 2.14  | 114.32      | 110.89   |
| 4   | B     | 1314 | MAN  | C1-O5-C5 | 2.15  | 115.30      | 112.14   |
| 4   | B     | 1340 | MAN  | C1-O5-C5 | 2.16  | 115.32      | 112.14   |
| 4   | A     | 1313 | MAN  | C1-O5-C5 | 2.18  | 115.35      | 112.14   |
| 2   | B     | 1316 | NAG  | C3-C4-C5 | 2.18  | 114.12      | 110.23   |
| 2   | A     | 1315 | NAG  | C3-C4-C5 | 2.22  | 114.19      | 110.23   |
| 3   | B     | 1313 | BMA  | C2-C3-C4 | 2.25  | 114.97      | 111.05   |
| 4   | B     | 1314 | MAN  | C1-C2-C3 | 2.28  | 112.32      | 109.55   |
| 4   | B     | 1336 | MAN  | C1-O5-C5 | 2.29  | 115.50      | 112.14   |
| 3   | A     | 1312 | BMA  | C2-C3-C4 | 2.29  | 115.04      | 111.05   |
| 4   | A     | 1333 | MAN  | C1-O5-C5 | 2.30  | 115.52      | 112.14   |
| 2   | A     | 1301 | NAG  | C2-N2-C7 | 2.32  | 126.12      | 123.11   |
| 4   | A     | 1313 | MAN  | C1-C2-C3 | 2.33  | 112.37      | 109.55   |
| 2   | B     | 1301 | NAG  | C2-N2-C7 | 2.33  | 126.13      | 123.11   |
| 2   | B     | 1312 | NAG  | C4-C3-C2 | 2.33  | 114.96      | 111.34   |
| 2   | A     | 1311 | NAG  | C4-C3-C2 | 2.33  | 114.96      | 111.34   |
| 4   | B     | 1334 | MAN  | C1-C2-C3 | 2.40  | 112.46      | 109.55   |
| 4   | B     | 1326 | MAN  | C1-O5-C5 | 2.40  | 115.67      | 112.14   |
| 2   | A     | 1305 | NAG  | C4-C3-C2 | 2.43  | 115.12      | 111.34   |
| 4   | B     | 1308 | MAN  | C1-C2-C3 | 2.47  | 112.54      | 109.55   |
| 2   | B     | 1305 | NAG  | C4-C3-C2 | 2.49  | 115.20      | 111.34   |
| 2   | A     | 1327 | NAG  | C4-C3-C2 | 2.61  | 115.39      | 111.34   |
| 2   | B     | 1329 | NAG  | C4-C3-C2 | 2.61  | 115.40      | 111.34   |
| 4   | B     | 1308 | MAN  | C1-O5-C5 | 2.63  | 116.01      | 112.14   |
| 2   | B     | 1324 | NAG  | C4-C3-C2 | 2.64  | 115.44      | 111.34   |
| 2   | B     | 1338 | NAG  | C4-C3-C2 | 2.64  | 115.44      | 111.34   |
| 2   | A     | 1335 | NAG  | C4-C3-C2 | 2.65  | 115.45      | 111.34   |
| 2   | A     | 1322 | NAG  | C4-C3-C2 | 2.65  | 115.46      | 111.34   |
| 4   | A     | 1304 | MAN  | C1-C2-C3 | 2.67  | 112.79      | 109.55   |
| 2   | B     | 1323 | NAG  | C4-C3-C2 | 2.68  | 115.50      | 111.34   |
| 2   | A     | 1323 | NAG  | C4-C3-C2 | 2.68  | 115.51      | 111.34   |
| 4   | B     | 1304 | MAN  | C1-C2-C3 | 2.69  | 112.81      | 109.55   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4   | A     | 1308 | MAN  | C1-C2-C3 | 2.70 | 112.82      | 109.55   |
| 4   | B     | 1309 | MAN  | C1-C2-C3 | 2.70 | 112.83      | 109.55   |
| 4   | A     | 1333 | MAN  | C1-C2-C3 | 2.71 | 112.83      | 109.55   |
| 2   | A     | 1311 | NAG  | C1-O5-C5 | 2.74 | 116.18      | 112.14   |
| 4   | B     | 1336 | MAN  | C1-C2-C3 | 2.76 | 112.89      | 109.55   |
| 3   | A     | 1328 | BMA  | C1-C2-C3 | 2.76 | 112.89      | 109.55   |
| 3   | B     | 1330 | BMA  | C1-C2-C3 | 2.77 | 112.91      | 109.55   |
| 2   | B     | 1312 | NAG  | C1-O5-C5 | 2.78 | 116.23      | 112.14   |
| 3   | A     | 1316 | BMA  | C2-C3-C4 | 2.84 | 116.00      | 111.05   |
| 4   | A     | 1340 | MAN  | C1-C2-C3 | 2.87 | 113.03      | 109.55   |
| 3   | B     | 1317 | BMA  | C2-C3-C4 | 2.87 | 116.05      | 111.05   |
| 4   | B     | 1343 | MAN  | C1-C2-C3 | 2.89 | 113.05      | 109.55   |
| 2   | A     | 1326 | NAG  | C4-C3-C2 | 2.90 | 115.84      | 111.34   |
| 2   | A     | 1321 | NAG  | C4-C3-C2 | 2.90 | 115.85      | 111.34   |
| 2   | B     | 1328 | NAG  | C4-C3-C2 | 2.92 | 115.86      | 111.34   |
| 2   | A     | 1335 | NAG  | C3-C4-C5 | 2.92 | 115.43      | 110.23   |
| 2   | B     | 1338 | NAG  | C3-C4-C5 | 2.93 | 115.45      | 110.23   |
| 3   | A     | 1328 | BMA  | C1-O5-C5 | 2.93 | 116.45      | 112.14   |
| 2   | B     | 1322 | NAG  | C4-C3-C2 | 2.94 | 115.90      | 111.34   |
| 4   | B     | 1310 | MAN  | C1-C2-C3 | 2.98 | 113.17      | 109.55   |
| 3   | B     | 1330 | BMA  | C1-O5-C5 | 2.99 | 116.54      | 112.14   |
| 3   | B     | 1333 | BMA  | C3-C4-C5 | 3.00 | 115.57      | 110.23   |
| 4   | B     | 1340 | MAN  | C1-C2-C3 | 3.01 | 113.20      | 109.55   |
| 3   | A     | 1331 | BMA  | C3-C4-C5 | 3.02 | 115.60      | 110.23   |
| 4   | A     | 1309 | MAN  | C1-C2-C3 | 3.02 | 113.21      | 109.55   |
| 4   | B     | 1321 | MAN  | C1-C2-C3 | 3.03 | 113.22      | 109.55   |
| 4   | A     | 1337 | MAN  | C1-C2-C3 | 3.04 | 113.23      | 109.55   |
| 4   | A     | 1320 | MAN  | C1-C2-C3 | 3.05 | 113.25      | 109.55   |
| 2   | B     | 1301 | NAG  | C3-C4-C5 | 3.06 | 115.68      | 110.23   |
| 2   | B     | 1331 | NAG  | C1-O5-C5 | 3.06 | 116.64      | 112.14   |
| 2   | A     | 1329 | NAG  | C1-O5-C5 | 3.06 | 116.64      | 112.14   |
| 2   | A     | 1301 | NAG  | C3-C4-C5 | 3.08 | 115.72      | 110.23   |
| 4   | B     | 1310 | MAN  | C1-O5-C5 | 3.13 | 116.74      | 112.14   |
| 4   | A     | 1309 | MAN  | C1-O5-C5 | 3.13 | 116.74      | 112.14   |
| 3   | B     | 1317 | BMA  | C1-C2-C3 | 3.28 | 113.53      | 109.55   |
| 3   | A     | 1316 | BMA  | C1-C2-C3 | 3.33 | 113.59      | 109.55   |
| 4   | B     | 1321 | MAN  | C1-O5-C5 | 3.40 | 117.14      | 112.14   |
| 4   | A     | 1320 | MAN  | C1-O5-C5 | 3.42 | 117.16      | 112.14   |
| 2   | A     | 1314 | NAG  | C4-C3-C2 | 3.53 | 116.82      | 111.34   |
| 2   | B     | 1315 | NAG  | C4-C3-C2 | 3.55 | 116.84      | 111.34   |
| 4   | A     | 1339 | MAN  | C1-C2-C3 | 3.60 | 113.92      | 109.55   |
| 4   | B     | 1342 | MAN  | C1-C2-C3 | 3.60 | 113.92      | 109.55   |

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| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 2   | A     | 1310 | NAG  | C4-C3-C2 | 3.64 | 116.99      | 111.34   |
| 2   | B     | 1311 | NAG  | C4-C3-C2 | 3.64 | 116.99      | 111.34   |
| 2   | A     | 1306 | NAG  | C1-O5-C5 | 3.69 | 117.57      | 112.14   |
| 2   | B     | 1306 | NAG  | C1-O5-C5 | 3.71 | 117.59      | 112.14   |
| 3   | B     | 1317 | BMA  | C3-C4-C5 | 3.73 | 116.87      | 110.23   |
| 3   | A     | 1316 | BMA  | C3-C4-C5 | 3.76 | 116.93      | 110.23   |
| 3   | B     | 1325 | BMA  | C1-C2-C3 | 3.89 | 114.27      | 109.55   |
| 3   | A     | 1324 | BMA  | C1-C2-C3 | 3.89 | 114.27      | 109.55   |
| 4   | A     | 1319 | MAN  | C1-O5-C5 | 3.90 | 117.88      | 112.14   |
| 4   | B     | 1320 | MAN  | C1-O5-C5 | 3.94 | 117.93      | 112.14   |
| 3   | A     | 1324 | BMA  | C1-O5-C5 | 4.27 | 118.43      | 112.14   |
| 3   | B     | 1325 | BMA  | C1-O5-C5 | 4.31 | 118.47      | 112.14   |
| 4   | B     | 1335 | MAN  | C1-C2-C3 | 4.34 | 114.81      | 109.55   |
| 4   | A     | 1332 | MAN  | C1-C2-C3 | 4.34 | 114.81      | 109.55   |
| 2   | B     | 1302 | NAG  | C4-C3-C2 | 4.40 | 118.16      | 111.34   |
| 2   | A     | 1302 | NAG  | C4-C3-C2 | 4.42 | 118.20      | 111.34   |
| 2   | B     | 1301 | NAG  | C4-C3-C2 | 4.67 | 118.58      | 111.34   |
| 2   | A     | 1301 | NAG  | C4-C3-C2 | 4.67 | 118.58      | 111.34   |
| 3   | A     | 1312 | BMA  | C1-C2-C3 | 7.42 | 118.54      | 109.55   |
| 3   | B     | 1313 | BMA  | C1-C2-C3 | 7.45 | 118.58      | 109.55   |

All (2) chirality outliers are listed below:

| Mol | Chain | Res  | Type | Atom |
|-----|-------|------|------|------|
| 2   | B     | 1337 | NAG  | C1   |
| 2   | A     | 1334 | NAG  | C1   |

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 2   | A     | 1301 | NAG  | 1       | 0            |
| 2   | A     | 1314 | NAG  | 3       | 0            |
| 2   | A     | 1315 | NAG  | 1       | 0            |
| 4   | A     | 1320 | MAN  | 1       | 0            |
| 2   | B     | 1301 | NAG  | 1       | 0            |
| 2   | B     | 1315 | NAG  | 1       | 0            |
| 2   | B     | 1316 | NAG  | 1       | 0            |
| 4   | B     | 1321 | MAN  | 1       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|-----|-------|------------------|
| 1   | B     | 7                |
| 1   | A     | 6                |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1     | A     | 1147:ASP  | C      | 1148:PRO  | N      | 3.75         |
| 1     | A     | 1043:THR  | C      | 1044:GLU  | N      | 2.21         |
| 1     | B     | 658:ASN   | C      | 659:CYS   | N      | 2.12         |
| 1     | A     | 704:CYS   | C      | 705:PRO   | N      | 2.07         |
| 1     | A     | 658:ASN   | C      | 659:CYS   | N      | 2.04         |
| 1     | B     | 561:CYS   | C      | 562:VAL   | N      | 1.99         |
| 1     | B     | 1147:ASP  | C      | 1148:PRO  | N      | 1.96         |
| 1     | B     | 859:CYS   | C      | 860:THR   | N      | 1.76         |
| 1     | A     | 510:VAL   | C      | 511:GLU   | N      | 1.75         |
| 1     | B     | 1043:THR  | C      | 1044:GLU  | N      | 1.64         |
| 1     | B     | 957:VAL   | C      | 958:THR   | N      | 1.61         |
| 1     | B     | 510:VAL   | C      | 511:GLU   | N      | 1.19         |
| 1     | A     | 859:CYS   | C      | 860:THR   | N      | 0.89         |

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|------------|-----|-----------------------|-------|
| 1   | A     | 1171/1212 (96%) | 8.80   | 1099 (93%) | 0 1 | 241, 248, 360, 360    | 0     |
| 1   | B     | 1171/1212 (96%) | 9.89   | 1117 (95%) | 0 1 | 243, 247, 397, 397    | 0     |
| All | All   | 2342/2424 (96%) | 9.35   | 2216 (94%) | 0 1 | 241, 248, 365, 397    | 0     |

All (2216) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1073 | THR  | 44.3 |
| 1   | B     | 1068 | GLY  | 40.0 |
| 1   | B     | 835  | CYS  | 37.1 |
| 1   | A     | 1070 | ASN  | 36.1 |
| 1   | B     | 1203 | GLN  | 35.6 |
| 1   | B     | 1200 | SER  | 35.0 |
| 1   | B     | 1173 | ASN  | 34.3 |
| 1   | A     | 1083 | TYR  | 33.7 |
| 1   | B     | 1208 | ALA  | 33.3 |
| 1   | B     | 1171 | GLY  | 33.3 |
| 1   | B     | 1073 | THR  | 33.2 |
| 1   | A     | 1129 | ASP  | 32.4 |
| 1   | B     | 1106 | SER  | 32.4 |
| 1   | B     | 1105 | PRO  | 32.3 |
| 1   | B     | 1108 | ASP  | 32.1 |
| 1   | B     | 1043 | THR  | 31.5 |
| 1   | B     | 1082 | LYS  | 31.4 |
| 1   | B     | 827  | GLY  | 30.7 |
| 1   | B     | 1182 | SER  | 30.4 |
| 1   | B     | 1122 | ASP  | 30.4 |
| 1   | A     | 1123 | GLU  | 30.1 |
| 1   | B     | 1148 | PRO  | 30.0 |
| 1   | A     | 1045 | ASP  | 30.0 |
| 1   | B     | 1123 | GLU  | 29.9 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1122 | ASP  | 29.8 |
| 1   | A     | 970  | PRO  | 29.7 |
| 1   | B     | 829  | CYS  | 29.4 |
| 1   | B     | 1083 | TYR  | 29.4 |
| 1   | B     | 1107 | ILE  | 29.0 |
| 1   | A     | 1043 | THR  | 27.8 |
| 1   | B     | 1070 | ASN  | 27.7 |
| 1   | A     | 555  | ALA  | 27.7 |
| 1   | B     | 1119 | GLU  | 27.5 |
| 1   | B     | 675  | CYS  | 27.4 |
| 1   | B     | 1080 | ARG  | 27.2 |
| 1   | A     | 987  | GLY  | 27.0 |
| 1   | B     | 1087 | GLU  | 26.9 |
| 1   | A     | 1082 | LYS  | 26.9 |
| 1   | B     | 1170 | LYS  | 26.9 |
| 1   | B     | 1202 | THR  | 26.7 |
| 1   | A     | 1072 | ALA  | 26.6 |
| 1   | B     | 1207 | GLU  | 26.6 |
| 1   | A     | 872  | GLY  | 26.4 |
| 1   | B     | 1061 | GLY  | 26.2 |
| 1   | B     | 1109 | ASN  | 26.1 |
| 1   | B     | 969  | GLY  | 26.1 |
| 1   | B     | 1089 | GLU  | 25.9 |
| 1   | B     | 1045 | ASP  | 25.8 |
| 1   | A     | 343  | GLN  | 25.7 |
| 1   | B     | 1178 | ALA  | 25.7 |
| 1   | B     | 826  | CYS  | 25.7 |
| 1   | B     | 1176 | PRO  | 25.5 |
| 1   | B     | 1147 | ASP  | 25.4 |
| 1   | B     | 970  | PRO  | 25.4 |
| 1   | B     | 507  | GLN  | 25.4 |
| 1   | B     | 1166 | PRO  | 25.3 |
| 1   | B     | 1174 | LEU  | 25.2 |
| 1   | B     | 1081 | ALA  | 25.1 |
| 1   | B     | 1058 | ASN  | 25.0 |
| 1   | B     | 1046 | PRO  | 24.9 |
| 1   | A     | 675  | CYS  | 24.9 |
| 1   | B     | 1118 | GLY  | 24.9 |
| 1   | B     | 90   | ASN  | 24.8 |
| 1   | A     | 1084 | GLY  | 24.7 |
| 1   | B     | 1077 | PRO  | 24.7 |
| 1   | B     | 1069 | THR  | 24.6 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1074 | VAL  | 24.3 |
| 1   | B     | 836  | SER  | 24.2 |
| 1   | B     | 1149 | VAL  | 23.9 |
| 1   | B     | 1067 | THR  | 23.8 |
| 1   | B     | 530  | CYS  | 23.8 |
| 1   | B     | 807  | CYS  | 23.8 |
| 1   | A     | 966  | PRO  | 23.7 |
| 1   | A     | 1016 | GLY  | 23.7 |
| 1   | B     | 1150 | LEU  | 23.6 |
| 1   | B     | 1198 | THR  | 23.5 |
| 1   | B     | 1226 | PHE  | 23.4 |
| 1   | B     | 1177 | PRO  | 23.4 |
| 1   | B     | 1175 | LEU  | 23.1 |
| 1   | B     | 160  | SER  | 23.1 |
| 1   | A     | 658  | ASN  | 23.0 |
| 1   | B     | 1104 | ALA  | 23.0 |
| 1   | B     | 545  | CYS  | 23.0 |
| 1   | A     | 1178 | ALA  | 22.8 |
| 1   | A     | 530  | CYS  | 22.8 |
| 1   | B     | 698  | VAL  | 22.7 |
| 1   | B     | 1129 | ASP  | 22.5 |
| 1   | B     | 1121 | PRO  | 22.5 |
| 1   | B     | 876  | GLY  | 22.5 |
| 1   | A     | 873  | PRO  | 22.5 |
