



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:06 AM UTC

PDB ID : 1FVF / pdb\_00001fvf  
Title : CRYSTAL STRUCTURE ANALYSIS OF NEURONAL SEC1 FROM THE SQUID L. PEALEI  
Authors : Bracher, A.; Weissenhorn, W.  
Deposited on : 2000-09-19  
Resolution : 3.20 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Percentile statistics          | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| CCP4                           | : | 9.0.010 (Gargrove)                                               |
| Density-Fitness                | : | 1.0.12                                                           |
| Ideal geometry (proteins)      | : | Engh & Huber (2001)                                              |
| Ideal geometry (DNA, RNA)      | : | Parkinson et al. (1996)                                          |
| Validation Pipeline (wwPDB-VP) | : | 2.49                                                             |

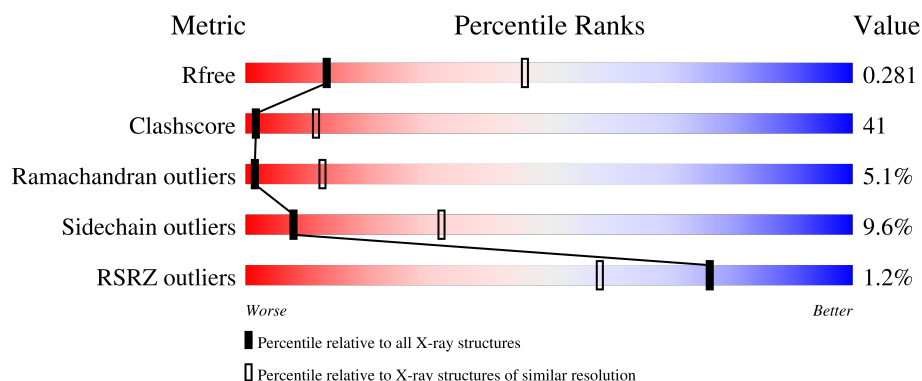
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| $R_{free}$            | 180053                      | 1466 (3.20-3.20)                                      |
| Clashscore            | 190562                      | 1573 (3.20-3.20)                                      |
| Ramachandran outliers | 187476                      | 1548 (3.20-3.20)                                      |
| Sidechain outliers    | 187428                      | 1547 (3.20-3.20)                                      |
| RSRZ outliers         | 180081                      | 1466 (3.20-3.20)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 591    |                  |
| 1   | B     | 591    |                  |

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8786 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.

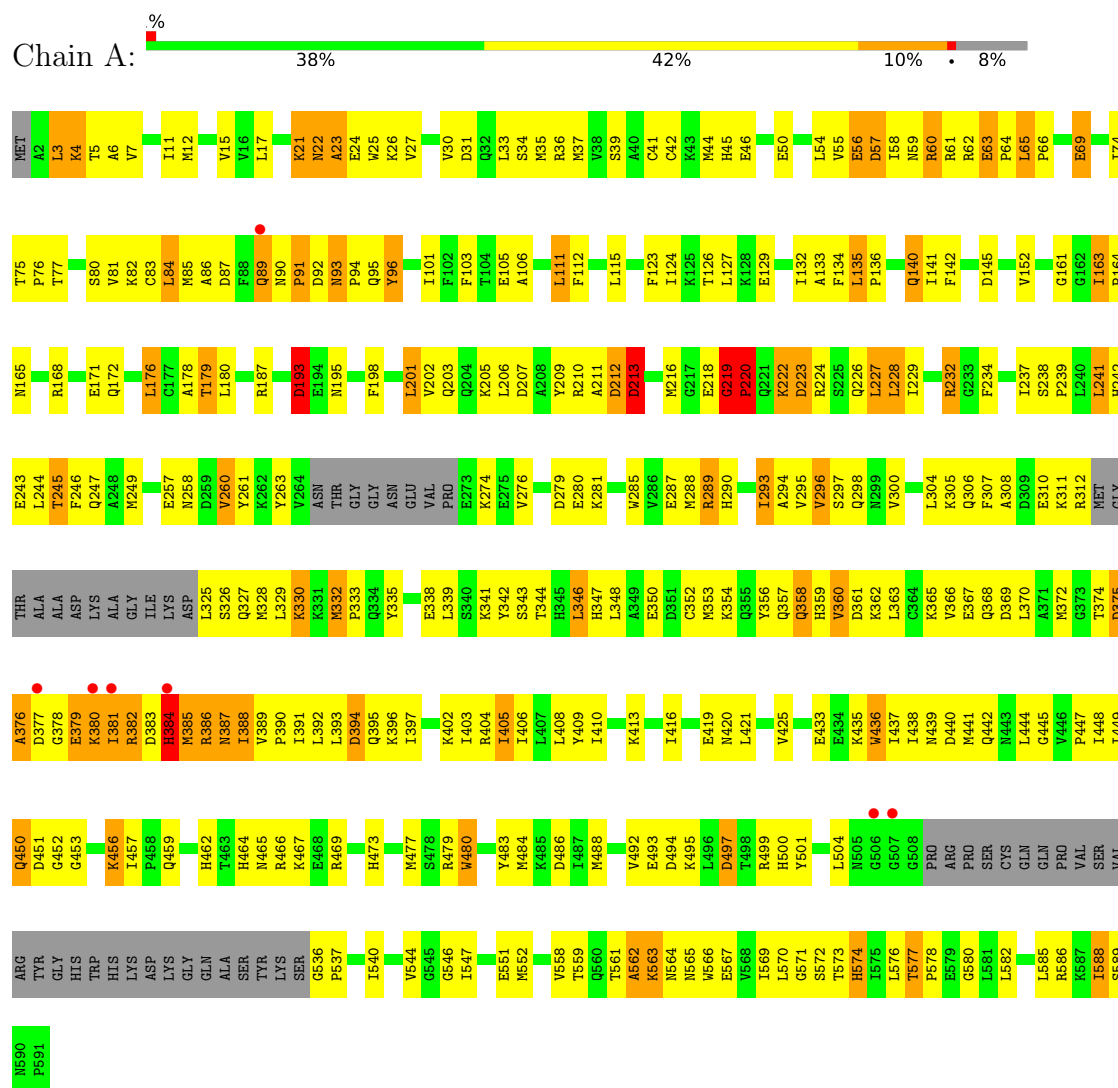
- Molecule 1 is a protein called SEC1.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 543      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4393  | 2783 | 759 | 823 | 28 |         |         |       |
| 1   | B     | 543      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 4393  | 2783 | 759 | 823 | 28 |         |         |       |

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: SEC1



|      |      |      |      |      |      |      |      |     |
|------|------|------|------|------|------|------|------|-----|
| K587 | SER  | I448 | T374 | R312 | H242 | G162 | I75  | MET |
| I588 | VAL  | I449 | D375 | MEI  | E243 | I163 | P76  | A2  |
| S589 | ARG  | Q450 | A376 | GLY  | I244 | P164 |      | L3  |