| 1   | B     | 1060 | GLY  | 22.4 |
| 1   | B     | 987  | GLY  | 22.4 |
| 1   | B     | 658  | ASN  | 22.3 |
| 1   | A     | 897  | GLY  | 22.2 |
| 1   | A     | 150  | PRO  | 22.2 |
| 1   | A     | 1094 | VAL  | 22.1 |
| 1   | B     | 1084 | GLY  | 22.0 |
| 1   | A     | 1069 | THR  | 22.0 |
| 1   | B     | 677  | TRP  | 22.0 |
| 1   | A     | 531  | GLY  | 22.0 |
| 1   | A     | 988  | SER  | 22.0 |
| 1   | B     | 1056 | SER  | 21.9 |
| 1   | B     | 1145 | TYR  | 21.9 |
| 1   | A     | 1112 | ARG  | 21.9 |
| 1   | B     | 1066 | VAL  | 21.8 |
| 1   | B     | 919  | VAL  | 21.8 |
| 1   | B     | 1218 | THR  | 21.8 |
| 1   | A     | 1099 | THR  | 21.7 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1120 | ARG  | 21.7 |
| 1   | A     | 1093 | MET  | 21.5 |
| 1   | A     | 1074 | VAL  | 21.5 |
| 1   | A     | 529  | HIS  | 21.4 |
| 1   | B     | 1201 | GLU  | 21.2 |
| 1   | B     | 161  | VAL  | 21.1 |
| 1   | B     | 1165 | SER  | 21.1 |
| 1   | A     | 527  | ASP  | 21.1 |
| 1   | B     | 808  | PRO  | 21.1 |
| 1   | B     | 968  | ARG  | 21.1 |
| 1   | B     | 1047 | THR  | 21.0 |
| 1   | B     | 848  | SER  | 21.0 |
| 1   | B     | 817  | CYS  | 21.0 |
| 1   | B     | 665  | CYS  | 21.0 |
| 1   | A     | 1046 | PRO  | 21.0 |
| 1   | B     | 877  | GLY  | 21.0 |
| 1   | A     | 1018 | THR  | 20.9 |
| 1   | B     | 410  | ASN  | 20.9 |
| 1   | A     | 1068 | GLY  | 20.8 |
| 1   | B     | 1088 | ARG  | 20.8 |
| 1   | B     | 1092 | CYS  | 20.8 |
| 1   | B     | 308  | ARG  | 20.8 |
| 1   | B     | 1227 | SER  | 20.8 |
| 1   | A     | 1029 | ASN  | 20.6 |
| 1   | B     | 1144 | TYR  | 20.6 |
| 1   | B     | 159  | SER  | 20.5 |
| 1   | B     | 1206 | CYS  | 20.5 |
| 1   | B     | 555  | ALA  | 20.5 |
| 1   | B     | 1098 | THR  | 20.5 |
| 1   | A     | 1092 | CYS  | 20.4 |
| 1   | B     | 511  | GLU  | 20.4 |
| 1   | B     | 828  | TRP  | 20.3 |
| 1   | A     | 1148 | PRO  | 20.3 |
| 1   | B     | 529  | HIS  | 20.2 |
| 1   | B     | 1059 | SER  | 20.2 |
| 1   | A     | 1081 | ALA  | 20.2 |
| 1   | A     | 1056 | SER  | 20.1 |
| 1   | B     | 1168 | ILE  | 20.1 |
| 1   | B     | 527  | ASP  | 20.0 |
| 1   | B     | 1072 | ALA  | 20.0 |
| 1   | B     | 1127 | ILE  | 20.0 |
| 1   | A     | 1097 | ASP  | 19.9 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1199 | VAL  | 19.9 |
| 1   | B     | 686  | ASN  | 19.8 |
| 1   | A     | 1071 | LEU  | 19.8 |
| 1   | A     | 1109 | ASN  | 19.8 |
| 1   | B     | 1100 | MET  | 19.8 |
| 1   | A     | 196  | PHE  | 19.7 |
| 1   | A     | 969  | GLY  | 19.7 |
| 1   | B     | 806  | LYS  | 19.7 |
| 1   | B     | 668  | CYS  | 19.5 |
| 1   | B     | 1172 | ARG  | 19.5 |
| 1   | B     | 540  | SER  | 19.5 |
| 1   | B     | 1079 | ILE  | 19.5 |
| 1   | B     | 1050 | ARG  | 19.5 |
| 1   | A     | 554  | PHE  | 19.4 |
| 1   | B     | 89   | ASP  | 19.4 |
| 1   | B     | 1197 | LEU  | 19.4 |
| 1   | B     | 1071 | LEU  | 19.3 |
| 1   | B     | 849  | TRP  | 19.3 |
| 1   | A     | 90   | ASN  | 19.3 |
| 1   | A     | 159  | SER  | 19.2 |
| 1   | B     | 1062 | THR  | 19.1 |
| 1   | B     | 1169 | LEU  | 19.1 |
| 1   | B     | 669  | VAL  | 19.1 |
| 1   | A     | 1017 | HIS  | 19.0 |
| 1   | B     | 685  | THR  | 18.9 |
| 1   | B     | 878  | THR  | 18.9 |
| 1   | A     | 971  | LEU  | 18.7 |
| 1   | A     | 826  | CYS  | 18.7 |
| 1   | A     | 835  | CYS  | 18.7 |
| 1   | A     | 989  | ASP  | 18.6 |
| 1   | B     | 333  | GLU  | 18.5 |
| 1   | A     | 1047 | THR  | 18.5 |
| 1   | B     | 1044 | GLU  | 18.5 |
| 1   | B     | 1093 | MET  | 18.5 |
| 1   | B     | 1094 | VAL  | 18.4 |
| 1   | A     | 1177 | PRO  | 18.4 |
| 1   | A     | 1019 | PRO  | 18.4 |
| 1   | A     | 965  | SER  | 18.3 |
| 1   | A     | 540  | SER  | 18.3 |
| 1   | A     | 1067 | THR  | 18.3 |
| 1   | B     | 684  | CYS  | 18.2 |
| 1   | B     | 1210 | ASN  | 18.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1176 | PRO  | 18.2 |
| 1   | A     | 541  | ARG  | 18.1 |
| 1   | A     | 1130 | ASN  | 18.1 |
| 1   | A     | 545  | CYS  | 18.1 |
| 1   | A     | 410  | ASN  | 18.0 |
| 1   | A     | 1141 | SER  | 18.0 |
| 1   | A     | 533  | CYS  | 18.0 |
| 1   | A     | 871  | THR  | 17.9 |
| 1   | A     | 342  | GLY  | 17.9 |
| 1   | B     | 1221 | ALA  | 17.9 |
| 1   | B     | 1204 | LEU  | 17.8 |
| 1   | A     | 1096 | ASN  | 17.8 |
| 1   | B     | 1219 | VAL  | 17.8 |
| 1   | A     | 1146 | PRO  | 17.8 |
| 1   | B     | 1042 | TYR  | 17.8 |
| 1   | B     | 879  | ARG  | 17.7 |
| 1   | A     | 1023 | PRO  | 17.7 |
| 1   | B     | 1041 | ASN  | 17.7 |
| 1   | A     | 91   | GLU  | 17.7 |
| 1   | A     | 1100 | MET  | 17.7 |
| 1   | B     | 1097 | ASP  | 17.6 |
| 1   | A     | 1080 | ARG  | 17.6 |
| 1   | A     | 698  | VAL  | 17.6 |
| 1   | A     | 160  | SER  | 17.5 |
| 1   | B     | 875  | GLN  | 17.5 |
| 1   | A     | 957  | VAL  | 17.5 |
| 1   | B     | 1102 | CYS  | 17.4 |
| 1   | B     | 888  | GLY  | 17.4 |
| 1   | B     | 1222 | GLY  | 17.4 |
| 1   | A     | 632  | ASP  | 17.4 |
| 1   | A     | 1182 | SER  | 17.4 |
| 1   | A     | 1145 | TYR  | 17.3 |
| 1   | B     | 40   | ARG  | 17.3 |
| 1   | A     | 919  | VAL  | 17.3 |
| 1   | B     | 1103 | ARG  | 17.2 |
| 1   | A     | 807  | CYS  | 17.2 |
| 1   | A     | 899  | HIS  | 17.1 |
| 1   | A     | 197  | PRO  | 17.1 |
| 1   | B     | 91   | GLU  | 17.1 |
| 1   | A     | 276  | PHE  | 17.0 |
| 1   | B     | 1143 | LEU  | 17.0 |
| 1   | A     | 1015 | PRO  | 17.0 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 869  | PRO  | 17.0 |
| 1   | A     | 434  | ALA  | 17.0 |
| 1   | A     | 1121 | PRO  | 17.0 |
| 1   | B     | 1078 | ARG  | 17.0 |
| 1   | B     | 859  | CYS  | 16.9 |
| 1   | A     | 858  | ARG  | 16.9 |
| 1   | B     | 873  | PRO  | 16.9 |
| 1   | B     | 1023 | PRO  | 16.8 |
| 1   | B     | 696  | GLY  | 16.8 |
| 1   | B     | 676  | HIS  | 16.8 |
| 1   | B     | 988  | SER  | 16.8 |
| 1   | A     | 633  | GLN  | 16.7 |
| 1   | B     | 967  | SER  | 16.6 |
| 1   | A     | 1030 | ARG  | 16.6 |
| 1   | A     | 870  | GLU  | 16.6 |
| 1   | B     | 1183 | ARG  | 16.6 |
| 1   | A     | 1066 | VAL  | 16.6 |
| 1   | B     | 805  | TYR  | 16.5 |
| 1   | B     | 975  | THR  | 16.5 |
| 1   | A     | 333  | GLU  | 16.5 |
| 1   | A     | 1128 | MET  | 16.5 |
| 1   | B     | 541  | ARG  | 16.4 |
| 1   | A     | 1140 | SER  | 16.4 |
| 1   | B     | 632  | ASP  | 16.4 |
| 1   | B     | 1117 | LEU  | 16.4 |
| 1   | B     | 1205 | LEU  | 16.4 |
| 1   | A     | 1111 | LYS  | 16.4 |
| 1   | A     | 986  | ALA  | 16.4 |
| 1   | B     | 978  | GLY  | 16.4 |
| 1   | A     | 161  | VAL  | 16.3 |
| 1   | B     | 1022 | ALA  | 16.3 |
| 1   | B     | 1055 | TRP  | 16.3 |
| 1   | A     | 827  | GLY  | 16.3 |
| 1   | B     | 673  | PHE  | 16.2 |
| 1   | A     | 1102 | CYS  | 16.2 |
| 1   | B     | 273  | GLU  | 16.2 |
| 1   | A     | 193  | SER  | 16.2 |
| 1   | A     | 1147 | ASP  | 16.2 |
| 1   | B     | 1086 | ILE  | 16.1 |
| 1   | A     | 1044 | GLU  | 16.1 |
| 1   | A     | 817  | CYS  | 16.1 |
| 1   | B     | 924  | ASP  | 16.1 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1099 | THR  | 16.0 |
| 1   | B     | 986  | ALA  | 16.0 |
| 1   | B     | 434  | ALA  | 16.0 |
| 1   | A     | 878  | THR  | 15.9 |
| 1   | B     | 631  | GLY  | 15.9 |
| 1   | B     | 510  | VAL  | 15.9 |
| 1   | A     | 1089 | GLU  | 15.9 |
| 1   | A     | 556  | SER  | 15.8 |
| 1   | B     | 531  | GLY  | 15.8 |
| 1   | B     | 1128 | MET  | 15.8 |
| 1   | A     | 1183 | ARG  | 15.8 |
| 1   | A     | 657  | TYR  | 15.8 |
| 1   | A     | 859  | CYS  | 15.8 |
| 1   | A     | 133  | GLN  | 15.8 |
| 1   | A     | 1062 | THR  | 15.6 |
| 1   | B     | 1049 | LEU  | 15.6 |
| 1   | B     | 1065 | THR  | 15.6 |
| 1   | A     | 1088 | ARG  | 15.6 |
| 1   | B     | 1195 | CYS  | 15.6 |
| 1   | A     | 1058 | ASN  | 15.6 |
| 1   | B     | 1125 | GLY  | 15.6 |
| 1   | A     | 506  | THR  | 15.6 |
| 1   | A     | 879  | ARG  | 15.6 |
| 1   | B     | 664  | SER  | 15.5 |
| 1   | B     | 1090 | ASN  | 15.5 |
| 1   | A     | 553  | ARG  | 15.4 |
| 1   | A     | 978  | GLY  | 15.4 |
| 1   | A     | 1042 | TYR  | 15.4 |
| 1   | B     | 414  | GLY  | 15.4 |
| 1   | B     | 772  | TYR  | 15.4 |
| 1   | B     | 699  | ASN  | 15.3 |
| 1   | B     | 1152 | PRO  | 15.3 |
| 1   | A     | 874  | ARG  | 15.3 |
| 1   | A     | 1181 | ASN  | 15.3 |
| 1   | A     | 431  | GLY  | 15.3 |
| 1   | A     | 975  | THR  | 15.3 |
| 1   | A     | 1077 | PRO  | 15.2 |
| 1   | B     | 513  | CYS  | 15.2 |
| 1   | B     | 1167 | LEU  | 15.2 |
| 1   | B     | 553  | ARG  | 15.2 |
| 1   | A     | 1095 | TYR  | 15.2 |
| 1   | A     | 699  | ASN  | 15.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 425  | PHE  | 15.2 |
| 1   | B     | 1185 | ASN  | 15.1 |
| 1   | A     | 433  | THR  | 15.1 |
| 1   | A     | 278  | SER  | 15.1 |
| 1   | A     | 511  | GLU  | 15.1 |
| 1   | A     | 308  | ARG  | 15.1 |
| 1   | B     | 670  | ASN  | 15.1 |
| 1   | B     | 678  | CYS  | 15.1 |
| 1   | A     | 676  | HIS  | 15.0 |
| 1   | B     | 1186 | TYR  | 15.0 |
| 1   | B     | 318  | PRO  | 15.0 |
| 1   | B     | 1130 | ASN  | 15.0 |
| 1   | B     | 332  | GLU  | 15.0 |
| 1   | B     | 659  | CYS  | 14.9 |
| 1   | A     | 936  | GLU  | 14.9 |
| 1   | B     | 1019 | PRO  | 14.9 |
| 1   | A     | 968  | ARG  | 14.9 |
| 1   | A     | 851  | HIS  | 14.9 |
| 1   | B     | 1209 | PRO  | 14.9 |
| 1   | B     | 948  | ALA  | 14.9 |
| 1   | A     | 677  | TRP  | 14.8 |
| 1   | B     | 858  | ARG  | 14.9 |
| 1   | B     | 1052 | ASP  | 14.9 |
| 1   | B     | 343  | GLN  | 14.8 |
| 1   | A     | 673  | PHE  | 14.8 |
| 1   | B     | 512  | SER  | 14.8 |
| 1   | B     | 1146 | PRO  | 14.8 |
| 1   | A     | 857  | SER  | 14.8 |
| 1   | B     | 680  | TYR  | 14.8 |
| 1   | B     | 130  | SER  | 14.8 |
| 1   | A     | 382  | SER  | 14.7 |
| 1   | B     | 1131 | VAL  | 14.7 |
| 1   | A     | 277  | THR  | 14.7 |
| 1   | B     | 1018 | THR  | 14.7 |
| 1   | A     | 1151 | GLU  | 14.7 |
| 1   | B     | 131  | ALA  | 14.7 |
| 1   | A     | 923  | GLY  | 14.6 |
| 1   | A     | 1020 | GLY  | 14.6 |
| 1   | B     | 554  | PHE  | 14.6 |
| 1   | A     | 1057 | ILE  | 14.6 |
| 1   | B     | 966  | PRO  | 14.6 |
| 1   | A     | 1125 | GLY  | 14.5 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 274  | HIS  | 14.5 |
| 1   | A     | 89   | ASP  | 14.5 |
| 1   | B     | 1039 | LYS  | 14.5 |
| 1   | A     | 1075 | ARG  | 14.5 |
| 1   | A     | 1098 | THR  | 14.5 |
| 1   | B     | 633  | GLN  | 14.5 |
| 1   | A     | 1007 | ARG  | 14.5 |
| 1   | A     | 74   | GLY  | 14.4 |
| 1   | A     | 1150 | LEU  | 14.4 |
| 1   | B     | 885  | GLU  | 14.4 |
| 1   | B     | 150  | PRO  | 14.3 |
| 1   | B     | 630  | GLN  | 14.3 |
| 1   | A     | 814  | CYS  | 14.3 |
| 1   | B     | 196  | PHE  | 14.3 |
| 1   | B     | 657  | TYR  | 14.3 |
| 1   | A     | 500  | MET  | 14.2 |
| 1   | A     | 956  | PHE  | 14.2 |
| 1   | B     | 74   | GLY  | 14.2 |
| 1   | B     | 1085 | GLY  | 14.2 |
| 1   | A     | 808  | PRO  | 14.1 |
| 1   | A     | 149  | GLU  | 14.1 |
| 1   | A     | 536  | HIS  | 14.1 |
| 1   | B     | 819  | LYS  | 14.1 |
| 1   | A     | 392  | GLY  | 14.1 |
| 1   | A     | 1107 | ILE  | 14.1 |
| 1   | B     | 923  | GLY  | 14.1 |
| 1   | A     | 528  | PRO  | 14.1 |
| 1   | B     | 857  | SER  | 14.1 |
| 1   | B     | 1021 | SER  | 14.0 |
| 1   | B     | 1124 | ILE  | 14.0 |
| 1   | A     | 811  | ARG  | 14.0 |
| 1   | A     | 818  | LEU  | 14.0 |
| 1   | B     | 354  | ALA  | 13.9 |
| 1   | B     | 1075 | ARG  | 13.9 |
| 1   | B     | 278  | SER  | 13.9 |
| 1   | A     | 1113 | SER  | 13.9 |
| 1   | B     | 241  | ASP  | 13.9 |
| 1   | B     | 433  | THR  | 13.9 |
| 1   | A     | 94   | TYR  | 13.9 |
| 1   | A     | 680  | TYR  | 13.8 |
| 1   | A     | 876  | GLY  | 13.8 |
| 1   | A     | 705  | PRO  | 13.8 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 133  | GLN  | 13.8 |
| 1   | B     | 162  | ARG  | 13.8 |
| 1   | B     | 1057 | ILE  | 13.8 |
| 1   | A     | 512  | SER  | 13.8 |
| 1   | A     | 896  | LEU  | 13.8 |
| 1   | A     | 1144 | TYR  | 13.8 |
| 1   | A     | 414  | GLY  | 13.8 |
| 1   | B     | 1114 | PRO  | 13.7 |
| 1   | B     | 869  | PRO  | 13.7 |
| 1   | B     | 1017 | HIS  | 13.7 |
| 1   | B     | 1179 | PRO  | 13.7 |
| 1   | B     | 1030 | ARG  | 13.7 |
| 1   | A     | 1131 | VAL  | 13.6 |
| 1   | A     | 430  | ASP  | 13.6 |
| 1   | A     | 522  | CYS  | 13.6 |
| 1   | A     | 594  | VAL  | 13.6 |
| 1   | A     | 532  | TRP  | 13.6 |
| 1   | B     | 1112 | ARG  | 13.6 |
| 1   | A     | 93   | CYS  | 13.5 |
| 1   | A     | 75   | ASN  | 13.5 |
| 1   | B     | 1029 | ASN  | 13.5 |
| 1   | A     | 901  | GLY  | 13.5 |
| 1   | B     | 672  | SER  | 13.4 |
| 1   | A     | 875  | GLN  | 13.4 |
| 1   | A     | 1105 | PRO  | 13.4 |
| 1   | A     | 795  | ASP  | 13.4 |
| 1   | A     | 1127 | ILE  | 13.4 |
| 1   | B     | 1116 | GLU  | 13.4 |
| 1   | B     | 395  | ASN  | 13.4 |
| 1   | A     | 539  | CYS  | 13.4 |
| 1   | A     | 704  | CYS  | 13.4 |
| 1   | A     | 964  | VAL  | 13.4 |
| 1   | B     | 547  | ARG  | 13.4 |
| 1   | A     | 595  | ASN  | 13.3 |
| 1   | B     | 1184 | LEU  | 13.3 |
| 1   | A     | 974  | GLY  | 13.3 |
| 1   | B     | 378  | GLU  | 13.3 |
| 1   | B     | 1217 | VAL  | 13.3 |
| 1   | B     | 263  | THR  | 13.3 |
| 1   | B     | 506  | THR  | 13.3 |
| 1   | A     | 98   | SER  | 13.2 |
| 1   | A     | 615  | CYS  | 13.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 1065 | THR  | 13.2 |
| 1   | A     | 1022 | ALA  | 13.2 |
| 1   | A     | 542  | GLN  | 13.2 |
| 1   | B     | 240  | PHE  | 13.2 |
| 1   | A     | 1142 | PHE  | 13.2 |
| 1   | B     | 525  | SER  | 13.2 |
| 1   | B     | 837  | LEU  | 13.2 |
| 1   | B     | 1142 | PHE  | 13.2 |
| 1   | A     | 499  | ALA  | 13.2 |
| 1   | B     | 75   | ASN  | 13.2 |
| 1   | B     | 704  | CYS  | 13.2 |
| 1   | A     | 151  | HIS  | 13.2 |
| 1   | B     | 1076 | GLU  | 13.2 |
| 1   | A     | 888  | GLY  | 13.1 |
| 1   | A     | 924  | ASP  | 13.1 |
| 1   | A     | 48   | GLY  | 13.1 |
| 1   | A     | 178  | GLN  | 13.1 |
| 1   | B     | 862  | PRO  | 13.1 |
| 1   | B     | 824  | PHE  | 13.1 |
| 1   | A     | 525  | SER  | 13.1 |
| 1   | B     | 825  | GLU  | 13.1 |
| 1   | B     | 533  | CYS  | 13.1 |
| 1   | B     | 1196 | ILE  | 13.1 |
| 1   | B     | 1151 | GLU  | 13.0 |
| 1   | B     | 1016 | GLY  | 13.0 |
| 1   | A     | 1179 | PRO  | 13.0 |
| 1   | A     | 260  | GLN  | 13.0 |
| 1   | B     | 1040 | TYR  | 13.0 |
| 1   | B     | 1013 | THR  | 13.0 |
| 1   | B     | 593  | GLY  | 13.0 |
| 1   | A     | 1052 | ASP  | 13.0 |
| 1   | A     | 815  | GLY  | 12.9 |
| 1   | B     | 546  | GLU  | 12.9 |
| 1   | A     | 938  | CYS  | 12.9 |
| 1   | B     | 539  | CYS  | 12.9 |
| 1   | B     | 687  | ASN  | 12.9 |
| 1   | B     | 528  | PRO  | 12.9 |
| 1   | A     | 507  | GLN  | 12.9 |
| 1   | B     | 884  | GLY  | 12.9 |
| 1   | B     | 1020 | GLY  | 12.9 |
| 1   | A     | 940  | ARG  | 12.9 |
| 1   | A     | 177  | GLY  | 12.9 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 955  | THR  | 12.9 |
| 1   | B     | 697  | ARG  | 12.9 |
| 1   | B     | 180  | GLN  | 12.9 |
| 1   | A     | 131  | ALA  | 12.8 |
| 1   | B     | 556  | SER  | 12.8 |
| 1   | B     | 274  | HIS  | 12.8 |
| 1   | B     | 393  | CYS  | 12.8 |
| 1   | A     | 917  | GLN  | 12.8 |
| 1   | A     | 596  | CYS  | 12.8 |
| 1   | B     | 537  | SER  | 12.8 |
| 1   | A     | 1050 | ARG  | 12.8 |
| 1   | B     | 674  | PRO  | 12.8 |
| 1   | A     | 546  | GLU  | 12.8 |
| 1   | B     | 276  | PHE  | 12.8 |
| 1   | A     | 1031 | ALA  | 12.8 |
| 1   | A     | 381  | LEU  | 12.8 |
| 1   | A     | 972  | SER  | 12.8 |
| 1   | A     | 1008 | GLU  | 12.8 |
| 1   | A     | 1114 | PRO  | 12.7 |
| 1   | A     | 877  | GLY  | 12.7 |
| 1   | B     | 1064 | LEU  | 12.7 |
| 1   | A     | 712  | HIS  | 12.7 |
| 1   | A     | 353  | SER  | 12.7 |
| 1   | B     | 444  | THR  | 12.7 |
| 1   | A     | 132  | SER  | 12.7 |
| 1   | A     | 189  | ILE  | 12.7 |
| 1   | B     | 111  | ASN  | 12.7 |
| 1   | B     | 41   | THR  | 12.7 |
| 1   | B     | 850  | MET  | 12.7 |
| 1   | B     | 971  | LEU  | 12.6 |
| 1   | A     | 474  | GLU  | 12.6 |
| 1   | B     | 501  | THR  | 12.6 |
| 1   | A     | 311  | GLN  | 12.6 |
| 1   | A     | 399  | GLN  | 12.6 |
| 1   | B     | 415  | GLY  | 12.6 |
| 1   | B     | 532  | TRP  | 12.6 |
| 1   | A     | 907  | PRO  | 12.5 |
| 1   | B     | 132  | SER  | 12.5 |
| 1   | B     | 1110 | PRO  | 12.5 |
| 1   | B     | 425  | PHE  | 12.5 |
| 1   | A     | 967  | SER  | 12.5 |
| 1   | B     | 823  | ARG  | 12.5 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 1223 | GLY  | 12.5 |
| 1   | A     | 1040 | TYR  | 12.5 |
| 1   | A     | 557  | ASP  | 12.5 |
| 1   | B     | 402  | ASP  | 12.4 |
| 1   | A     | 534  | VAL  | 12.4 |
| 1   | B     | 693  | PHE  | 12.4 |
| 1   | A     | 602  | THR  | 12.4 |
| 1   | B     | 863  | LYS  | 12.4 |
| 1   | B     | 1188 | VAL  | 12.4 |
| 1   | A     | 898  | VAL  | 12.4 |
| 1   | B     | 295  | GLU  | 12.4 |
| 1   | B     | 478  | ALA  | 12.4 |
| 1   | B     | 834  | ARG  | 12.4 |
| 1   | A     | 959  | PRO  | 12.4 |
| 1   | B     | 695  | GLU  | 12.4 |
| 1   | A     | 958  | THR  | 12.3 |
| 1   | B     | 92   | LYS  | 12.3 |
| 1   | A     | 908  | VAL  | 12.3 |
| 1   | B     | 163  | GLU  | 12.3 |
| 1   | A     | 157  | TYR  | 12.3 |
| 1   | A     | 603  | GLU  | 12.3 |
| 1   | A     | 655  | VAL  | 12.3 |
| 1   | B     | 309  | LEU  | 12.3 |
| 1   | B     | 874  | ARG  | 12.3 |
| 1   | B     | 995  | GLY  | 12.3 |
| 1   | A     | 1101 | VAL  | 12.3 |
| 1   | B     | 820  | ALA  | 12.3 |
| 1   | A     | 1048 | ILE  | 12.3 |
| 1   | A     | 152  | HIS  | 12.3 |
| 1   | B     | 105  | GLY  | 12.3 |
| 1   | B     | 438  | TYR  | 12.3 |
| 1   | B     | 536  | HIS  | 12.3 |
| 1   | B     | 603  | GLU  | 12.2 |
| 1   | B     | 818  | LEU  | 12.2 |
| 1   | A     | 432  | LEU  | 12.2 |
| 1   | A     | 813  | SER  | 12.2 |
| 1   | B     | 1126 | PHE  | 12.2 |
| 1   | A     | 980  | GLU  | 12.2 |
| 1   | B     | 485  | LEU  | 12.2 |
| 1   | A     | 240  | PHE  | 12.2 |
| 1   | A     | 1110 | PRO  | 12.2 |
| 1   | B     | 682  | HIS  | 12.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 523  | LEU  | 12.2 |
| 1   | A     | 766  | GLN  | 12.1 |
| 1   | B     | 339  | PHE  | 12.1 |
| 1   | B     | 82   | HIS  | 12.1 |
| 1   | A     | 130  | SER  | 12.1 |
| 1   | A     | 47   | TRP  | 12.1 |
| 1   | A     | 828  | TRP  | 12.1 |
| 1   | B     | 974  | GLY  | 12.1 |
| 1   | A     | 406  | GLY  | 12.1 |
| 1   | B     | 812  | GLN  | 12.1 |
| 1   | B     | 671  | GLY  | 12.1 |
| 1   | A     | 190  | ASP  | 12.1 |
| 1   | A     | 862  | PRO  | 12.1 |
| 1   | B     | 588  | PRO  | 12.1 |
| 1   | B     | 1091 | SER  | 12.0 |
| 1   | A     | 263  | THR  | 12.0 |
| 1   | B     | 977  | ILE  | 12.0 |
| 1   | B     | 68   | ARG  | 12.0 |
| 1   | B     | 317  | ARG  | 12.0 |
| 1   | B     | 307  | TYR  | 12.0 |
| 1   | A     | 631  | GLY  | 12.0 |
| 1   | B     | 534  | VAL  | 12.0 |
| 1   | B     | 936  | GLU  | 11.9 |
| 1   | B     | 329  | ALA  | 11.9 |
| 1   | B     | 93   | CYS  | 11.9 |
| 1   | B     | 933  | ALA  | 11.9 |
| 1   | A     | 400  | ILE  | 11.9 |
| 1   | A     | 1124 | ILE  | 11.9 |
| 1   | A     | 641  | LYS  | 11.9 |
| 1   | B     | 705  | PRO  | 11.9 |
| 1   | A     | 1055 | TRP  | 11.9 |
| 1   | A     | 583  | GLN  | 11.9 |
| 1   | B     | 851  | HIS  | 11.8 |
| 1   | A     | 861  | ASP  | 11.8 |
| 1   | A     | 819  | LYS  | 11.8 |
| 1   | A     | 939  | VAL  | 11.8 |
| 1   | A     | 1164 | SER  | 11.8 |
| 1   | B     | 353  | SER  | 11.8 |
| 1   | B     | 392  | GLY  | 11.8 |
| 1   | B     | 976  | TRP  | 11.8 |
| 1   | B     | 920  | CYS  | 11.8 |
| 1   | A     | 136  | CYS  | 11.8 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 149  | GLU  | 11.8 |
| 1   | B     | 634  | ARG  | 11.8 |
| 1   | B     | 515  | GLN  | 11.8 |
| 1   | A     | 1184 | LEU  | 11.8 |
| 1   | A     | 1076 | GLU  | 11.8 |
| 1   | B     | 1014 | PRO  | 11.7 |
| 1   | A     | 642  | SER  | 11.7 |
| 1   | B     | 98   | SER  | 11.7 |
| 1   | B     | 815  | GLY  | 11.7 |
| 1   | A     | 487  | ASP  | 11.7 |
| 1   | B     | 886  | ASN  | 11.7 |
| 1   | A     | 679  | LYS  | 11.7 |
| 1   | A     | 510  | VAL  | 11.7 |
| 1   | A     | 513  | CYS  | 11.7 |
| 1   | A     | 350  | PRO  | 11.7 |
| 1   | B     | 663  | GLN  | 11.7 |
| 1   | A     | 162  | ARG  | 11.7 |
| 1   | B     | 476  | VAL  | 11.6 |
| 1   | B     | 477  | VAL  | 11.6 |
| 1   | B     | 1096 | ASN  | 11.6 |
| 1   | A     | 332  | GLU  | 11.6 |
| 1   | A     | 476  | VAL  | 11.6 |
| 1   | B     | 1113 | SER  | 11.6 |
| 1   | A     | 1024 | ILE  | 11.6 |
| 1   | B     | 662  | HIS  | 11.6 |
| 1   | A     | 413  | LEU  | 11.6 |
| 1   | B     | 811  | ARG  | 11.6 |
| 1   | A     | 573  | VAL  | 11.6 |
| 1   | B     | 500  | MET  | 11.6 |
| 1   | A     | 228  | LYS  | 11.6 |
| 1   | A     | 229  | ILE  | 11.6 |
| 1   | A     | 836  | SER  | 11.6 |
| 1   | B     | 1053 | PRO  | 11.5 |
| 1   | A     | 426  | VAL  | 11.5 |
| 1   | A     | 275  | PHE  | 11.5 |
| 1   | B     | 483  | PRO  | 11.5 |
| 1   | A     | 95   | PRO  | 11.5 |
| 1   | A     | 523  | LEU  | 11.5 |
| 1   | A     | 449  | GLY  | 11.5 |
| 1   | B     | 148  | GLY  | 11.5 |
| 1   | B     | 692  | ALA  | 11.5 |
| 1   | A     | 860  | THR  | 11.5 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 504  | GLN  | 11.5 |
| 1   | A     | 354  | ALA  | 11.4 |
| 1   | A     | 1079 | ILE  | 11.4 |
| 1   | A     | 656  | PHE  | 11.4 |
| 1   | A     | 1186 | TYR  | 11.4 |
| 1   | B     | 1194 | PRO  | 11.4 |
| 1   | B     | 1010 | ARG  | 11.4 |
| 1   | A     | 886  | ASN  | 11.4 |
| 1   | A     | 1116 | GLU  | 11.4 |
| 1   | B     | 890  | ARG  | 11.4 |
| 1   | A     | 479  | GLN  | 11.3 |
| 1   | B     | 1220 | ARG  | 11.3 |
| 1   | A     | 900  | VAL  | 11.3 |
| 1   | B     | 412  | PRO  | 11.3 |
| 1   | A     | 192  | LYS  | 11.3 |
| 1   | A     | 570  | ASN  | 11.3 |
| 1   | B     | 502  | GLU  | 11.3 |
| 1   | B     | 76   | LEU  | 11.2 |
| 1   | B     | 771  | SER  | 11.2 |
| 1   | A     | 96   | PRO  | 11.2 |
| 1   | A     | 895  | ARG  | 11.2 |
| 1   | B     | 993  | SER  | 11.2 |
| 1   | A     | 424  | LEU  | 11.2 |
| 1   | B     | 99   | VAL  | 11.2 |
| 1   | A     | 344  | LYS  | 11.2 |
| 1   | A     | 893  | ASP  | 11.2 |
| 1   | A     | 912  | TYR  | 11.2 |
| 1   | B     | 1101 | VAL  | 11.1 |
| 1   | B     | 277  | THR  | 11.1 |
| 1   | B     | 509  | PRO  | 11.1 |
| 1   | B     | 947  | ARG  | 11.1 |
| 1   | A     | 820  | ALA  | 11.1 |
| 1   | B     | 306  | GLU  | 11.1 |
| 1   | A     | 973  | GLY  | 11.1 |
| 1   | B     | 907  | PRO  | 11.1 |
| 1   | A     | 812  | GLN  | 11.1 |
| 1   | B     | 413  | LEU  | 11.1 |
| 1   | A     | 1171 | GLY  | 11.0 |
| 1   | B     | 1048 | ILE  | 11.0 |
| 1   | A     | 99   | VAL  | 11.0 |
| 1   | A     | 380  | LYS  | 11.0 |
| 1   | A     | 543  | ASP  | 11.0 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 662  | HIS  | 11.0 |
| 1   | A     | 427  | ASP  | 11.0 |
| 1   | B     | 526  | ARG  | 11.0 |
| 1   | A     | 273  | GLU  | 11.0 |
| 1   | A     | 682  | HIS  | 11.0 |
| 1   | B     | 400  | ILE  | 11.0 |
| 1   | B     | 562  | VAL  | 11.0 |
| 1   | A     | 593  | GLY  | 11.0 |
| 1   | B     | 110  | ASP  | 11.0 |
| 1   | A     | 903  | VAL  | 10.9 |
| 1   | A     | 1027 | ASN  | 10.9 |
| 1   | B     | 700  | MET  | 10.9 |
| 1   | A     | 1064 | LEU  | 10.9 |
| 1   | A     | 1054 | GLU  | 10.9 |
| 1   | B     | 484  | ILE  | 10.9 |
| 1   | B     | 543  | ASP  | 10.9 |
| 1   | B     | 1181 | ASN  | 10.9 |
| 1   | A     | 383  | LEU  | 10.9 |
| 1   | B     | 925  | ALA  | 10.9 |
| 1   | A     | 1106 | SER  | 10.9 |
| 1   | A     | 472  | ALA  | 10.9 |
| 1   | B     | 426  | VAL  | 10.9 |
| 1   | B     | 376  | ARG  | 10.9 |
| 1   | B     | 972  | SER  | 10.9 |
| 1   | A     | 1087 | GLU  | 10.9 |
| 1   | A     | 1120 | ARG  | 10.8 |
| 1   | A     | 995  | GLY  | 10.8 |
| 1   | B     | 535  | LEU  | 10.8 |
| 1   | B     | 841  | CYS  | 10.8 |
| 1   | B     | 548  | ALA  | 10.8 |
| 1   | A     | 1078 | ARG  | 10.8 |
| 1   | A     | 604  | THR  | 10.8 |
| 1   | A     | 665  | CYS  | 10.8 |
| 1   | A     | 92   | LYS  | 10.8 |
| 1   | B     | 1024 | ILE  | 10.8 |
| 1   | A     | 663  | GLN  | 10.8 |
| 1   | B     | 482  | ASN  | 10.8 |
| 1   | B     | 656  | PHE  | 10.8 |
| 1   | B     | 861  | ASP  | 10.8 |
| 1   | B     | 917  | GLN  | 10.8 |
| 1   | A     | 1126 | PHE  | 10.8 |
| 1   | A     | 634  | ARG  | 10.7 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 486  | ARG  | 10.7 |
| 1   | B     | 809  | ALA  | 10.7 |
| 1   | B     | 889  | LEU  | 10.7 |
| 1   | B     | 627  | THR  | 10.7 |
| 1   | B     | 479  | GLN  | 10.7 |
| 1   | B     | 980  | GLU  | 10.7 |
| 1   | A     | 412  | PRO  | 10.7 |
| 1   | B     | 714  | TYR  | 10.7 |
| 1   | B     | 114  | LYS  | 10.7 |
| 1   | A     | 484  | ILE  | 10.7 |
| 1   | A     | 1061 | GLY  | 10.7 |
| 1   | B     | 310  | VAL  | 10.7 |
| 1   | B     | 778  | SER  | 10.7 |
| 1   | A     | 706  | GLN  | 10.7 |
| 1   | A     | 566  | VAL  | 10.7 |
| 1   | B     | 683  | VAL  | 10.7 |
| 1   | A     | 674  | PRO  | 10.6 |
| 1   | A     | 1004 | ARG  | 10.6 |
| 1   | B     | 151  | HIS  | 10.6 |
| 1   | B     | 908  | VAL  | 10.6 |
| 1   | B     | 260  | GLN  | 10.6 |
| 1   | B     | 832  | GLU  | 10.6 |
| 1   | B     | 190  | ASP  | 10.6 |
| 1   | A     | 686  | ASN  | 10.6 |