| N590 | TYR  | D451 | D377 | THR  | T245 | N165 | S80  | K4  |
| P591 | GLY  | G452 | G378 | ALA  | F246 | V81  | K82  | T5  |
|      | HIS  | G453 | E379 | ALA  | Q247 | R168 | C93  | A6  |
|      | TRP  |      | K380 | ASP  | K248 | C169 | L84  | V7  |
|      | HIS  | K456 | I381 | LYS  | K249 | A170 |      |     |
|      | LYS  | I457 | R382 | ALA  | E257 | E171 | R85  | I11 |
|      | LYS  | Q458 | D383 | GLY  | E258 | L176 | A86  | M12 |
|      | LYS  | Q459 | H384 | I1E  | L177 | C177 | D87  |     |
|      | GLN  | H462 | M385 | LYS  | D259 | A178 | F88  | V15 |
|      | ALA  | I463 | R386 | ASP  | V260 | D92  | N90  | V16 |
|      | SER  | H464 | I387 | L325 | Y261 | T179 | P91  | L17 |
|      | TYR  | N465 | V388 | S326 | K262 | L180 |      |     |
|      | LYS  | R466 | P390 | M328 | V264 | R187 | N93  | K21 |
|      | SER  | R467 | I391 | K330 | ASN  |      | P94  | N22 |
|      | G536 | R468 | L392 | K331 | THR  | D193 | E24  | A23 |
| P537 | P537 | R469 | L393 | M332 | GLY  | E194 | O95  | E24 |
|      | I540 | H473 | D394 | M333 | GLY  | N195 | Y96  | W25 |
|      | V544 | M477 | K395 | P333 | ASN  | F198 | I101 | K26 |
| G545 | G545 | S478 | Q396 | Q334 | GLU  | F102 | F103 | V27 |
| G546 | G546 | R479 | K397 | Y335 | VAL  | T104 | E105 | V30 |
| I547 | I547 | W480 | K402 | Q336 | PRO  | L201 | A106 | D31 |
| E551 | E551 | Y483 | I403 | K337 | E273 | V202 |      | Q32 |
| M552 | M552 | M484 | R404 | E338 | K274 | Q203 |      | L33 |
| R553 | R553 | D486 | I405 | L339 | E275 | Q204 |      | S34 |
|      | V558 | I487 | I406 | S340 | V276 | K205 |      | M35 |
| T559 | T559 | M488 | L407 | K341 | D279 | L206 |      | R36 |
| A562 | A562 | D494 | L408 | S342 | E280 | D207 |      | M37 |
| K563 | K563 | K495 | I410 | T344 | K281 | K208 |      | V38 |
| N564 | N564 | L496 | I411 | H345 | W285 | Y209 |      | S39 |
| W566 | W566 | D497 | H412 | L346 | E287 | R210 |      | A40 |
| E567 | E567 | T498 | K413 | H347 | W288 | A211 |      | C41 |
| V568 | V568 | R499 | I416 | L348 | E289 | I124 |      | C42 |
| I569 | I569 | H500 | N420 |      | H290 | T126 |      | M44 |
| L570 | L570 | F503 | L421 |      | Q291 | L127 |      | H45 |
| G571 | G571 | L504 | V425 |      | E292 | E129 |      | E46 |
| S572 | S572 | N505 | E433 |      | T293 | N131 |      | E50 |
| T573 | T573 | K435 | E434 |      | K294 | I132 |      | L54 |
| H574 | H574 | W436 | W436 |      | V295 | A133 |      | V55 |
| I575 | I575 | G506 | I437 |      | W296 | F134 |      | E56 |
| L576 | L576 | G507 | I438 |      | S297 | L135 |      | D57 |
| T577 | T577 | G508 | I439 |      | Q298 | P136 |      | I58 |