| 1   | B     | 432  | LEU  | 10.6 |
| 1   | B     | 440  | TYR  | 10.6 |
| 1   | B     | 542  | GLN  | 10.6 |
| 1   | A     | 477  | VAL  | 10.6 |
| 1   | A     | 990  | VAL  | 10.6 |
| 1   | B     | 1025 | VAL  | 10.6 |
| 1   | A     | 100  | GLN  | 10.5 |
| 1   | A     | 195  | TYR  | 10.5 |
| 1   | A     | 904  | LEU  | 10.5 |
| 1   | A     | 701  | SER  | 10.5 |
| 1   | A     | 885  | GLU  | 10.5 |
| 1   | A     | 1091 | SER  | 10.5 |
| 1   | A     | 548  | ALA  | 10.5 |
| 1   | A     | 732  | GLN  | 10.5 |
| 1   | B     | 228  | LYS  | 10.5 |
| 1   | A     | 393  | CYS  | 10.5 |
| 1   | A     | 809  | ALA  | 10.4 |
| 1   | A     | 341  | GLN  | 10.4 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 342  | GLY  | 10.4 |
| 1   | A     | 1119 | GLU  | 10.4 |
| 1   | A     | 191  | GLY  | 10.4 |
| 1   | B     | 963  | ARG  | 10.4 |
| 1   | B     | 1164 | SER  | 10.4 |
| 1   | B     | 104  | HIS  | 10.4 |
| 1   | A     | 295  | GLU  | 10.4 |
| 1   | B     | 152  | HIS  | 10.4 |
| 1   | A     | 672  | SER  | 10.4 |
| 1   | B     | 814  | CYS  | 10.4 |
| 1   | A     | 372  | GLN  | 10.4 |
| 1   | A     | 616  | HIS  | 10.4 |
| 1   | B     | 1004 | ARG  | 10.4 |
| 1   | A     | 208  | GLU  | 10.4 |
| 1   | B     | 49   | LEU  | 10.4 |
| 1   | A     | 501  | THR  | 10.3 |
| 1   | B     | 766  | GLN  | 10.3 |
| 1   | A     | 97   | PRO  | 10.3 |
| 1   | A     | 920  | CYS  | 10.3 |
| 1   | B     | 1225 | GLU  | 10.3 |
| 1   | B     | 65   | ALA  | 10.3 |
| 1   | B     | 316  | SER  | 10.3 |
| 1   | A     | 217  | VAL  | 10.3 |
| 1   | B     | 1051 | ILE  | 10.3 |
| 1   | B     | 816  | LEU  | 10.3 |
| 1   | A     | 697  | ARG  | 10.3 |
| 1   | B     | 1137 | LEU  | 10.3 |
| 1   | B     | 341  | GLN  | 10.3 |
| 1   | B     | 504  | GLN  | 10.3 |
| 1   | A     | 889  | LEU  | 10.3 |
| 1   | B     | 427  | ASP  | 10.3 |
| 1   | B     | 864  | ILE  | 10.2 |
| 1   | B     | 691  | CYS  | 10.2 |
| 1   | A     | 293  | TYR  | 10.2 |
| 1   | B     | 301  | GLU  | 10.2 |
| 1   | B     | 189  | ILE  | 10.2 |
| 1   | B     | 262  | ASP  | 10.2 |
| 1   | B     | 1009 | ILE  | 10.2 |
| 1   | B     | 1224 | PHE  | 10.2 |
| 1   | A     | 352  | GLU  | 10.2 |
| 1   | B     | 197  | PRO  | 10.2 |
| 1   | A     | 375  | TYR  | 10.2 |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 681  | ARG  | 10.2 |
| 1   | B     | 157  | TYR  | 10.2 |
| 1   | B     | 396  | SER  | 10.2 |
| 1   | B     | 844  | ASP  | 10.2 |
| 1   | A     | 572  | SER  | 10.2 |
| 1   | A     | 1013 | THR  | 10.2 |
| 1   | B     | 999  | CYS  | 10.2 |
| 1   | A     | 498  | TYR  | 10.2 |
| 1   | B     | 456  | ARG  | 10.2 |
| 1   | B     | 901  | GLY  | 10.2 |
| 1   | A     | 1152 | PRO  | 10.2 |
| 1   | A     | 526  | ARG  | 10.2 |
| 1   | A     | 963  | ARG  | 10.1 |
| 1   | A     | 485  | LEU  | 10.1 |
| 1   | B     | 660  | SER  | 10.1 |
| 1   | A     | 568  | PRO  | 10.1 |
| 1   | B     | 1007 | ARG  | 10.1 |
| 1   | A     | 110  | ASP  | 10.1 |
| 1   | B     | 311  | GLN  | 10.1 |
| 1   | A     | 405  | CYS  | 10.1 |
| 1   | B     | 39   | PHE  | 10.1 |
| 1   | B     | 767  | ASN  | 10.1 |
| 1   | B     | 401  | ASP  | 10.1 |
| 1   | A     | 731  | PRO  | 10.0 |
| 1   | B     | 503  | LYS  | 10.0 |
| 1   | A     | 1149 | VAL  | 10.0 |
| 1   | B     | 258  | THR  | 10.0 |
| 1   | B     | 915  | ALA  | 10.0 |
| 1   | A     | 298  | ILE  | 10.0 |
| 1   | B     | 459  | LEU  | 10.0 |
| 1   | B     | 706  | GLN  | 10.0 |
| 1   | B     | 701  | SER  | 10.0 |
| 1   | A     | 451  | ARG  | 10.0 |
| 1   | B     | 795  | ASP  | 10.0 |
| 1   | A     | 1104 | ALA  | 10.0 |
| 1   | A     | 473  | TYR  | 9.9  |
| 1   | A     | 1032 | GLN  | 9.9  |
| 1   | B     | 208  | GLU  | 9.9  |
| 1   | B     | 891  | PHE  | 9.9  |
| 1   | B     | 352  | GLU  | 9.9  |
| 1   | A     | 915  | ALA  | 9.9  |
| 1   | A     | 1053 | PRO  | 9.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 911  | GLU  | 9.9  |
| 1   | B     | 48   | GLY  | 9.9  |
| 1   | B     | 275  | PHE  | 9.9  |
| 1   | B     | 97   | PRO  | 9.9  |
| 1   | B     | 1132 | ARG  | 9.9  |
| 1   | A     | 1175 | LEU  | 9.9  |
| 1   | B     | 346  | ARG  | 9.9  |
| 1   | B     | 381  | LEU  | 9.9  |
| 1   | A     | 905  | CYS  | 9.9  |
| 1   | A     | 537  | SER  | 9.9  |
| 1   | B     | 1008 | GLU  | 9.9  |
| 1   | A     | 1028 | ILE  | 9.9  |
| 1   | A     | 1060 | GLY  | 9.9  |
| 1   | A     | 606  | SER  | 9.9  |
| 1   | A     | 891  | PHE  | 9.8  |
| 1   | A     | 617  | SER  | 9.8  |
| 1   | A     | 581  | VAL  | 9.8  |
| 1   | A     | 209  | GLU  | 9.8  |
| 1   | A     | 716  | PRO  | 9.8  |
| 1   | A     | 979  | ILE  | 9.8  |
| 1   | B     | 667  | ALA  | 9.8  |
| 1   | A     | 648  | LYS  | 9.8  |
| 1   | B     | 1015 | PRO  | 9.8  |
| 1   | A     | 668  | CYS  | 9.8  |
| 1   | A     | 398  | LEU  | 9.8  |
| 1   | A     | 1143 | LEU  | 9.8  |
| 1   | A     | 137  | GLN  | 9.8  |
| 1   | B     | 962  | TYR  | 9.8  |
| 1   | B     | 644  | GLU  | 9.8  |
| 1   | A     | 571  | VAL  | 9.8  |
| 1   | A     | 390  | GLU  | 9.7  |
| 1   | A     | 71   | LYS  | 9.7  |
| 1   | B     | 439  | ASP  | 9.7  |
| 1   | A     | 659  | CYS  | 9.7  |
| 1   | B     | 679  | LYS  | 9.7  |
| 1   | B     | 965  | SER  | 9.7  |
| 1   | A     | 1103 | ARG  | 9.7  |
| 1   | B     | 871  | THR  | 9.7  |
| 1   | B     | 375  | TYR  | 9.7  |
| 1   | A     | 580  | LEU  | 9.7  |
| 1   | B     | 994  | ILE  | 9.7  |
| 1   | A     | 562  | VAL  | 9.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 508  | VAL  | 9.6  |
| 1   | B     | 457  | LYS  | 9.6  |
| 1   | A     | 309  | LEU  | 9.6  |
| 1   | A     | 158  | LEU  | 9.6  |
| 1   | A     | 448  | ALA  | 9.6  |
| 1   | A     | 407  | GLN  | 9.6  |
| 1   | B     | 813  | SER  | 9.6  |
| 1   | B     | 1136 | VAL  | 9.6  |
| 1   | A     | 478  | ALA  | 9.6  |
| 1   | B     | 1011 | CYS  | 9.6  |
| 1   | B     | 1190 | ILE  | 9.6  |
| 1   | A     | 457  | LYS  | 9.6  |
| 1   | B     | 100  | GLN  | 9.6  |
| 1   | A     | 454  | ARG  | 9.6  |
| 1   | B     | 264  | GLN  | 9.6  |
| 1   | A     | 1021 | SER  | 9.6  |
| 1   | A     | 852  | ALA  | 9.6  |
| 1   | B     | 463  | ALA  | 9.6  |
| 1   | B     | 460  | VAL  | 9.6  |
| 1   | A     | 1086 | ILE  | 9.6  |
| 1   | A     | 282  | ARG  | 9.5  |
| 1   | B     | 94   | TYR  | 9.5  |
| 1   | B     | 242  | ILE  | 9.5  |
| 1   | A     | 411  | GLN  | 9.5  |
| 1   | A     | 711  | THR  | 9.5  |
| 1   | A     | 456  | ARG  | 9.5  |
| 1   | B     | 243  | TYR  | 9.5  |
| 1   | B     | 843  | ALA  | 9.5  |
| 1   | A     | 932  | ASP  | 9.5  |
| 1   | B     | 604  | THR  | 9.5  |
| 1   | A     | 660  | SER  | 9.4  |
| 1   | A     | 1085 | GLY  | 9.4  |
| 1   | B     | 1095 | TYR  | 9.4  |
| 1   | B     | 437  | ALA  | 9.4  |
| 1   | A     | 713  | ILE  | 9.4  |
| 1   | A     | 49   | LEU  | 9.4  |
| 1   | A     | 544  | ALA  | 9.4  |
| 1   | B     | 411  | GLN  | 9.4  |
| 1   | A     | 925  | ALA  | 9.4  |
| 1   | B     | 586  | ASN  | 9.4  |
| 1   | B     | 71   | LYS  | 9.4  |
| 1   | B     | 84   | THR  | 9.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 70   | TYR  | 9.4  |
| 1   | B     | 498  | TYR  | 9.4  |
| 1   | B     | 394  | ILE  | 9.4  |
| 1   | A     | 618  | PRO  | 9.4  |
| 1   | A     | 1063 | LEU  | 9.4  |
| 1   | A     | 40   | ARG  | 9.4  |
| 1   | A     | 831  | ALA  | 9.4  |
| 1   | A     | 614  | HIS  | 9.3  |
| 1   | A     | 661  | VAL  | 9.3  |
| 1   | B     | 344  | LYS  | 9.3  |
| 1   | B     | 921  | GLU  | 9.3  |
| 1   | B     | 1111 | LYS  | 9.3  |
| 1   | B     | 839  | HIS  | 9.3  |
| 1   | A     | 312  | ASP  | 9.3  |
| 1   | B     | 112  | VAL  | 9.3  |
| 1   | A     | 567  | GLN  | 9.3  |
| 1   | B     | 516  | TYR  | 9.3  |
| 1   | B     | 860  | THR  | 9.3  |
| 1   | B     | 469  | PRO  | 9.3  |
| 1   | B     | 872  | GLY  | 9.3  |
| 1   | B     | 979  | ILE  | 9.3  |
| 1   | B     | 602  | THR  | 9.3  |
| 1   | A     | 981  | GLY  | 9.3  |
| 1   | B     | 831  | ALA  | 9.3  |
| 1   | A     | 471  | LEU  | 9.2  |
| 1   | A     | 977  | ILE  | 9.2  |
| 1   | B     | 918  | ILE  | 9.2  |
| 1   | A     | 569  | ARG  | 9.2  |
| 1   | B     | 441  | GLN  | 9.2  |
| 1   | A     | 816  | LEU  | 9.2  |
| 1   | B     | 842  | PRO  | 9.2  |
| 1   | B     | 96   | PRO  | 9.2  |
| 1   | B     | 956  | PHE  | 9.2  |
| 1   | B     | 589  | ASP  | 9.2  |
| 1   | B     | 158  | LEU  | 9.2  |
| 1   | B     | 379  | GLY  | 9.2  |
| 1   | B     | 840  | HIS  | 9.2  |
| 1   | B     | 340  | ALA  | 9.2  |
| 1   | A     | 438  | TYR  | 9.2  |
| 1   | A     | 73   | SER  | 9.2  |
| 1   | A     | 535  | LEU  | 9.2  |
| 1   | A     | 768  | SER  | 9.1  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 605  | GLU  | 9.1  |
| 1   | A     | 726  | ALA  | 9.1  |
| 1   | B     | 985  | ASN  | 9.1  |
| 1   | A     | 921  | GLU  | 9.1  |
| 1   | B     | 939  | VAL  | 9.1  |
| 1   | B     | 1189 | LEU  | 9.1  |
| 1   | B     | 688  | ALA  | 9.1  |
| 1   | A     | 582  | LEU  | 9.1  |
| 1   | B     | 195  | TYR  | 9.1  |
| 1   | B     | 573  | VAL  | 9.1  |
| 1   | A     | 565  | THR  | 9.1  |
| 1   | B     | 931  | HIS  | 9.1  |
| 1   | A     | 922  | ILE  | 9.1  |
| 1   | B     | 245  | VAL  | 9.1  |
| 1   | A     | 502  | GLU  | 9.1  |
| 1   | A     | 931  | HIS  | 9.1  |
| 1   | A     | 1049 | LEU  | 9.1  |
| 1   | B     | 385  | TRP  | 9.1  |
| 1   | A     | 825  | GLU  | 9.1  |
| 1   | A     | 703  | ASP  | 9.1  |
| 1   | A     | 318  | PRO  | 9.1  |
| 1   | A     | 423  | PRO  | 9.1  |
| 1   | B     | 934  | LEU  | 9.0  |
| 1   | B     | 932  | ASP  | 9.0  |
| 1   | B     | 69   | ILE  | 9.0  |
| 1   | B     | 912  | TYR  | 9.0  |
| 1   | B     | 930  | ALA  | 9.0  |
| 1   | A     | 1222 | GLY  | 9.0  |
| 1   | B     | 716  | PRO  | 9.0  |
| 1   | B     | 229  | ILE  | 9.0  |
| 1   | A     | 1009 | ILE  | 9.0  |
| 1   | A     | 306  | GLU  | 9.0  |
| 1   | A     | 317  | ARG  | 9.0  |
| 1   | A     | 985  | ASN  | 9.0  |
| 1   | B     | 496  | TYR  | 8.9  |
| 1   | A     | 1137 | LEU  | 8.9  |
| 1   | B     | 905  | CYS  | 8.9  |
| 1   | A     | 918  | ILE  | 8.9  |
| 1   | A     | 1010 | ARG  | 8.9  |
| 1   | B     | 204  | LEU  | 8.9  |
| 1   | A     | 1014 | PRO  | 8.9  |
| 1   | B     | 946  | TYR  | 8.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 961  | PHE  | 8.9  |
| 1   | A     | 930  | ALA  | 8.9  |
| 1   | A     | 868  | SER  | 8.9  |
| 1   | B     | 935  | VAL  | 8.9  |
| 1   | A     | 194  | GLU  | 8.9  |
| 1   | B     | 596  | CYS  | 8.9  |
| 1   | B     | 54   | VAL  | 8.9  |
| 1   | B     | 81   | ALA  | 8.9  |
| 1   | B     | 649  | PHE  | 8.9  |
| 1   | B     | 838  | ARG  | 8.9  |
| 1   | A     | 954  | PHE  | 8.9  |
| 1   | A     | 1207 | GLU  | 8.9  |
| 1   | B     | 488  | LEU  | 8.9  |
| 1   | A     | 401  | ASP  | 8.9  |
| 1   | A     | 719  | VAL  | 8.8  |
| 1   | A     | 806  | LYS  | 8.8  |
| 1   | A     | 135  | ILE  | 8.8  |
| 1   | A     | 517  | THR  | 8.8  |
| 1   | A     | 261  | LEU  | 8.8  |
| 1   | B     | 1193 | THR  | 8.8  |
| 1   | A     | 937  | VAL  | 8.8  |
| 1   | B     | 964  | VAL  | 8.8  |
| 1   | B     | 852  | ALA  | 8.8  |
| 1   | B     | 594  | VAL  | 8.8  |
| 1   | A     | 198  | THR  | 8.8  |
| 1   | B     | 382  | SER  | 8.8  |
| 1   | B     | 209  | GLU  | 8.8  |
| 1   | A     | 714  | TYR  | 8.8  |
| 1   | B     | 380  | LYS  | 8.8  |
| 1   | B     | 830  | VAL  | 8.8  |
| 1   | B     | 188  | PRO  | 8.8  |
| 1   | B     | 106  | LEU  | 8.7  |
| 1   | B     | 424  | LEU  | 8.7  |
| 1   | B     | 486  | ARG  | 8.7  |
| 1   | A     | 1041 | ASN  | 8.7  |
| 1   | B     | 587  | VAL  | 8.7  |
| 1   | A     | 39   | PHE  | 8.7  |
| 1   | A     | 805  | TYR  | 8.7  |
| 1   | A     | 444  | THR  | 8.7  |
| 1   | B     | 1216 | LYS  | 8.7  |
| 1   | B     | 821  | ASP  | 8.7  |
| 1   | A     | 1174 | LEU  | 8.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 218  | TYR  | 8.7  |
| 1   | B     | 707  | ILE  | 8.7  |
| 1   | A     | 509  | PRO  | 8.7  |
| 1   | B     | 1031 | ALA  | 8.7  |
| 1   | A     | 902  | LYS  | 8.7  |
| 1   | B     | 661  | VAL  | 8.7  |
| 1   | B     | 272  | GLY  | 8.6  |
| 1   | A     | 245  | VAL  | 8.6  |
| 1   | B     | 445  | VAL  | 8.6  |
| 1   | B     | 361  | ARG  | 8.6  |
| 1   | B     | 973  | GLY  | 8.6  |
| 1   | B     | 916  | GLU  | 8.6  |
| 1   | B     | 449  | GLY  | 8.6  |
| 1   | B     | 60   | GLU  | 8.6  |
| 1   | A     | 355  | LEU  | 8.6  |
| 1   | B     | 648  | LYS  | 8.6  |
| 1   | A     | 960  | THR  | 8.6  |
| 1   | B     | 490  | LEU  | 8.6  |
| 1   | A     | 402  | ASP  | 8.6  |
| 1   | A     | 70   | TYR  | 8.6  |
| 1   | B     | 136  | CYS  | 8.6  |
| 1   | A     | 685  | THR  | 8.6  |
| 1   | A     | 650  | ALA  | 8.6  |
| 1   | B     | 296  | PHE  | 8.6  |
| 1   | B     | 732  | GLN  | 8.6  |
| 1   | A     | 310  | VAL  | 8.6  |
| 1   | B     | 302  | GLN  | 8.6  |
| 1   | A     | 643  | LYS  | 8.5  |
| 1   | A     | 756  | LEU  | 8.5  |
| 1   | B     | 1115 | PRO  | 8.5  |
| 1   | B     | 1134 | LEU  | 8.5  |
| 1   | B     | 42   | PHE  | 8.5  |
| 1   | B     | 666  | LEU  | 8.5  |
| 1   | A     | 947  | ARG  | 8.5  |
| 1   | A     | 340  | ALA  | 8.5  |
| 1   | B     | 992  | VAL  | 8.5  |
| 1   | A     | 794  | ILE  | 8.5  |
| 1   | A     | 850  | MET  | 8.5  |
| 1   | B     | 436  | ALA  | 8.5  |
| 1   | A     | 519  | CYS  | 8.5  |
| 1   | A     | 649  | PHE  | 8.5  |
| 1   | A     | 887  | LEU  | 8.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 880  | LEU  | 8.5  |
| 1   | A     | 597  | SER  | 8.5  |
| 1   | B     | 887  | LEU  | 8.5  |
| 1   | B     | 1028 | ILE  | 8.5  |
| 1   | B     | 1135 | LEU  | 8.5  |
| 1   | A     | 384  | PRO  | 8.5  |
| 1   | A     | 385  | TRP  | 8.5  |
| 1   | A     | 505  | VAL  | 8.5  |
| 1   | A     | 516  | TYR  | 8.5  |
| 1   | A     | 475  | SER  | 8.5  |
| 1   | B     | 724  | THR  | 8.5  |
| 1   | B     | 731  | PRO  | 8.5  |
| 1   | B     | 73   | SER  | 8.5  |
| 1   | A     | 916  | GLU  | 8.4  |
| 1   | B     | 1033 | LEU  | 8.4  |
| 1   | B     | 293  | TYR  | 8.4  |
| 1   | A     | 948  | ALA  | 8.4  |
| 1   | B     | 721  | LYS  | 8.4  |
| 1   | A     | 724  | THR  | 8.4  |
| 1   | A     | 134  | GLY  | 8.4  |
| 1   | A     | 294  | VAL  | 8.4  |
| 1   | A     | 538  | ILE  | 8.4  |
| 1   | A     | 1173 | ASN  | 8.4  |
| 1   | A     | 982  | SER  | 8.4  |
| 1   | A     | 669  | VAL  | 8.4  |
| 1   | A     | 994  | ILE  | 8.4  |
| 1   | A     | 155  | GLU  | 8.4  |
| 1   | B     | 330  | GLU  | 8.4  |
| 1   | A     | 810  | LEU  | 8.4  |
| 1   | A     | 1206 | CYS  | 8.4  |
| 1   | A     | 894  | VAL  | 8.3  |
| 1   | B     | 239  | ALA  | 8.3  |
| 1   | A     | 52   | LEU  | 8.3  |
| 1   | B     | 328  | LEU  | 8.3  |
| 1   | B     | 1187 | THR  | 8.3  |
| 1   | A     | 678  | CYS  | 8.3  |
| 1   | A     | 911  | GLU  | 8.3  |
| 1   | A     | 262  | ASP  | 8.3  |
| 1   | B     | 729  | ASN  | 8.3  |
| 1   | A     | 239  | ALA  | 8.3  |
| 1   | B     | 338  | VAL  | 8.3  |
| 1   | B     | 645  | THR  | 8.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 101  | SER  | 8.3  |
| 1   | A     | 588  | PRO  | 8.3  |
| 1   | A     | 202  | ARG  | 8.3  |
| 1   | A     | 1025 | VAL  | 8.2  |
| 1   | A     | 102  | CYS  | 8.2  |
| 1   | B     | 883  | THR  | 8.2  |
| 1   | B     | 922  | ILE  | 8.2  |
| 1   | A     | 1033 | LEU  | 8.2  |
| 1   | B     | 62   | TYR  | 8.2  |
| 1   | B     | 355  | LEU  | 8.2  |
| 1   | A     | 1051 | ILE  | 8.2  |
| 1   | A     | 41   | THR  | 8.2  |
| 1   | B     | 167  | MET  | 8.2  |
| 1   | B     | 390  | GLU  | 8.2  |
| 1   | B     | 187  | THR  | 8.2  |
| 1   | A     | 42   | PHE  | 8.2  |
| 1   | B     | 524  | GLY  | 8.1  |
| 1   | A     | 62   | TYR  | 8.1  |
| 1   | A     | 503  | LYS  | 8.1  |
| 1   | B     | 383  | LEU  | 8.1  |
| 1   | B     | 192  | LYS  | 8.1  |
| 1   | B     | 900  | VAL  | 8.1  |
| 1   | A     | 226  | GLN  | 8.1  |
| 1   | A     | 1108 | ASP  | 8.1  |
| 1   | B     | 954  | PHE  | 8.1  |
| 1   | B     | 538  | ILE  | 8.1  |
| 1   | B     | 300  | CYS  | 8.1  |
| 1   | B     | 870  | GLU  | 8.0  |
| 1   | A     | 729  | ASN  | 8.0  |
| 1   | A     | 1134 | LEU  | 8.0  |
| 1   | B     | 703  | ASP  | 8.0  |
| 1   | B     | 770  | TYR  | 8.0  |
| 1   | A     | 880  | LEU  | 8.0  |
| 1   | B     | 937  | VAL  | 8.0  |
| 1   | B     | 822  | PRO  | 8.0  |
| 1   | A     | 187  | THR  | 8.0  |
| 1   | A     | 684  | CYS  | 8.0  |
| 1   | B     | 44   | ALA  | 8.0  |
| 1   | B     | 499  | ALA  | 8.0  |
| 1   | B     | 184  | PHE  | 8.0  |
| 1   | A     | 842  | PRO  | 8.0  |
| 1   | B     | 983  | HIS  | 8.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 558  | LEU  | 8.0  |
| 1   | A     | 779  | ASP  | 8.0  |
| 1   | A     | 983  | HIS  | 8.0  |
| 1   | B     | 990  | VAL  | 8.0  |
| 1   | A     | 733  | PRO  | 8.0  |
| 1   | B     | 957  | VAL  | 8.0  |
| 1   | A     | 945  | HIS  | 8.0  |
| 1   | A     | 188  | PRO  | 8.0  |
| 1   | B     | 377  | GLY  | 8.0  |
| 1   | A     | 483  | PRO  | 8.0  |
| 1   | B     | 489  | VAL  | 8.0  |
| 1   | A     | 740  | TYR  | 8.0  |
| 1   | B     | 350  | PRO  | 7.9  |
| 1   | B     | 803  | HIS  | 7.9  |
| 1   | B     | 88   | GLU  | 7.9  |
| 1   | A     | 584  | ALA  | 7.9  |
| 1   | B     | 226  | GLN  | 7.9  |
| 1   | B     | 198  | THR  | 7.9  |
| 1   | B     | 1133 | THR  | 7.9  |
| 1   | B     | 61   | VAL  | 7.9  |
| 1   | B     | 989  | ASP  | 7.9  |
| 1   | A     | 627  | THR  | 7.9  |
| 1   | A     | 644  | GLU  | 7.9  |
| 1   | A     | 469  | PRO  | 7.9  |
| 1   | B     | 1063 | LEU  | 7.9  |
| 1   | A     | 76   | LEU  | 7.9  |
| 1   | B     | 470  | ALA  | 7.9  |
| 1   | A     | 906  | SER  | 7.9  |
| 1   | B     | 47   | TRP  | 7.8  |
| 1   | A     | 330  | GLU  | 7.8  |
| 1   | B     | 202  | ARG  | 7.8  |
| 1   | B     | 643  | LYS  | 7.8  |
| 1   | A     | 863  | LYS  | 7.8  |
| 1   | A     | 796  | ASN  | 7.8  |
| 1   | A     | 1170 | LYS  | 7.8  |
| 1   | A     | 1202 | THR  | 7.8  |
| 1   | B     | 868  | SER  | 7.8  |
| 1   | B     | 938  | CYS  | 7.8  |
| 1   | B     | 563  | GLN  | 7.8  |
| 1   | A     | 623  | VAL  | 7.8  |
| 1   | A     | 368  | LYS  | 7.8  |
| 1   | A     | 1217 | VAL  | 7.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 339  | PHE  | 7.8  |
| 1   | A     | 435  | VAL  | 7.8  |
| 1   | A     | 69   | ILE  | 7.8  |
| 1   | B     | 495  | GLN  | 7.8  |
| 1   | A     | 1180 | GLY  | 7.8  |
| 1   | A     | 237  | PHE  | 7.8  |
| 1   | B     | 544  | ALA  | 7.7  |
| 1   | B     | 1141 | SER  | 7.7  |
| 1   | A     | 264  | GLN  | 7.7  |
| 1   | A     | 721  | LYS  | 7.7  |
| 1   | B     | 867  | LEU  | 7.7  |
| 1   | B     | 298  | ILE  | 7.7  |
| 1   | A     | 801  | GLN  | 7.7  |
| 1   | B     | 384  | PRO  | 7.7  |
| 1   | B     | 1034 | SER  | 7.7  |
| 1   | A     | 1139 | SER  | 7.7  |
| 1   | A     | 933  | ALA  | 7.7  |
| 1   | A     | 156  | HIS  | 7.7  |
| 1   | B     | 118  | LEU  | 7.7  |
| 1   | B     | 929  | ARG  | 7.7  |
| 1   | B     | 181  | ALA  | 7.7  |
| 1   | A     | 991  | ALA  | 7.7  |
| 1   | A     | 764  | GLN  | 7.7  |
| 1   | A     | 824  | PHE  | 7.7  |
| 1   | A     | 338  | VAL  | 7.7  |
| 1   | A     | 561  | CYS  | 7.7  |
| 1   | B     | 717  | VAL  | 7.6  |
| 1   | B     | 804  | LEU  | 7.6  |
| 1   | A     | 725  | LEU  | 7.6  |
| 1   | B     | 642  | SER  | 7.6  |
| 1   | B     | 505  | VAL  | 7.6  |
| 1   | A     | 111  | ASN  | 7.6  |
| 1   | B     | 259  | LEU  | 7.6  |
| 1   | A     | 757  | ARG  | 7.6  |
| 1   | A     | 707  | ILE  | 7.6  |
| 1   | A     | 346  | ARG  | 7.6  |
| 1   | A     | 429  | GLU  | 7.6  |
| 1   | B     | 458  | ILE  | 7.6  |
| 1   | B     | 164  | ALA  | 7.6  |
| 1   | B     | 193  | SER  | 7.6  |
| 1   | A     | 881  | THR  | 7.6  |
| 1   | B     | 628  | GLN  | 7.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 524  | GLY  | 7.6  |
| 1   | B     | 359  | THR  | 7.6  |
| 1   | B     | 1140 | SER  | 7.6  |
| 1   | B     | 626  | ILE  | 7.6  |
| 1   | A     | 238  | PRO  | 7.6  |
| 1   | B     | 955  | THR  | 7.5  |
| 1   | A     | 770  | TYR  | 7.5  |
| 1   | A     | 180  | GLN  | 7.5  |
| 1   | B     | 388  | ASN  | 7.5  |
| 1   | B     | 898  | VAL  | 7.5  |
| 1   | B     | 722  | PRO  | 7.5  |
| 1   | A     | 613  | ILE  | 7.5  |
| 1   | A     | 459  | LEU  | 7.5  |
| 1   | B     | 1054 | GLU  | 7.5  |
| 1   | B     | 833  | ARG  | 7.5  |
| 1   | A     | 654  | PHE  | 7.5  |
| 1   | A     | 683  | VAL  | 7.5  |
| 1   | A     | 460  | VAL  | 7.5  |
| 1   | B     | 959  | PRO  | 7.4  |
| 1   | A     | 803  | HIS  | 7.4  |
| 1   | A     | 976  | TRP  | 7.4  |
| 1   | A     | 370  | ARG  | 7.4  |
| 1   | A     | 148  | GLY  | 7.4  |
| 1   | A     | 54   | VAL  | 7.4  |
| 1   | B     | 135  | ILE  | 7.4  |
| 1   | A     | 1059 | SER  | 7.4  |
| 1   | A     | 388  | ASN  | 7.4  |
| 1   | A     | 288  | PRO  | 7.4  |
| 1   | B     | 102  | CYS  | 7.4  |
| 1   | A     | 882  | ILE  | 7.4  |
| 1   | B     | 709  | PRO  | 7.4  |
| 1   | B     | 113  | ASN  | 7.4  |
| 1   | A     | 841  | CYS  | 7.4  |
| 1   | B     | 1032 | GLN  | 7.4  |
| 1   | A     | 488  | LEU  | 7.4  |
| 1   | A     | 752  | ARG  | 7.4  |
| 1   | A     | 717  | VAL  | 7.4  |
| 1   | B     | 926  | SER  | 7.4  |
| 1   | B     | 958  | THR  | 7.4  |
| 1   | A     | 612  | ARG  | 7.4  |
| 1   | B     | 168  | ALA  | 7.4  |
| 1   | A     | 926  | SER  | 7.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 423  | PRO  | 7.4  |
| 1   | B     | 186  | GLY  | 7.3  |
| 1   | B     | 561  | CYS  | 7.3  |
| 1   | B     | 137  | GLN  | 7.3  |
| 1   | B     | 487  | ASP  | 7.3  |
| 1   | A     | 515  | GLN  | 7.3  |
| 1   | B     | 185  | VAL  | 7.3  |
| 1   | B     | 299  | GLY  | 7.3  |
| 1   | A     | 1118 | GLY  | 7.3  |
| 1   | A     | 101  | SER  | 7.3  |
| 1   | A     | 914  | SER  | 7.3  |
| 1   | A     | 1090 | ASN  | 7.3  |
| 1   | A     | 1169 | LEU  | 7.3  |
| 1   | B     | 519  | CYS  | 7.3  |
| 1   | A     | 909  | GLU  | 7.3  |
| 1   | A     | 495  | GLN  | 7.3  |
| 1   | B     | 95   | PRO  | 7.3  |
| 1   | A     | 81   | ALA  | 7.3  |
| 1   | A     | 437  | ALA  | 7.3  |
| 1   | A     | 216  | PHE  | 7.3  |
| 1   | A     | 744  | PHE  | 7.3  |
| 1   | A     | 1204 | LEU  | 7.3  |
| 1   | B     | 435  | VAL  | 7.2  |
| 1   | A     | 379  | GLY  | 7.2  |
| 1   | B     | 560  | GLN  | 7.2  |
| 1   | B     | 882  | ILE  | 7.2  |
| 1   | A     | 409  | PHE  | 7.2  |
| 1   | B     | 448  | ALA  | 7.2  |
| 1   | B     | 72   | LEU  | 7.2  |
| 1   | A     | 1003 | TRP  | 7.2  |
| 1   | B     | 998  | PRO  | 7.2  |
| 1   | A     | 508  | VAL  | 7.2  |
| 1   | A     | 258  | THR  | 7.2  |
| 1   | B     | 928  | LEU  | 7.2  |
| 1   | B     | 279  | LYS  | 7.2  |
| 1   | A     | 112  | VAL  | 7.2  |
| 1   | A     | 700  | MET  | 7.2  |
| 1   | A     | 72   | LEU  | 7.2  |
| 1   | B     | 1153 | LEU  | 7.2  |
| 1   | A     | 82   | HIS  | 7.2  |
| 1   | B     | 203  | ARG  | 7.2  |
| 1   | A     | 687  | ASN  | 7.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 394  | ILE  | 7.2  |
| 1   | A     | 838  | ARG  | 7.2  |
| 1   | B     | 961  | PHE  | 7.1  |
| 1   | A     | 1221 | ALA  | 7.1  |
| 1   | B     | 416  | THR  | 7.1  |
| 1   | B     | 845  | SER  | 7.1  |
| 1   | A     | 598  | PHE  | 7.1  |
| 1   | B     | 319  | GLY  | 7.1  |
| 1   | A     | 953  | ARG  | 7.1  |
| 1   | B     | 472  | ALA  | 7.1  |
| 1   | A     | 439  | ASP  | 7.1  |
| 1   | A     | 283  | LEU  | 7.1  |
| 1   | B     | 801  | GLN  | 7.1  |
| 1   | B     | 950  | SER  | 7.1  |
| 1   | A     | 778  | SER  | 7.1  |
| 1   | B     | 598  | PHE  | 7.1  |
| 1   | A     | 639  | TYR  | 7.1  |
| 1   | A     | 549  | GLU  | 7.1  |
| 1   | A     | 253  | PHE  | 7.1  |
| 1   | B     | 282  | ARG  | 7.1  |
| 1   | B     | 50   | THR  | 7.1  |
| 1   | A     | 587  | VAL  | 7.0  |
| 1   | B     | 592  | ALA  | 7.0  |
| 1   | A     | 1216 | LYS  | 7.0  |
| 1   | A     | 601  | PHE  | 7.0  |
| 1   | B     | 552  | GLN  | 7.0  |
| 1   | B     | 238  | PRO  | 7.0  |
| 1   | B     | 443  | ARG  | 7.0  |
| 1   | A     | 1026 | ILE  | 7.0  |
| 1   | A     | 163  | GLU  | 7.0  |
| 1   | A     | 227  | LEU  | 7.0  |
| 1   | A     | 552  | GLN  | 7.0  |
| 1   | A     | 447  | PHE  | 7.0  |
| 1   | B     | 171  | LEU  | 7.0  |
| 1   | B     | 1191 | GLY  | 7.0  |
| 1   | A     | 146  | LYS  | 7.0  |
| 1   | A     | 351  | LYS  | 7.0  |
| 1   | B     | 927  | THR  | 7.0  |
| 1   | A     | 455  | ILE  | 7.0  |
| 1   | B     | 337  | THR  | 7.0  |
| 1   | B     | 331  | ASP  | 7.0  |
| 1   | A     | 391  | LEU  | 7.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 497  | LEU  | 7.0  |
| 1   | B     | 66   | VAL  | 7.0  |
| 1   | B     | 981  | GLY  | 7.0  |
| 1   | A     | 443  | ARG  | 7.0  |
| 1   | B     | 940  | ARG  | 6.9  |
| 1   | B     | 1035 | ASN  | 6.9  |
| 1   | A     | 307  | TYR  | 6.9  |
| 1   | A     | 738  | ARG  | 6.9  |
| 1   | A     | 890  | ARG  | 6.9  |
| 1   | B     | 83   | VAL  | 6.9  |
| 1   | A     | 849  | TRP  | 6.9  |
| 1   | B     | 453  | GLY  | 6.9  |
| 1   | B     | 802  | ALA  | 6.9  |
| 1   | A     | 334  | VAL  | 6.9  |
| 1   | B     | 904  | LEU  | 6.9  |
| 1   | B     | 374  | CYS  | 6.9  |
| 1   | A     | 408  | ASP  | 6.9  |
| 1   | A     | 758  | PHE  | 6.9  |
| 1   | A     | 450  | THR  | 6.9  |
| 1   | A     | 984  | LEU  | 6.9  |
| 1   | B     | 447  | PHE  | 6.9  |
| 1   | B     | 780  | LEU  | 6.9  |
| 1   | B     | 480  | GLU  | 6.9  |
| 1   | A     | 440  | TYR  | 6.9  |