| P578 | P578 | PRO  | N440 |      | D361 | Q140 |      | N59 |
| E579 | E579 | ARG  | D440 |      | K362 | R60  |      | R61 |
| G580 | G580 | SER  | M441 |      | L363 | R62  |      | R62 |
| I581 | I581 | CYS  | Q442 |      | C364 | E63  |      | E63 |
| L582 | L582 | GLN  | N443 |      | K365 | L65  |      | L65 |
|      |      | PRO  | L444 |      | V366 | P66  |      | P66 |
| L585 | L585 | GLN  | G445 |      | E367 | E69  |      | E69 |
| R586 | R586 | VAL  | V446 |      | Q368 | I74  |      | I74 |
|      |      |      | P447 |      | D369 |      |      |     |
|      |      |      |      |      | F307 |      |      |     |
|      |      |      |      |      | A308 |      |      |     |
|      |      |      |      |      | D309 |      |      |     |
|      |      |      |      |      | E310 |      |      |     |
|      |      |      |      |      | L240 |      |      |     |
|      |      |      |      |      | G161 |      |      |     |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 31 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 118.52Å 118.52Å 192.62Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 12.00 – 3.20<br>12.00 – 3.20                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 95.7 (12.00-3.20)<br>93.7 (12.00-3.20)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 3.54 (at 3.21Å)                                             | Xtriage          |
| Refinement program                                                      | CNS                                                         | Depositor        |
| R, $R_{free}$                                                           | 0.243 , 0.288<br>0.240 , 0.281                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1202 reflections (4.85%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 81.3                                                        | Xtriage          |
| Anisotropy                                                              | 0.105                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.33 , 59.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$ | Xtriage          |
| Estimated twinning fraction                                             | 0.022 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 8786                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 66.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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

### 5.1 Standard geometry

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

| Mol | Chain | Bond lengths |               | Bond angles |                 |
|-----|-------|--------------|---------------|-------------|-----------------|
|     |       | RMSZ         | # $ Z  > 5$   | RMSZ        | # $ Z  > 5$     |
| 1   | A     | 0.53         | 0/4481        | 1.05        | 31/6050 (0.5%)  |
| 1   | B     | 0.50         | 1/4481 (0.0%) | 1.05        | 30/6050 (0.5%)  |
| All | All   | 0.51         | 1/8962 (0.0%) | 1.05        | 61/12100 (0.5%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1   | B     | 544 | VAL  | CA-CB | 5.39 | 1.59        | 1.53     |

All (61) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 193 | ASP  | N-CA-C    | 10.02 | 122.28      | 111.36   |
| 1   | B     | 193 | ASP  | N-CA-C    | 9.85  | 121.78      | 111.14   |
| 1   | A     | 207 | ASP  | N-CA-C    | -8.84 | 101.62      | 111.07   |
| 1   | A     | 346 | LEU  | N-CA-C    | -8.52 | 101.96      | 111.07   |
| 1   | B     | 207 | ASP  | N-CA-C    | -8.36 | 102.12      | 111.07   |
| 1   | B     | 360 | VAL  | N-CA-C    | 8.34  | 118.43      | 110.42   |
| 1   | B     | 346 | LEU  | N-CA-C    | -8.00 | 102.25      | 110.97   |
| 1   | A     | 360 | VAL  | N-CA-C    | 7.99  | 118.09      | 110.42   |
| 1   | B     | 459 | GLN  | CA-C-N    | 7.79  | 127.51      | 119.56   |
| 1   | B     | 459 | GLN  | C-N-CA    | 7.79  | 127.51      | 119.56   |
| 1   | A     | 459 | GLN  | CA-C-N    | 7.51  | 127.22      | 119.56   |
| 1   | A     | 459 | GLN  | C-N-CA    | 7.51  | 127.22      | 119.56   |
| 1   | A     | 499 | ARG  | N-CA-C    | -7.26 | 104.39      | 113.18   |
| 1   | B     | 499 | ARG  | N-CA-C    | -6.99 | 104.72      | 113.18   |
| 1   | A     | 480 | TRP  | N-CA-C    | 6.89  | 121.09      | 110.20   |
| 1   | A     | 218 | GLU  | N-CA-C    | 6.75  | 119.27      | 108.41   |
| 1   | B     | 65  | LEU  | CA-C-N    | 6.70  | 128.22      | 119.84   |
| 1   | B     | 65  | LEU  | C-N-CA    | 6.70  | 128.22      | 119.84   |
| 1   | B     | 480 | TRP  | N-CA-C    | 6.67  | 120.74      | 110.20   |
| 1   | B     | 224 | ARG  | N-CA-C    | -6.66 | 105.13      | 113.18   |
| 1   | B     | 404 | ARG  | NE-CZ-NH2 | 6.64  | 125.18      | 119.20   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | B     | 218 | GLU  | N-CA-C    | 6.60  | 119.03      | 108.41   |
| 1   | A     | 65  | LEU  | CA-C-N    | 6.50  | 127.96      | 119.84   |
| 1   | A     | 65  | LEU  | C-N-CA    | 6.50  | 127.96      | 119.84   |
| 1   | A     | 224 | ARG  | N-CA-C    | -6.48 | 105.37      | 113.28   |
| 1   | B     | 404 | ARG  | NE-CZ-NH1 | -6.47 | 115.03      | 121.50   |
| 1   | A     | 3   | LEU  | N-CA-C    | -6.43 | 104.36      | 111.82   |