| 1   | B     | 752  | ARG  | 6.9  |
| 1   | A     | 688  | ALA  | 6.9  |
| 1   | A     | 695  | GLU  | 6.9  |
| 1   | A     | 1188 | VAL  | 6.9  |
| 1   | A     | 797  | PRO  | 6.9  |
| 1   | B     | 428  | LYS  | 6.9  |
| 1   | A     | 271  | ALA  | 6.9  |
| 1   | A     | 1198 | THR  | 6.9  |
| 1   | B     | 1000 | SER  | 6.9  |
| 1   | B     | 1026 | ILE  | 6.9  |
| 1   | A     | 292  | SER  | 6.9  |
| 1   | A     | 518  | SER  | 6.9  |
| 1   | B     | 949  | LEU  | 6.9  |
| 1   | B     | 146  | LYS  | 6.9  |
| 1   | B     | 894  | VAL  | 6.8  |
| 1   | B     | 856  | SER  | 6.8  |
| 1   | A     | 520  | GLU  | 6.8  |
| 1   | B     | 63   | VAL  | 6.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 629  | GLY  | 6.8  |
| 1   | A     | 560  | GLN  | 6.8  |
| 1   | A     | 834  | ARG  | 6.8  |
| 1   | B     | 261  | LEU  | 6.8  |
| 1   | B     | 166  | SER  | 6.8  |
| 1   | B     | 372  | GLN  | 6.8  |
| 1   | B     | 1001 | PHE  | 6.8  |
| 1   | A     | 715  | VAL  | 6.8  |
| 1   | A     | 331  | ASP  | 6.8  |
| 1   | B     | 454  | ARG  | 6.8  |
| 1   | B     | 906  | SER  | 6.8  |
| 1   | B     | 623  | VAL  | 6.8  |
| 1   | B     | 200  | SER  | 6.8  |
| 1   | A     | 1218 | THR  | 6.8  |
| 1   | A     | 490  | LEU  | 6.8  |
| 1   | A     | 892  | GLU  | 6.8  |
| 1   | A     | 179  | GLY  | 6.8  |
| 1   | A     | 1172 | ARG  | 6.8  |
| 1   | B     | 756  | LEU  | 6.8  |
| 1   | A     | 284  | CYS  | 6.8  |
| 1   | A     | 396  | SER  | 6.8  |
| 1   | B     | 294  | VAL  | 6.8  |
| 1   | A     | 201  | SER  | 6.7  |
| 1   | A     | 214  | PHE  | 6.7  |
| 1   | A     | 763  | LEU  | 6.7  |
| 1   | A     | 574  | THR  | 6.7  |
| 1   | A     | 664  | SER  | 6.7  |
| 1   | A     | 1167 | LEU  | 6.7  |
| 1   | A     | 329  | ALA  | 6.7  |
| 1   | A     | 962  | TYR  | 6.7  |
| 1   | A     | 622  | GLU  | 6.7  |
| 1   | B     | 334  | VAL  | 6.7  |
| 1   | A     | 415  | GLY  | 6.7  |
| 1   | A     | 946  | TYR  | 6.7  |
| 1   | A     | 867  | LEU  | 6.7  |
| 1   | B     | 124  | ARG  | 6.7  |
| 1   | A     | 494  | ARG  | 6.7  |
| 1   | A     | 935  | VAL  | 6.7  |
| 1   | A     | 547  | ARG  | 6.7  |
| 1   | A     | 1219 | VAL  | 6.7  |
| 1   | A     | 670  | ASN  | 6.7  |
| 1   | B     | 514  | VAL  | 6.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 461  | ASP  | 6.7  |
| 1   | A     | 299  | GLY  | 6.7  |
| 1   | B     | 464  | ASN  | 6.6  |
| 1   | B     | 191  | GLY  | 6.6  |
| 1   | A     | 730  | LEU  | 6.6  |
| 1   | A     | 470  | ALA  | 6.6  |
| 1   | B     | 129  | GLY  | 6.6  |
| 1   | B     | 571  | VAL  | 6.6  |
| 1   | A     | 1001 | PHE  | 6.6  |
| 1   | B     | 358  | PHE  | 6.6  |
| 1   | B     | 903  | VAL  | 6.6  |
| 1   | A     | 61   | VAL  | 6.6  |
| 1   | B     | 984  | LEU  | 6.6  |
| 1   | B     | 169  | GLY  | 6.6  |
| 1   | A     | 1205 | LEU  | 6.6  |
| 1   | B     | 713  | ILE  | 6.6  |
| 1   | A     | 802  | ALA  | 6.6  |
| 1   | B     | 138  | PHE  | 6.5  |
| 1   | B     | 201  | SER  | 6.5  |
| 1   | B     | 781  | PRO  | 6.5  |
| 1   | B     | 451  | ARG  | 6.5  |
| 1   | A     | 579  | PRO  | 6.5  |
| 1   | B     | 237  | PHE  | 6.5  |
| 1   | A     | 236  | LYS  | 6.5  |
| 1   | B     | 779  | ASP  | 6.5  |
| 1   | A     | 336  | PHE  | 6.5  |
| 1   | A     | 837  | LEU  | 6.5  |
| 1   | B     | 650  | ALA  | 6.5  |
| 1   | A     | 144  | LEU  | 6.5  |
| 1   | B     | 244  | TYR  | 6.5  |
| 1   | A     | 1132 | ARG  | 6.5  |
| 1   | A     | 114  | LYS  | 6.5  |
| 1   | A     | 251  | GLU  | 6.5  |
| 1   | B     | 475  | SER  | 6.5  |
| 1   | A     | 746  | ILE  | 6.4  |
| 1   | A     | 1133 | THR  | 6.4  |
| 1   | A     | 203  | ARG  | 6.4  |
| 1   | A     | 44   | ALA  | 6.4  |
| 1   | A     | 640  | LEU  | 6.4  |
| 1   | B     | 257  | LEU  | 6.4  |
| 1   | A     | 404  | PHE  | 6.4  |
| 1   | A     | 1039 | LYS  | 6.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 641  | LYS  | 6.4  |
| 1   | A     | 480  | GLU  | 6.4  |
| 1   | A     | 608  | LEU  | 6.4  |
| 1   | B     | 522  | CYS  | 6.4  |
| 1   | A     | 997  | ARG  | 6.4  |
| 1   | B     | 43   | VAL  | 6.4  |
| 1   | B     | 53   | VAL  | 6.4  |
| 1   | B     | 847  | ALA  | 6.4  |
| 1   | A     | 1011 | CYS  | 6.3  |
| 1   | B     | 715  | VAL  | 6.3  |
| 1   | A     | 60   | GLU  | 6.3  |
| 1   | A     | 279  | LYS  | 6.3  |
| 1   | A     | 1115 | PRO  | 6.3  |
| 1   | B     | 572  | SER  | 6.3  |
| 1   | A     | 1002 | SER  | 6.3  |
| 1   | B     | 430  | ASP  | 6.3  |
| 1   | B     | 810  | LEU  | 6.3  |
| 1   | B     | 214  | PHE  | 6.3  |
| 1   | B     | 710  | SER  | 6.3  |
| 1   | A     | 607  | ILE  | 6.3  |
| 1   | A     | 739  | GLY  | 6.3  |
| 1   | B     | 364  | LYS  | 6.3  |
| 1   | B     | 893  | ASP  | 6.3  |
| 1   | B     | 205  | MET  | 6.3  |
| 1   | B     | 182  | LYS  | 6.3  |
| 1   | B     | 902  | LYS  | 6.3  |
| 1   | B     | 134  | GLY  | 6.3  |
| 1   | B     | 281  | VAL  | 6.3  |
| 1   | A     | 751  | ALA  | 6.3  |
| 1   | A     | 452  | SER  | 6.3  |
| 1   | B     | 468  | ARG  | 6.3  |
| 1   | A     | 575  | MET  | 6.3  |
| 1   | A     | 696  | GLY  | 6.3  |
| 1   | A     | 200  | SER  | 6.2  |
| 1   | B     | 723  | ILE  | 6.2  |
| 1   | B     | 865  | LEU  | 6.2  |
| 1   | A     | 285  | VAL  | 6.2  |
| 1   | A     | 463  | ALA  | 6.2  |
| 1   | A     | 272  | GLY  | 6.2  |
| 1   | A     | 832  | GLU  | 6.2  |
| 1   | A     | 1201 | GLU  | 6.2  |
| 1   | A     | 124  | ARG  | 6.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 265  | LEU  | 6.2  |
| 1   | B     | 446  | VAL  | 6.2  |
| 1   | A     | 626  | ILE  | 6.2  |
| 1   | A     | 104  | HIS  | 6.2  |
| 1   | A     | 804  | LEU  | 6.2  |
| 1   | A     | 374  | CYS  | 6.2  |
| 1   | A     | 723  | ILE  | 6.2  |
| 1   | B     | 251  | GLU  | 6.2  |
| 1   | A     | 428  | LYS  | 6.2  |
| 1   | B     | 720  | VAL  | 6.2  |
| 1   | A     | 397  | PRO  | 6.2  |
| 1   | A     | 241  | ASP  | 6.2  |
| 1   | A     | 349  | PRO  | 6.2  |
| 1   | A     | 1034 | SER  | 6.2  |
| 1   | B     | 997  | ARG  | 6.2  |
| 1   | A     | 844  | ASP  | 6.2  |
| 1   | A     | 43   | VAL  | 6.1  |
| 1   | B     | 991  | ALA  | 6.1  |
| 1   | A     | 830  | VAL  | 6.1  |
| 1   | B     | 52   | LEU  | 6.1  |
| 1   | B     | 694  | LEU  | 6.1  |
| 1   | A     | 337  | THR  | 6.1  |
| 1   | A     | 1166 | PRO  | 6.1  |
| 1   | B     | 87   | VAL  | 6.1  |
| 1   | B     | 473  | TYR  | 6.1  |
| 1   | B     | 290  | PHE  | 6.1  |
| 1   | B     | 610  | ASP  | 6.1  |
| 1   | B     | 982  | SER  | 6.1  |
| 1   | B     | 914  | SER  | 6.1  |
| 1   | B     | 730  | LEU  | 6.1  |
| 1   | A     | 80   | ARG  | 6.1  |
| 1   | B     | 109  | THR  | 6.1  |
| 1   | B     | 1003 | TRP  | 6.1  |
| 1   | B     | 471  | LEU  | 6.1  |
| 1   | B     | 725  | LEU  | 6.1  |
| 1   | A     | 184  | PHE  | 6.1  |
| 1   | A     | 482  | ASN  | 6.0  |
| 1   | B     | 595  | ASN  | 6.0  |
| 1   | B     | 708  | LEU  | 6.0  |
| 1   | B     | 712  | HIS  | 6.0  |
| 1   | B     | 1027 | ASN  | 6.0  |
| 1   | A     | 63   | VAL  | 6.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 67   | ASN  | 6.0  |
| 1   | B     | 280  | ILE  | 6.0  |
| 1   | A     | 753  | VAL  | 6.0  |
| 1   | A     | 722  | PRO  | 6.0  |
| 1   | A     | 445  | VAL  | 6.0  |
| 1   | B     | 726  | ALA  | 6.0  |
| 1   | A     | 371  | ILE  | 6.0  |
| 1   | A     | 259  | LEU  | 6.0  |
| 1   | A     | 453  | GLY  | 6.0  |
| 1   | B     | 297  | PRO  | 6.0  |
| 1   | B     | 494  | ARG  | 6.0  |
| 1   | B     | 1038 | VAL  | 6.0  |
| 1   | A     | 718  | GLY  | 6.0  |
| 1   | B     | 256  | TYR  | 6.0  |
| 1   | A     | 645  | THR  | 5.9  |
| 1   | B     | 793  | VAL  | 5.9  |
| 1   | A     | 693  | PHE  | 5.9  |
| 1   | A     | 564  | LEU  | 5.9  |
| 1   | B     | 590  | LEU  | 5.9  |
| 1   | B     | 1012 | LEU  | 5.9  |
| 1   | B     | 147  | LEU  | 5.9  |
| 1   | A     | 840  | HIS  | 5.9  |
| 1   | B     | 455  | ILE  | 5.9  |
| 1   | A     | 302  | GLN  | 5.9  |
| 1   | B     | 953  | ARG  | 5.9  |
| 1   | B     | 360  | LEU  | 5.9  |
| 1   | A     | 625  | PRO  | 5.9  |
| 1   | B     | 782  | VAL  | 5.9  |
| 1   | B     | 605  | GLU  | 5.9  |
| 1   | B     | 719  | VAL  | 5.9  |
| 1   | B     | 116  | LEU  | 5.9  |
| 1   | A     | 458  | ILE  | 5.9  |
| 1   | A     | 1117 | LEU  | 5.9  |
| 1   | B     | 397  | PRO  | 5.9  |
| 1   | B     | 312  | ASP  | 5.9  |
| 1   | B     | 794  | ILE  | 5.8  |
| 1   | B     | 289  | LYS  | 5.8  |
| 1   | B     | 183  | LEU  | 5.8  |
| 1   | A     | 387  | LEU  | 5.8  |
| 1   | A     | 928  | LEU  | 5.8  |
| 1   | B     | 702  | GLU  | 5.8  |
| 1   | A     | 839  | HIS  | 5.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 129  | GLY  | 5.8  |
| 1   | A     | 563  | GLN  | 5.8  |
| 1   | A     | 1224 | PHE  | 5.8  |
| 1   | B     | 368  | LYS  | 5.8  |
| 1   | B     | 271  | ALA  | 5.8  |
| 1   | A     | 250  | SER  | 5.8  |
| 1   | A     | 164  | ALA  | 5.8  |
| 1   | B     | 611  | GLY  | 5.8  |
| 1   | B     | 117  | LEU  | 5.8  |
| 1   | B     | 305  | VAL  | 5.8  |
| 1   | B     | 285  | VAL  | 5.8  |
| 1   | A     | 681  | ARG  | 5.8  |
| 1   | B     | 742  | CYS  | 5.8  |
| 1   | B     | 419  | ILE  | 5.8  |
| 1   | A     | 291  | TYR  | 5.8  |
| 1   | A     | 1208 | ALA  | 5.7  |
| 1   | B     | 647  | LYS  | 5.7  |
| 1   | A     | 86   | PRO  | 5.7  |
| 1   | A     | 624  | ALA  | 5.7  |
| 1   | A     | 934  | LEU  | 5.7  |
| 1   | A     | 702  | GLU  | 5.7  |
| 1   | B     | 952  | LYS  | 5.7  |
| 1   | A     | 782  | VAL  | 5.7  |
| 1   | B     | 389  | LYS  | 5.7  |
| 1   | B     | 796  | ASN  | 5.7  |
| 1   | B     | 399  | GLN  | 5.7  |
| 1   | B     | 216  | PHE  | 5.7  |
| 1   | A     | 66   | VAL  | 5.7  |
| 1   | B     | 227  | LEU  | 5.7  |
| 1   | A     | 316  | SER  | 5.7  |
| 1   | A     | 913  | ILE  | 5.7  |
| 1   | A     | 246  | TYR  | 5.7  |
| 1   | A     | 395  | ASN  | 5.7  |
| 1   | B     | 566  | VAL  | 5.7  |
| 1   | B     | 115  | LEU  | 5.6  |
| 1   | A     | 252  | GLN  | 5.6  |
| 1   | B     | 336  | PHE  | 5.6  |
| 1   | B     | 119  | ASP  | 5.6  |
| 1   | B     | 315  | LEU  | 5.6  |
| 1   | B     | 895  | ARG  | 5.6  |
| 1   | A     | 833  | ARG  | 5.6  |
| 1   | A     | 1135 | LEU  | 5.6  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 106  | LEU  | 5.6  |
| 1   | B     | 288  | PRO  | 5.6  |
| 1   | B     | 754  | THR  | 5.6  |
| 1   | B     | 170  | VAL  | 5.6  |
| 1   | B     | 1002 | SER  | 5.6  |
| 1   | B     | 899  | HIS  | 5.6  |
| 1   | B     | 624  | ALA  | 5.6  |
| 1   | A     | 249  | ARG  | 5.6  |
| 1   | B     | 253  | PHE  | 5.6  |
| 1   | A     | 765  | CYS  | 5.6  |
| 1   | A     | 1220 | ARG  | 5.6  |
| 1   | B     | 322  | LEU  | 5.6  |
| 1   | A     | 692  | ALA  | 5.6  |
| 1   | A     | 359  | THR  | 5.6  |
| 1   | B     | 398  | LEU  | 5.6  |
| 1   | A     | 219  | GLN  | 5.6  |
| 1   | A     | 754  | THR  | 5.6  |
| 1   | B     | 618  | PRO  | 5.6  |
| 1   | B     | 757  | ARG  | 5.6  |
| 1   | A     | 600  | ASP  | 5.5  |
| 1   | A     | 199  | LEU  | 5.5  |
| 1   | B     | 172  | ILE  | 5.5  |
| 1   | B     | 141  | LEU  | 5.5  |
| 1   | B     | 945  | HIS  | 5.5  |
| 1   | B     | 59   | GLY  | 5.5  |
| 1   | B     | 391  | LEU  | 5.5  |
| 1   | A     | 489  | VAL  | 5.5  |
| 1   | B     | 786  | VAL  | 5.5  |
| 1   | A     | 496  | TYR  | 5.5  |
| 1   | B     | 747  | PRO  | 5.5  |
| 1   | B     | 474  | GLU  | 5.5  |
| 1   | A     | 767  | ASN  | 5.5  |
| 1   | A     | 1190 | ILE  | 5.5  |
| 1   | A     | 550  | GLU  | 5.5  |
| 1   | B     | 155  | GLU  | 5.5  |
| 1   | B     | 517  | THR  | 5.5  |
| 1   | B     | 909  | GLU  | 5.5  |
| 1   | A     | 798  | GLN  | 5.5  |
| 1   | B     | 855  | GLY  | 5.5  |
| 1   | B     | 217  | VAL  | 5.5  |
| 1   | B     | 570  | ASN  | 5.5  |
| 1   | A     | 319  | GLY  | 5.4  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 800  | ILE  | 5.4  |
| 1   | A     | 154  | LYS  | 5.4  |
| 1   | A     | 1199 | VAL  | 5.4  |
| 1   | B     | 233  | THR  | 5.4  |
| 1   | A     | 728  | ARG  | 5.4  |
| 1   | A     | 497  | LEU  | 5.4  |
| 1   | A     | 1006 | SER  | 5.4  |
| 1   | A     | 301  | GLU  | 5.4  |
| 1   | A     | 864  | ILE  | 5.4  |
| 1   | B     | 349  | PRO  | 5.4  |
| 1   | B     | 199  | LEU  | 5.4  |
| 1   | A     | 611  | GLY  | 5.4  |
| 1   | B     | 85   | GLY  | 5.4  |
| 1   | A     | 265  | LEU  | 5.4  |
| 1   | A     | 710  | SER  | 5.4  |
| 1   | A     | 783  | ASN  | 5.4  |
| 1   | B     | 252  | GLN  | 5.4  |
| 1   | A     | 551  | PRO  | 5.3  |
| 1   | B     | 951  | PRO  | 5.3  |
| 1   | A     | 599  | GLU  | 5.3  |
| 1   | A     | 436  | ALA  | 5.3  |
| 1   | A     | 927  | THR  | 5.3  |
| 1   | A     | 781  | PRO  | 5.3  |
| 1   | A     | 829  | CYS  | 5.3  |