| 1   | B     | 3   | LEU  | N-CA-C    | -6.24 | 104.58      | 111.82   |
| 1   | B     | 69  | GLU  | N-CA-C    | -6.23 | 102.14      | 110.55   |
| 1   | A     | 57  | ASP  | N-CA-C    | 6.16  | 118.02      | 109.15   |
| 1   | A     | 135 | LEU  | CA-C-N    | 6.00  | 127.34      | 119.84   |
| 1   | A     | 135 | LEU  | C-N-CA    | 6.00  | 127.34      | 119.84   |
| 1   | B     | 56  | GLU  | N-CA-C    | 5.92  | 117.53      | 108.42   |
| 1   | A     | 341 | LYS  | N-CA-C    | -5.91 | 104.53      | 110.97   |
| 1   | A     | 69  | GLU  | N-CA-C    | -5.81 | 102.71      | 110.55   |
| 1   | A     | 501 | TYR  | CA-C-N    | 5.80  | 125.77      | 120.03   |
| 1   | A     | 501 | TYR  | C-N-CA    | 5.80  | 125.77      | 120.03   |
| 1   | B     | 63  | GLU  | CA-C-N    | 5.78  | 125.69      | 119.85   |
| 1   | B     | 63  | GLU  | C-N-CA    | 5.78  | 125.69      | 119.85   |
| 1   | A     | 56  | GLU  | N-CA-C    | 5.67  | 117.15      | 108.42   |
| 1   | B     | 341 | LYS  | N-CA-C    | -5.62 | 104.85      | 110.97   |
| 1   | B     | 161 | GLY  | N-CA-C    | -5.59 | 106.78      | 115.67   |
| 1   | A     | 161 | GLY  | N-CA-C    | -5.59 | 106.78      | 115.67   |
| 1   | B     | 213 | ASP  | CA-C-N    | 5.57  | 125.66      | 119.87   |
| 1   | B     | 213 | ASP  | C-N-CA    | 5.57  | 125.66      | 119.87   |
| 1   | A     | 176 | LEU  | N-CA-C    | -5.48 | 105.22      | 111.14   |
| 1   | A     | 213 | ASP  | CA-C-N    | 5.41  | 125.50      | 119.87   |
| 1   | A     | 213 | ASP  | C-N-CA    | 5.41  | 125.50      | 119.87   |
| 1   | B     | 176 | LEU  | N-CA-C    | -5.40 | 105.31      | 111.14   |
| 1   | A     | 124 | ILE  | N-CA-C    | 5.23  | 114.79      | 107.37   |
| 1   | A     | 63  | GLU  | CA-C-N    | 5.22  | 125.12      | 119.85   |
| 1   | A     | 63  | GLU  | C-N-CA    | 5.22  | 125.12      | 119.85   |
| 1   | B     | 169 | CYS  | N-CA-C    | -5.22 | 105.67      | 111.36   |
| 1   | B     | 245 | THR  | N-CA-C    | -5.18 | 101.27      | 109.76   |
| 1   | B     | 57  | ASP  | N-CA-C    | 5.11  | 117.10      | 109.59   |
| 1   | B     | 131 | ASN  | N-CA-C    | 5.10  | 118.28      | 111.24   |
| 1   | A     | 245 | THR  | N-CA-C    | -5.09 | 101.41      | 109.76   |
| 1   | A     | 219 | GLY  | CA-C-N    | 5.01  | 126.11      | 119.84   |
| 1   | A     | 219 | GLY  | C-N-CA    | 5.01  | 126.11      | 119.84   |
| 1   | B     | 450 | GLN  | N-CA-C    | 5.01  | 121.47      | 110.80   |
| 1   | B     | 124 | ILE  | N-CA-C    | 5.01  | 114.48      | 107.37   |

There are no chirality outliers.

There are no planarity outliers.

## 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     | 4393  | 0        | 4393     | 371     | 0            |
| 1   | B     | 4393  | 0        | 4393     | 374     | 0            |
| All | All   | 8786  | 0        | 8786     | 721     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (721) 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:209:TYR:HB3  | 1:A:216:MET:HE1  | 1.42                     | 1.02              |
| 1:A:89:GLN:HE21  | 1:A:89:GLN:HA    | 1.25                     | 1.00              |
| 1:B:89:GLN:HE21  | 1:B:89:GLN:HA    | 1.27                     | 0.98              |
| 1:B:209:TYR:HB3  | 1:B:216:MET:HE1  | 1.43                     | 0.98              |
| 1:A:577:THR:HG22 | 1:A:580:GLY:H    | 1.32                     | 0.94              |
| 1:B:577:THR:HG22 | 1:B:580:GLY:H    | 1.33                     | 0.94              |
| 1:B:305:LYS:HG3  | 1:B:306:GLN:H    | 1.35                     | 0.90              |
| 1:A:305:LYS:HG3  | 1:A:306:GLN:N    | 1.85                     | 0.90              |
| 1:A:330:LYS:HZ1  | 1:A:330:LYS:HA   | 1.36                     | 0.89              |
| 1:A:305:LYS:HG3  | 1:A:306:GLN:H    | 1.36                     | 0.89              |
| 1:B:163:ILE:H    | 1:B:163:ILE:HD12 | 1.39                     | 0.87              |
| 1:B:305:LYS:HG3  | 1:B:306:GLN:N    | 1.87                     | 0.87              |
| 1:B:54:LEU:HD23  | 1:B:55:VAL:N     | 1.89                     | 0.87              |
| 1:A:163:ILE:HD12 | 1:A:163:ILE:H    | 1.40                     | 0.86              |
| 1:B:54:LEU:HD23  | 1:B:55:VAL:H     | 1.41                     | 0.84              |
| 1:B:439:ASN:HA   | 1:B:448:ILE:CD1  | 2.07                     | 0.84              |
| 1:A:330:LYS:HA   | 1:A:330:LYS:NZ   | 1.92                     | 0.84              |
| 1:A:308:ALA:HB1  | 1:B:305:LYS:HB3  | 1.60                     | 0.83              |
| 1:A:54:LEU:HD23  | 1:A:55:VAL:N     | 1.94                     | 0.83              |
| 1:A:439:ASN:HA   | 1:A:448:ILE:CD1  | 2.08                     | 0.83              |
| 1:A:54:LEU:HD23  | 1:A:55:VAL:H     | 1.45                     | 0.82              |
| 1:B:372:MET:HE1  | 1:B:480:TRP:HB2  | 1.63                     | 0.81              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:380:LYS:O    | 1:B:381:ILE:HG23 | 1.80                     | 0.81              |
| 1:B:330:LYS:NZ   | 1:B:330:LYS:HA   | 1.95                     | 0.81              |
| 1:B:540:ILE:HD13 | 1:B:569:ILE:HB   | 1.61                     | 0.80              |
| 1:B:433:GLU:H    | 1:B:433:GLU:CD   | 1.90                     | 0.80              |
| 1:A:380:LYS:O    | 1:A:381:ILE:HG23 | 1.82                     | 0.79              |
| 1:A:448:ILE:HG13 | 1:A:449:ILE:N    | 1.97                     | 0.79              |
| 1:A:362:LYS:HE3  | 1:A:397:ILE:HD11 | 1.64                     | 0.78              |
| 1:B:311:LYS:HG3  | 1:B:335:TYR:HE1  | 1.46                     | 0.78              |
| 1:B:330:LYS:HA   | 1:B:330:LYS:HZ1  | 1.48                     | 0.78              |
| 1:B:362:LYS:HE3  | 1:B:397:ILE:HD11 | 1.65                     | 0.78              |