| 1   | B     | 431  | GLY  | 5.3  |
| 1   | A     | 142  | ASP  | 5.3  |
| 1   | B     | 404  | PHE  | 5.3  |
| 1   | B     | 206  | ALA  | 5.3  |
| 1   | A     | 233  | THR  | 5.3  |
| 1   | B     | 608  | LEU  | 5.3  |
| 1   | A     | 514  | VAL  | 5.3  |
| 1   | B     | 125  | LEU  | 5.3  |
| 1   | A     | 254  | VAL  | 5.3  |
| 1   | A     | 771  | SER  | 5.3  |
| 1   | A     | 993  | SER  | 5.3  |
| 1   | A     | 153  | ARG  | 5.3  |
| 1   | A     | 727  | ALA  | 5.3  |
| 1   | A     | 290  | PHE  | 5.2  |
| 1   | A     | 171  | LEU  | 5.2  |
| 1   | A     | 53   | VAL  | 5.2  |
| 1   | B     | 1005 | ASN  | 5.2  |
| 1   | B     | 784  | LEU  | 5.2  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 118  | LEU  | 5.2  |
| 1   | B     | 417  | VAL  | 5.2  |
| 1   | A     | 691  | CYS  | 5.2  |
| 1   | A     | 356  | CYS  | 5.2  |
| 1   | B     | 387  | LEU  | 5.2  |
| 1   | A     | 88   | GLU  | 5.2  |
| 1   | A     | 742  | CYS  | 5.2  |
| 1   | B     | 744  | PHE  | 5.2  |
| 1   | A     | 720  | VAL  | 5.2  |
| 1   | A     | 328  | LEU  | 5.2  |
| 1   | A     | 345  | ASN  | 5.2  |
| 1   | A     | 786  | VAL  | 5.2  |
| 1   | A     | 992  | VAL  | 5.2  |
| 1   | A     | 300  | CYS  | 5.2  |
| 1   | A     | 481  | GLY  | 5.2  |
| 1   | A     | 289  | LYS  | 5.2  |
| 1   | A     | 772  | TYR  | 5.1  |
| 1   | B     | 165  | GLY  | 5.1  |
| 1   | B     | 321  | ALA  | 5.1  |
| 1   | A     | 141  | LEU  | 5.1  |
| 1   | A     | 313  | ALA  | 5.1  |
| 1   | A     | 389  | LYS  | 5.1  |
| 1   | A     | 77   | THR  | 5.1  |
| 1   | B     | 785  | SER  | 5.1  |
| 1   | A     | 745  | HIS  | 5.1  |
| 1   | B     | 127  | ALA  | 5.1  |
| 1   | B     | 520  | GLU  | 5.1  |
| 1   | B     | 758  | PHE  | 5.1  |
| 1   | A     | 647  | LYS  | 5.1  |
| 1   | A     | 367  | ILE  | 5.1  |
| 1   | B     | 753  | VAL  | 5.1  |
| 1   | A     | 68   | ARG  | 5.1  |
| 1   | B     | 1036 | PRO  | 5.1  |
| 1   | B     | 567  | GLN  | 5.0  |
| 1   | A     | 793  | VAL  | 5.0  |
| 1   | B     | 866  | LYS  | 5.0  |
| 1   | B     | 128  | CYS  | 5.0  |
| 1   | A     | 182  | LYS  | 5.0  |
| 1   | B     | 765  | CYS  | 5.0  |
| 1   | A     | 147  | LEU  | 5.0  |
| 1   | B     | 418  | THR  | 5.0  |
| 1   | B     | 450  | THR  | 5.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 557  | ASP  | 5.0  |
| 1   | B     | 881  | THR  | 5.0  |
| 1   | B     | 1006 | SER  | 5.0  |
| 1   | A     | 50   | THR  | 5.0  |
| 1   | A     | 823  | ARG  | 5.0  |
| 1   | A     | 461  | ASP  | 5.0  |
| 1   | A     | 856  | SER  | 5.0  |
| 1   | B     | 178  | GLN  | 5.0  |
| 1   | A     | 788  | TRP  | 5.0  |
| 1   | B     | 727  | ALA  | 5.0  |
| 1   | B     | 1180 | GLY  | 5.0  |
| 1   | A     | 799  | ASN  | 4.9  |
| 1   | A     | 1136 | VAL  | 4.9  |
| 1   | B     | 615  | CYS  | 4.9  |
| 1   | A     | 1035 | ASN  | 4.9  |
| 1   | A     | 225  | SER  | 4.9  |
| 1   | A     | 145  | PHE  | 4.9  |
| 1   | B     | 768  | SER  | 4.9  |
| 1   | B     | 1138 | ASN  | 4.9  |
| 1   | B     | 194  | GLU  | 4.9  |
| 1   | B     | 452  | SER  | 4.9  |
| 1   | A     | 441  | GLN  | 4.9  |
| 1   | B     | 601  | PHE  | 4.9  |
| 1   | A     | 315  | LEU  | 4.9  |
| 1   | B     | 773  | GLU  | 4.9  |
| 1   | B     | 625  | PRO  | 4.8  |
| 1   | B     | 462  | LEU  | 4.8  |
| 1   | B     | 640  | LEU  | 4.8  |
| 1   | A     | 747  | PRO  | 4.8  |
| 1   | B     | 763  | LEU  | 4.8  |
| 1   | B     | 64   | GLY  | 4.8  |
| 1   | B     | 345  | ASN  | 4.8  |
| 1   | A     | 320  | GLN  | 4.8  |
| 1   | B     | 549  | GLU  | 4.8  |
| 1   | A     | 1185 | ASN  | 4.8  |
| 1   | B     | 320  | GLN  | 4.8  |
| 1   | B     | 77   | THR  | 4.8  |
| 1   | B     | 777  | VAL  | 4.8  |
| 1   | A     | 105  | GLY  | 4.8  |
| 1   | A     | 335  | LEU  | 4.8  |
| 1   | A     | 638  | LEU  | 4.8  |
| 1   | A     | 694  | LEU  | 4.8  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 287  | ASP  | 4.8  |
| 1   | A     | 590  | LEU  | 4.8  |
| 1   | A     | 84   | THR  | 4.8  |
| 1   | A     | 51   | HIS  | 4.8  |
| 1   | A     | 884  | GLY  | 4.7  |
| 1   | B     | 734  | GLN  | 4.7  |
| 1   | A     | 1165 | SER  | 4.7  |
| 1   | A     | 1138 | ASN  | 4.7  |
| 1   | A     | 855  | GLY  | 4.7  |
| 1   | A     | 286  | ASN  | 4.7  |
| 1   | A     | 821  | ASP  | 4.7  |
| 1   | A     | 1005 | ASN  | 4.7  |
| 1   | B     | 746  | ILE  | 4.7  |
| 1   | B     | 86   | PRO  | 4.7  |
| 1   | B     | 764  | GLN  | 4.7  |
| 1   | A     | 734  | GLN  | 4.7  |
| 1   | B     | 751  | ALA  | 4.7  |
| 1   | A     | 666  | LEU  | 4.7  |
| 1   | B     | 367  | ILE  | 4.7  |
| 1   | A     | 213  | MET  | 4.7  |
| 1   | B     | 606  | SER  | 4.7  |
| 1   | A     | 468  | ARG  | 4.6  |
| 1   | B     | 177  | GLY  | 4.6  |
| 1   | A     | 78   | LEU  | 4.6  |
| 1   | A     | 305  | VAL  | 4.6  |
| 1   | B     | 126  | LEU  | 4.6  |
| 1   | B     | 246  | TYR  | 4.6  |
| 1   | B     | 409  | PHE  | 4.6  |
| 1   | A     | 138  | PHE  | 4.6  |
| 1   | B     | 365  | GLU  | 4.6  |
| 1   | B     | 292  | SER  | 4.6  |
| 1   | B     | 236  | LYS  | 4.6  |
| 1   | B     | 1192 | SER  | 4.6  |
| 1   | A     | 234  | LEU  | 4.6  |
| 1   | A     | 446  | VAL  | 4.6  |
| 1   | B     | 718  | GLY  | 4.6  |
| 1   | B     | 283  | LEU  | 4.5  |
| 1   | A     | 296  | PHE  | 4.5  |
| 1   | B     | 853  | HIS  | 4.5  |
| 1   | B     | 616  | HIS  | 4.5  |
| 1   | B     | 351  | LYS  | 4.5  |
| 1   | A     | 257  | LEU  | 4.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 521  | LEU  | 4.5  |
| 1   | A     | 168  | ALA  | 4.5  |
| 1   | A     | 87   | VAL  | 4.5  |
| 1   | A     | 784  | LEU  | 4.5  |
| 1   | B     | 575  | MET  | 4.5  |
| 1   | B     | 386  | LEU  | 4.5  |
| 1   | A     | 204  | LEU  | 4.5  |
| 1   | B     | 800  | ILE  | 4.5  |
| 1   | B     | 254  | VAL  | 4.5  |
| 1   | B     | 429  | GLU  | 4.5  |
| 1   | A     | 741  | GLU  | 4.4  |
| 1   | B     | 370  | ARG  | 4.4  |
| 1   | B     | 690  | ASP  | 4.4  |
| 1   | A     | 119  | ASP  | 4.4  |
| 1   | B     | 492  | PRO  | 4.4  |
| 1   | A     | 281  | VAL  | 4.4  |
| 1   | B     | 655  | VAL  | 4.4  |
| 1   | A     | 59   | GLY  | 4.4  |
| 1   | A     | 1168 | ILE  | 4.4  |
| 1   | A     | 462  | LEU  | 4.4  |
| 1   | B     | 324  | LYS  | 4.4  |
| 1   | A     | 358  | PHE  | 4.4  |
| 1   | B     | 225  | SER  | 4.4  |
| 1   | A     | 755  | ALA  | 4.4  |
| 1   | B     | 910  | SER  | 4.4  |
| 1   | A     | 109  | THR  | 4.3  |
| 1   | B     | 612  | ARG  | 4.3  |
| 1   | B     | 218  | TYR  | 4.3  |
| 1   | A     | 185  | VAL  | 4.3  |
| 1   | B     | 897  | GLY  | 4.3  |
| 1   | B     | 303  | ALA  | 4.3  |
| 1   | B     | 356  | CYS  | 4.3  |
| 1   | B     | 107  | GLY  | 4.3  |
| 1   | B     | 622  | GLU  | 4.3  |
| 1   | B     | 607  | ILE  | 4.3  |
| 1   | B     | 179  | GLY  | 4.3  |
| 1   | B     | 481  | GLY  | 4.3  |
| 1   | A     | 65   | ALA  | 4.3  |
| 1   | A     | 167  | MET  | 4.3  |
| 1   | A     | 785  | SER  | 4.3  |
| 1   | B     | 371  | ILE  | 4.3  |
| 1   | B     | 550  | GLU  | 4.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 492  | PRO  | 4.3  |
| 1   | A     | 230  | PRO  | 4.3  |
| 1   | A     | 464  | ASN  | 4.3  |
| 1   | B     | 255  | TYR  | 4.3  |
| 1   | B     | 357  | LEU  | 4.2  |
| 1   | B     | 613  | ILE  | 4.2  |
| 1   | A     | 79   | LEU  | 4.2  |
| 1   | A     | 366  | LYS  | 4.2  |
| 1   | A     | 737  | GLN  | 4.2  |
| 1   | B     | 422  | THR  | 4.2  |
| 1   | A     | 1012 | LEU  | 4.2  |
| 1   | B     | 323  | ALA  | 4.2  |
| 1   | B     | 156  | HIS  | 4.2  |
| 1   | B     | 960  | THR  | 4.2  |
| 1   | B     | 996  | GLY  | 4.2  |
| 1   | B     | 139  | LEU  | 4.2  |
| 1   | A     | 952  | LYS  | 4.2  |
| 1   | A     | 143  | ASP  | 4.2  |
| 1   | B     | 892  | GLU  | 4.1  |
| 1   | A     | 386  | LEU  | 4.1  |
| 1   | B     | 373  | SER  | 4.1  |
| 1   | B     | 846  | PRO  | 4.1  |
| 1   | A     | 769  | SER  | 4.1  |
| 1   | A     | 67   | ASN  | 4.1  |
| 1   | B     | 654  | PHE  | 4.1  |
| 1   | B     | 108  | SER  | 4.1  |
| 1   | A     | 128  | CYS  | 4.1  |
| 1   | B     | 407  | GLN  | 4.1  |
| 1   | A     | 635  | VAL  | 4.1  |
| 1   | B     | 366  | LYS  | 4.1  |
| 1   | A     | 780  | LEU  | 4.1  |
| 1   | A     | 224  | SER  | 4.0  |
| 1   | A     | 64   | GLY  | 4.0  |
| 1   | B     | 733  | PRO  | 4.0  |
| 1   | A     | 843  | ALA  | 4.0  |
| 1   | A     | 585  | TRP  | 4.0  |
| 1   | A     | 215  | GLY  | 4.0  |
| 1   | A     | 576  | SER  | 4.0  |
| 1   | B     | 335  | LEU  | 4.0  |
| 1   | A     | 1038 | VAL  | 4.0  |
| 1   | B     | 250  | SER  | 4.0  |
| 1   | B     | 80   | ARG  | 4.0  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 291  | TYR  | 4.0  |
| 1   | A     | 211  | ALA  | 4.0  |
| 1   | A     | 1203 | GLN  | 4.0  |
| 1   | A     | 491  | SER  | 4.0  |
| 1   | B     | 728  | ARG  | 4.0  |
| 1   | B     | 51   | HIS  | 4.0  |
| 1   | B     | 284  | CYS  | 3.9  |
| 1   | A     | 364  | LYS  | 3.9  |
| 1   | A     | 1209 | PRO  | 3.9  |
| 1   | B     | 144  | LEU  | 3.9  |
| 1   | A     | 578  | VAL  | 3.9  |
| 1   | A     | 242  | ILE  | 3.9  |
| 1   | A     | 748  | GLY  | 3.9  |
| 1   | B     | 797  | PRO  | 3.9  |
| 1   | A     | 708  | LEU  | 3.9  |
| 1   | A     | 1187 | THR  | 3.9  |
| 1   | A     | 1200 | SER  | 3.9  |
| 1   | A     | 1227 | SER  | 3.9  |
| 1   | B     | 154  | LYS  | 3.8  |
| 1   | B     | 248  | PHE  | 3.8  |
| 1   | B     | 493  | ASN  | 3.8  |
| 1   | B     | 363  | ILE  | 3.8  |
| 1   | A     | 248  | PHE  | 3.8  |
| 1   | B     | 491  | SER  | 3.8  |
| 1   | A     | 85   | GLY  | 3.8  |
| 1   | A     | 139  | LEU  | 3.8  |
| 1   | B     | 564  | LEU  | 3.8  |
| 1   | A     | 1189 | LEU  | 3.8  |
| 1   | A     | 592  | ALA  | 3.8  |
| 1   | B     | 420  | GLU  | 3.8  |
| 1   | A     | 325  | GLN  | 3.8  |
| 1   | B     | 230  | PRO  | 3.8  |
| 1   | A     | 651  | SER  | 3.7  |
| 1   | A     | 929  | ARG  | 3.7  |
| 1   | B     | 558  | LEU  | 3.7  |
| 1   | A     | 280  | ILE  | 3.7  |
| 1   | B     | 406  | GLY  | 3.7  |
| 1   | B     | 78   | LEU  | 3.7  |
| 1   | B     | 325  | GLN  | 3.7  |
| 1   | A     | 169  | GLY  | 3.7  |
| 1   | A     | 1197 | LEU  | 3.7  |
| 1   | B     | 224  | SER  | 3.7  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 896  | LEU  | 3.7  |
| 1   | B     | 591  | SER  | 3.7  |
| 1   | A     | 996  | GLY  | 3.6  |
| 1   | A     | 1210 | ASN  | 3.6  |
| 1   | B     | 568  | PRO  | 3.6  |
| 1   | B     | 79   | LEU  | 3.6  |
| 1   | B     | 580  | LEU  | 3.6  |
| 1   | A     | 667  | ALA  | 3.6  |
| 1   | B     | 942  | CYS  | 3.6  |
| 1   | A     | 357  | LEU  | 3.6  |
| 1   | A     | 127  | ALA  | 3.5  |
| 1   | B     | 597  | SER  | 3.5  |
| 1   | A     | 1000 | SER  | 3.5  |
| 1   | A     | 709  | PRO  | 3.5  |
| 1   | B     | 584  | ALA  | 3.5  |
| 1   | B     | 249  | ARG  | 3.5  |
| 1   | A     | 322  | LEU  | 3.5  |
| 1   | A     | 636  | VAL  | 3.5  |
| 1   | B     | 755  | ALA  | 3.5  |
| 1   | A     | 689  | ALA  | 3.4  |
| 1   | B     | 326  | LEU  | 3.4  |
| 1   | B     | 55   | HIS  | 3.4  |
| 1   | A     | 619  | SER  | 3.4  |
| 1   | A     | 125  | LEU  | 3.4  |
| 1   | B     | 614  | HIS  | 3.4  |
| 1   | B     | 743  | LEU  | 3.4  |
| 1   | A     | 244  | TYR  | 3.4  |
| 1   | A     | 999  | CYS  | 3.4  |
| 1   | A     | 113  | ASN  | 3.4  |
| 1   | A     | 140  | ARG  | 3.4  |
| 1   | A     | 416  | THR  | 3.4  |
| 1   | B     | 223  | VAL  | 3.4  |
| 1   | A     | 255  | TYR  | 3.3  |
| 1   | B     | 234  | LEU  | 3.3  |
| 1   | B     | 314  | TYR  | 3.3  |
| 1   | A     | 369  | GLU  | 3.3  |
| 1   | A     | 183  | LEU  | 3.3  |
| 1   | B     | 913  | ILE  | 3.3  |
| 1   | B     | 574  | THR  | 3.3  |
| 1   | B     | 211  | ALA  | 3.3  |
| 1   | B     | 585  | TRP  | 3.3  |
| 1   | A     | 777  | VAL  | 3.3  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 176  | PRO  | 3.3  |
| 1   | B     | 327  | GLY  | 3.3  |
| 1   | B     | 1037 | GLU  | 3.3  |
| 1   | A     | 762  | SER  | 3.3  |
| 1   | A     | 376  | ARG  | 3.3  |
| 1   | A     | 1226 | PHE  | 3.3  |
| 1   | A     | 671  | GLY  | 3.2  |
| 1   | A     | 883  | THR  | 3.2  |
| 1   | A     | 186  | GLY  | 3.2  |
| 1   | B     | 741  | GLU  | 3.2  |
| 1   | A     | 360  | LEU  | 3.2  |
| 1   | B     | 740  | TYR  | 3.2  |
| 1   | A     | 493  | ASN  | 3.2  |
| 1   | A     | 1195 | CYS  | 3.2  |
| 1   | A     | 170  | VAL  | 3.2  |
| 1   | B     | 565  | THR  | 3.2  |
| 1   | B     | 45   | SER  | 3.2  |
| 1   | A     | 172  | ILE  | 3.2  |
| 1   | B     | 582  | LEU  | 3.2  |
| 1   | B     | 581  | VAL  | 3.2  |
| 1   | A     | 646  | GLY  | 3.1  |
| 1   | A     | 949  | LEU  | 3.1  |
| 1   | B     | 745  | HIS  | 3.1  |
| 1   | B     | 247  | SER  | 3.1  |