| 1:A:372:MET:HE1  | 1:A:480:TRP:HB2  | 1.64                     | 0.78              |
| 1:B:439:ASN:HA   | 1:B:448:ILE:HD13 | 1.65                     | 0.77              |
| 1:A:311:LYS:HG3  | 1:A:335:TYR:HE1  | 1.50                     | 0.77              |
| 1:A:93:ASN:H     | 1:A:94:PRO:CD    | 1.97                     | 0.77              |
| 1:A:433:GLU:CD   | 1:A:433:GLU:H    | 1.93                     | 0.77              |
| 1:A:540:ILE:HD13 | 1:A:569:ILE:HB   | 1.66                     | 0.77              |
| 1:A:439:ASN:HA   | 1:A:448:ILE:HD13 | 1.65                     | 0.76              |
| 1:A:577:THR:HG22 | 1:A:580:GLY:N    | 2.01                     | 0.76              |
| 1:B:201:LEU:HD22 | 1:B:201:LEU:H    | 1.51                     | 0.76              |
| 1:A:89:GLN:HA    | 1:A:89:GLN:NE2   | 2.00                     | 0.76              |
| 1:B:577:THR:HG22 | 1:B:580:GLY:N    | 2.01                     | 0.75              |
| 1:B:448:ILE:HG13 | 1:B:449:ILE:N    | 2.00                     | 0.75              |
| 1:B:375:ASP:HA   | 1:B:479:ARG:NH1  | 2.02                     | 0.75              |
| 1:B:89:GLN:HA    | 1:B:89:GLN:NE2   | 2.01                     | 0.75              |
| 1:A:247:GLN:HB2  | 1:A:289:ARG:HB2  | 1.69                     | 0.74              |
| 1:B:93:ASN:H     | 1:B:94:PRO:CD    | 2.01                     | 0.74              |
| 1:B:86:ALA:HA    | 1:B:89:GLN:HB2   | 1.68                     | 0.74              |
| 1:A:374:THR:HB   | 1:A:378:GLY:HA2  | 1.68                     | 0.74              |
| 1:A:201:LEU:H    | 1:A:201:LEU:HD22 | 1.52                     | 0.74              |
| 1:A:133:ALA:HB1  | 1:A:172:GLN:HG2  | 1.70                     | 0.73              |
| 1:A:441:MET:HE1  | 1:A:444:LEU:HD22 | 1.71                     | 0.73              |
| 1:B:441:MET:HE1  | 1:B:444:LEU:HD22 | 1.70                     | 0.73              |
| 1:A:86:ALA:HA    | 1:A:89:GLN:HB2   | 1.71                     | 0.73              |
| 1:A:93:ASN:H     | 1:A:94:PRO:HD3   | 1.54                     | 0.73              |
| 1:A:305:LYS:HD2  | 1:B:312:ARG:HE   | 1.53                     | 0.73              |
| 1:A:276:VAL:HG21 | 1:A:344:THR:HG21 | 1.69                     | 0.72              |
| 1:B:374:THR:HB   | 1:B:378:GLY:HA2  | 1.68                     | 0.72              |
| 1:A:435:LYS:HD2  | 1:A:436:TRP:CZ3  | 2.23                     | 0.72              |
| 1:A:263:TYR:OH   | 1:A:274:LYS:HE3  | 1.90                     | 0.72              |
| 1:A:326:SER:HA   | 1:B:357:GLN:HE22 | 1.55                     | 0.72              |
| 1:B:382:ARG:HB2  | 1:B:386:ARG:HD2  | 1.70                     | 0.72              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:210:ARG:HG3  | 1:A:210:ARG:HH11 | 1.55                     | 0.71              |
| 1:A:382:ARG:HB2  | 1:A:386:ARG:HD2  | 1.71                     | 0.71              |
| 1:B:263:TYR:OH   | 1:B:274:LYS:HE3  | 1.91                     | 0.71              |
| 1:A:249:MET:CE   | 1:A:352:CYS:HB3  | 2.20                     | 0.70              |