| 1   | B     | 521  | LEU  | 3.1  |
| 1   | B     | 369  | GLU  | 3.1  |
| 1   | B     | 142  | ASP  | 3.1  |
| 1   | B     | 313  | ALA  | 3.1  |
| 1   | A     | 304  | GLY  | 3.0  |
| 1   | B     | 518  | SER  | 3.0  |
| 1   | A     | 126  | LEU  | 3.0  |
| 1   | A     | 314  | TYR  | 3.0  |
| 1   | B     | 569  | ARG  | 3.0  |
| 1   | A     | 1153 | LEU  | 3.0  |
| 1   | A     | 55   | HIS  | 3.0  |
| 1   | A     | 363  | ILE  | 3.0  |
| 1   | A     | 749  | SER  | 3.0  |
| 1   | A     | 1223 | GLY  | 3.0  |
| 1   | A     | 628  | GLN  | 3.0  |
| 1   | B     | 760  | SER  | 3.0  |
| 1   | B     | 405  | CYS  | 2.9  |
| 1   | B     | 599  | GLU  | 2.9  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | A     | 256  | TYR  | 2.9  |
| 1   | A     | 853  | HIS  | 2.9  |
| 1   | B     | 442  | GLY  | 2.9  |
| 1   | A     | 422  | THR  | 2.9  |
| 1   | A     | 577  | GLN  | 2.9  |
| 1   | B     | 38   | ALA  | 2.9  |
| 1   | B     | 711  | THR  | 2.9  |
| 1   | A     | 107  | GLY  | 2.8  |
| 1   | A     | 950  | SER  | 2.8  |
| 1   | A     | 1194 | PRO  | 2.8  |
| 1   | A     | 586  | ASN  | 2.8  |
| 1   | A     | 326  | LEU  | 2.8  |
| 1   | A     | 365  | GLU  | 2.8  |
| 1   | B     | 791  | ASN  | 2.8  |
| 1   | A     | 787  | VAL  | 2.8  |
| 1   | B     | 689  | ALA  | 2.8  |
| 1   | B     | 943  | SER  | 2.7  |
| 1   | B     | 609  | GLU  | 2.7  |
| 1   | B     | 639  | TYR  | 2.7  |
| 1   | A     | 419  | ILE  | 2.7  |
| 1   | B     | 46   | ASP  | 2.7  |
| 1   | B     | 121  | ALA  | 2.7  |
| 1   | A     | 116  | LEU  | 2.7  |
| 1   | B     | 173  | ALA  | 2.7  |
| 1   | B     | 213  | MET  | 2.7  |
| 1   | A     | 1191 | GLY  | 2.7  |
| 1   | B     | 304  | GLY  | 2.6  |
| 1   | A     | 243  | TYR  | 2.6  |
| 1   | B     | 775  | ASN  | 2.6  |
| 1   | A     | 621  | ARG  | 2.6  |
| 1   | B     | 617  | SER  | 2.6  |
| 1   | B     | 551  | PRO  | 2.6  |
| 1   | B     | 638  | LEU  | 2.6  |
| 1   | A     | 297  | PRO  | 2.6  |
| 1   | B     | 583  | GLN  | 2.6  |
| 1   | B     | 215  | GLY  | 2.6  |
| 1   | B     | 792  | PHE  | 2.6  |
| 1   | A     | 620  | ALA  | 2.6  |
| 1   | A     | 609  | GLU  | 2.5  |
| 1   | A     | 941  | ASP  | 2.5  |
| 1   | B     | 362  | ALA  | 2.5  |
| 1   | A     | 247  | SER  | 2.5  |

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| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 1   | B     | 37   | PRO  | 2.5  |
| 1   | B     | 941  | ASP  | 2.5  |
| 1   | A     | 942  | CYS  | 2.5  |
| 1   | A     | 303  | ALA  | 2.5  |
| 1   | A     | 761  | SER  | 2.4  |
| 1   | B     | 210  | ASP  | 2.4  |
| 1   | A     | 361  | ARG  | 2.4  |
| 1   | A     | 205  | MET  | 2.4  |
| 1   | B     | 123  | ASN  | 2.4  |
| 1   | B     | 145  | PHE  | 2.4  |
| 1   | A     | 743  | LEU  | 2.4  |
| 1   | A     | 117  | LEU  | 2.4  |
| 1   | A     | 377  | GLY  | 2.4  |
| 1   | B     | 219  | GLN  | 2.4  |
| 1   | B     | 122  | ALA  | 2.4  |
| 1   | A     | 845  | SER  | 2.4  |
| 1   | A     | 115  | LEU  | 2.3  |
| 1   | A     | 165  | GLY  | 2.3  |
| 1   | A     | 83   | VAL  | 2.3  |
| 1   | A     | 212  | ASP  | 2.3  |
| 1   | B     | 140  | ARG  | 2.3  |
| 1   | A     | 37   | PRO  | 2.3  |
| 1   | B     | 421  | GLY  | 2.3  |
| 1   | B     | 153  | ARG  | 2.3  |
| 1   | A     | 166  | SER  | 2.3  |
| 1   | A     | 848  | SER  | 2.3  |
| 1   | B     | 788  | TRP  | 2.3  |
| 1   | A     | 323  | ALA  | 2.3  |
| 1   | B     | 287  | ASP  | 2.2  |
| 1   | A     | 38   | ALA  | 2.2  |
| 1   | B     | 783  | ASN  | 2.2  |
| 1   | B     | 212  | ASP  | 2.2  |
| 1   | B     | 748  | GLY  | 2.2  |
| 1   | A     | 690  | ASP  | 2.2  |
| 1   | B     | 1139 | SER  | 2.2  |
| 1   | B     | 749  | SER  | 2.2  |
| 1   | B     | 759  | ASN  | 2.2  |
| 1   | B     | 58   | THR  | 2.2  |
| 1   | A     | 121  | ALA  | 2.1  |
| 1   | A     | 630  | GLN  | 2.1  |
| 1   | A     | 750  | PRO  | 2.1  |
| 1   | B     | 207  | ASN  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 120 | TYR  | 2.1  |
| 1   | A     | 589 | ASP  | 2.1  |
| 1   | A     | 378 | GLU  | 2.1  |
| 1   | A     | 220 | ASP  | 2.0  |
| 1   | B     | 737 | GLN  | 2.0  |
| 1   | A     | 944 | LEU  | 2.0  |
| 1   | A     | 223 | VAL  | 2.0  |
| 1   | A     | 951 | PRO  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|-------|----------------------------|-------|
| 2   | NAG  | A     | 1314 | 14/15 | 0.46  | 2.21 | 0.03  | 271,271,271,271            | 0     |
| 2   | NAG  | A     | 1301 | 14/15 | 0.44  | 1.71 | 0.01  | 242,242,242,242            | 0     |
| 2   | NAG  | B     | 1305 | 14/15 | 0.79  | 1.81 | -0.01 | 282,282,282,282            | 0     |
| 2   | NAG  | B     | 1315 | 14/15 | 0.48  | 2.13 | -0.19 | 282,282,282,282            | 0     |
| 2   | NAG  | B     | 1301 | 14/15 | 0.33  | 1.67 | -0.43 | 243,243,243,243            | 0     |
| 2   | NAG  | B     | 1331 | 14/15 | -0.52 | 3.55 | -0.58 | 308,308,308,308            | 0     |
| 2   | NAG  | A     | 1329 | 14/15 | -0.35 | 2.59 | -0.76 | 314,314,314,314            | 0     |
| 2   | NAG  | A     | 1305 | 14/15 | 0.59  | 1.75 | -1.15 | 271,271,271,271            | 0     |
| 2   | NAG  | B     | 1327 | 14/15 | 0.14  | 2.40 | -     | 270,270,270,270            | 0     |
| 2   | NAG  | A     | 1311 | 14/15 | 0.65  | 1.67 | -     | 271,271,271,271            | 0     |
| 3   | BMA  | B     | 1313 | 11/12 | 0.09  | 1.03 | -     | 282,282,282,282            | 0     |
| 2   | NAG  | A     | 1335 | 14/15 | 0.09  | 3.39 | -     | 359,359,359,359            | 0     |
| 2   | NAG  | A     | 1310 | 14/15 | 0.71  | 1.99 | -     | 271,271,271,271            | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 4   | MAN  | B     | 1336 | 11/12 | -0.34 | 1.17 | -    | 308,308,308,308             | 0     |
| 3   | BMA  | B     | 1317 | 11/12 | 0.73  | 0.94 | -    | 282,282,282,282             | 0     |
| 3   | BMA  | A     | 1328 | 11/12 | -0.16 | 0.89 | -    | 248,248,248,248             | 0     |
| 4   | MAN  | B     | 1340 | 11/12 | 0.09  | 1.51 | -    | 365,365,365,365             | 0     |
| 2   | NAG  | B     | 1322 | 14/15 | -0.01 | 1.98 | -    | 251,251,251,251             | 0     |
| 4   | MAN  | A     | 1340 | 11/12 | -0.30 | 1.60 | -    | 359,359,359,359             | 0     |
| 3   | BMA  | B     | 1330 | 11/12 | -0.10 | 1.55 | -    | 270,270,270,270             | 0     |
| 3   | BMA  | B     | 1333 | 11/12 | 0.04  | 1.39 | -    | 308,308,308,308             | 0     |
| 3   | BMA  | B     | 1325 | 11/12 | 0.71  | 0.54 | -    | 270,270,270,270             | 0     |
| 2   | NAG  | A     | 1323 | 14/15 | 0.59  | 0.62 | -    | 248,248,248,248             | 0     |
| 2   | NAG  | B     | 1329 | 14/15 | 0.63  | 1.51 | -    | 270,270,270,270             | 0     |
| 4   | MAN  | A     | 1318 | 11/12 | 0.41  | 0.72 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | B     | 1321 | 11/12 | -0.21 | 3.33 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | B     | 1306 | 14/15 | 0.77  | 2.40 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | B     | 1332 | 14/15 | -0.15 | 3.29 | -    | 308,308,308,308             | 0     |
| 4   | MAN  | A     | 1339 | 11/12 | -0.01 | 2.96 | -    | 359,359,359,359             | 0     |
| 2   | NAG  | B     | 1311 | 14/15 | 0.59  | 2.07 | -    | 282,282,282,282             | 0     |
| 4   | MAN  | B     | 1341 | 11/12 | 0.10  | 2.90 | -    | 365,365,365,365             | 0     |
| 3   | BMA  | A     | 1312 | 11/12 | 0.54  | 0.80 | -    | 271,271,271,271             | 0     |
| 3   | BMA  | B     | 1303 | 11/12 | 0.83  | 0.51 | -    | 243,243,243,243             | 0     |
| 2   | NAG  | B     | 1337 | 14/15 | -0.24 | 2.82 | -    | 365,365,365,365             | 0     |
| 4   | MAN  | A     | 1333 | 11/12 | -0.52 | 2.47 | -    | 314,314,314,314             | 0     |
| 3   | BMA  | B     | 1307 | 11/12 | 0.28  | 2.38 | -    | 282,282,282,282             | 0     |
| 4   | MAN  | A     | 1304 | 11/12 | 0.46  | 0.98 | -    | 242,242,242,242             | 0     |
| 2   | NAG  | A     | 1322 | 14/15 | 0.54  | 0.70 | -    | 248,248,248,248             | 0     |
| 4   | MAN  | B     | 1343 | 11/12 | -0.16 | 1.76 | -    | 365,365,365,365             | 0     |
| 4   | MAN  | A     | 1313 | 11/12 | 0.60  | 0.43 | -    | 271,271,271,271             | 0     |
| 2   | NAG  | A     | 1326 | 14/15 | 0.49  | 2.04 | -    | 248,248,248,248             | 0     |
| 2   | NAG  | A     | 1321 | 14/15 | 0.19  | 1.53 | -    | 240,240,240,240             | 0     |
| 4   | MAN  | A     | 1319 | 11/12 | 0.09  | 0.53 | -    | 271,271,271,271             | 0     |
| 2   | NAG  | B     | 1324 | 14/15 | 0.10  | 1.18 | -    | 270,270,270,270             | 0     |
| 3   | BMA  | A     | 1331 | 11/12 | -0.17 | 1.93 | -    | 314,314,314,314             | 0     |
| 4   | MAN  | B     | 1326 | 11/12 | 0.51  | 0.39 | -    | 270,270,270,270             | 0     |
| 4   | MAN  | A     | 1309 | 11/12 | 0.44  | 1.20 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | B     | 1318 | 11/12 | 0.76  | 1.10 | -    | 282,282,282,282             | 0     |
| 3   | BMA  | A     | 1303 | 11/12 | 0.51  | 1.03 | -    | 242,242,242,242             | 0     |
| 4   | MAN  | A     | 1337 | 11/12 | -0.30 | 1.50 | -    | 359,359,359,359             | 0     |
| 3   | BMA  | A     | 1336 | 11/12 | 0.10  | 2.79 | -    | 359,359,359,359             | 0     |
| 2   | NAG  | A     | 1306 | 14/15 | 0.82  | 1.29 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | B     | 1319 | 11/12 | 0.38  | 0.93 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | A     | 1302 | 14/15 | 0.76  | 1.03 | -    | 242,242,242,242             | 0     |
| 4   | MAN  | A     | 1332 | 11/12 | 0.18  | 2.39 | -    | 314,314,314,314             | 0     |

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| Mol | Type | Chain | Res  | Atoms | RSCC  | RSR  | LLDF | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|-------|------|------|-----------------------------|-------|
| 2   | NAG  | A     | 1325 | 14/15 | 0.10  | 0.83 | -    | 248,248,248,248             | 0     |
| 2   | NAG  | B     | 1316 | 14/15 | 0.83  | 1.39 | -    | 282,282,282,282             | 0     |
| 4   | MAN  | B     | 1309 | 11/12 | 0.29  | 1.67 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | B     | 1312 | 14/15 | 0.38  | 1.19 | -    | 282,282,282,282             | 0     |
| 3   | BMA  | A     | 1324 | 11/12 | 0.80  | 0.36 | -    | 248,248,248,248             | 0     |
| 4   | MAN  | B     | 1308 | 11/12 | 0.19  | 1.73 | -    | 282,282,282,282             | 0     |
| 4   | MAN  | B     | 1320 | 11/12 | 0.42  | 0.64 | -    | 282,282,282,282             | 0     |
| 4   | MAN  | A     | 1308 | 11/12 | 0.54  | 0.79 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | A     | 1320 | 11/12 | -0.02 | 1.13 | -    | 271,271,271,271             | 0     |
| 2   | NAG  | A     | 1327 | 14/15 | 0.59  | 1.92 | -    | 248,248,248,248             | 0     |
| 2   | NAG  | B     | 1323 | 14/15 | 0.01  | 0.96 | -    | 270,270,270,270             | 0     |
| 4   | MAN  | A     | 1338 | 11/12 | -0.04 | 2.37 | -    | 359,359,359,359             | 0     |
| 4   | MAN  | B     | 1342 | 11/12 | -0.54 | 3.79 | -    | 365,365,365,365             | 0     |
| 4   | MAN  | B     | 1314 | 11/12 | -0.03 | 1.35 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | A     | 1315 | 14/15 | 0.58  | 1.67 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | B     | 1310 | 11/12 | 0.19  | 0.92 | -    | 282,282,282,282             | 0     |
| 2   | NAG  | B     | 1302 | 14/15 | 0.85  | 0.89 | -    | 243,243,243,243             | 0     |
| 4   | MAN  | B     | 1334 | 11/12 | 0.34  | 0.40 | -    | 308,308,308,308             | 0     |
| 4   | MAN  | A     | 1317 | 11/12 | -0.03 | 0.98 | -    | 271,271,271,271             | 0     |
| 2   | NAG  | B     | 1338 | 14/15 | 0.19  | 2.87 | -    | 365,365,365,365             | 0     |
| 2   | NAG  | B     | 1328 | 14/15 | 0.72  | 1.08 | -    | 270,270,270,270             | 0     |
| 3   | BMA  | A     | 1316 | 11/12 | 0.70  | 1.08 | -    | 271,271,271,271             | 0     |
| 4   | MAN  | B     | 1335 | 11/12 | 0.43  | 1.53 | -    | 308,308,308,308             | 0     |
| 3   | BMA  | B     | 1339 | 11/12 | 0.24  | 2.98 | -    | 365,365,365,365             | 0     |
| 2   | NAG  | A     | 1334 | 14/15 | 0.10  | 2.66 | -    | 359,359,359,359             | 0     |
| 3   | BMA  | A     | 1307 | 11/12 | 0.68  | 0.78 | -    | 271,271,271,271             | 0     |
| 2   | NAG  | A     | 1330 | 14/15 | 0.24  | 2.91 | -    | 314,314,314,314             | 0     |
| 4   | MAN  | B     | 1304 | 11/12 | 0.75  | 0.54 | -    | 243,243,243,243             | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.