| 1:B:11:ILE:HD11  | 1:B:37:MET:HE2   | 1.73                     | 0.70              |
| 1:A:350:GLU:OE2  | 1:B:332:MET:HG2  | 1.90                     | 0.70              |
| 1:B:435:LYS:HD2  | 1:B:436:TRP:CZ3  | 2.27                     | 0.70              |
| 1:B:561:THR:C    | 1:B:563:LYS:H    | 2.00                     | 0.70              |
| 1:B:276:VAL:HG21 | 1:B:344:THR:HG21 | 1.71                     | 0.70              |
| 1:B:379:GLU:HG3  | 1:B:380:LYS:H    | 1.56                     | 0.70              |
| 1:A:558:VAL:O    | 1:A:561:THR:HG22 | 1.92                     | 0.69              |
| 1:B:249:MET:CE   | 1:B:352:CYS:HB3  | 2.22                     | 0.69              |
| 1:A:11:ILE:HD11  | 1:A:37:MET:HE2   | 1.73                     | 0.69              |
| 1:B:247:GLN:HB2  | 1:B:289:ARG:HB2  | 1.72                     | 0.69              |
| 1:B:558:VAL:O    | 1:B:561:THR:HG22 | 1.93                     | 0.69              |
| 1:B:288:MET:HE2  | 1:B:300:VAL:CG2  | 2.22                     | 0.69              |
| 1:A:379:GLU:HG3  | 1:A:380:LYS:H    | 1.58                     | 0.69              |
| 1:B:93:ASN:H     | 1:B:94:PRO:HD3   | 1.57                     | 0.69              |
| 1:B:134:PHE:CE1  | 1:B:176:LEU:HA   | 2.28                     | 0.69              |
| 1:A:249:MET:HE3  | 1:A:352:CYS:HB3  | 1.76                     | 0.68              |
| 1:B:187:ARG:HD2  | 1:B:226:GLN:OE1  | 1.93                     | 0.68              |
| 1:A:375:ASP:HA   | 1:A:479:ARG:NH1  | 2.08                     | 0.68              |
| 1:B:564:ASN:HB3  | 1:B:566:TRP:HD1  | 1.59                     | 0.68              |
| 1:B:210:ARG:HG3  | 1:B:210:ARG:HH11 | 1.59                     | 0.68              |
| 1:A:288:MET:HE2  | 1:A:300:VAL:CG2  | 2.24                     | 0.68              |
| 1:A:62:ARG:HD3   | 1:A:62:ARG:N     | 2.08                     | 0.67              |
| 1:A:187:ARG:HD2  | 1:A:226:GLN:OE1  | 1.95                     | 0.67              |
| 1:A:279:ASP:OD2  | 1:A:281:LYS:HE2  | 1.95                     | 0.67              |
| 1:B:62:ARG:N     | 1:B:62:ARG:HD3   | 2.09                     | 0.67              |
| 1:A:356:TYR:HA   | 1:A:360:VAL:HB   | 1.75                     | 0.67              |
| 1:A:577:THR:CG2  | 1:A:580:GLY:H    | 2.07                     | 0.67              |
| 1:A:339:LEU:HD11 | 1:B:304:LEU:HD21 | 1.77                     | 0.67              |
| 1:A:564:ASN:HB3  | 1:A:566:TRP:HD1  | 1.58                     | 0.67              |
| 1:A:386:ARG:O    | 1:A:388:ILE:N    | 2.28                     | 0.66              |
| 1:A:441:MET:CE   | 1:A:444:LEU:HD22 | 2.25                     | 0.66              |
| 1:B:379:GLU:HG3  | 1:B:380:LYS:N    | 2.11                     | 0.66              |
| 1:B:279:ASP:OD2  | 1:B:281:LYS:HE2  | 1.96                     | 0.66              |
| 1:A:328:MET:HE3  | 1:B:353:MET:HE1  | 1.77                     | 0.66              |
| 1:B:356:TYR:HA   | 1:B:360:VAL:HB   | 1.76                     | 0.66              |
| 1:A:448:ILE:HG13 | 1:A:449:ILE:H    | 1.61                     | 0.66              |
| 1:B:386:ARG:O    | 1:B:388:ILE:N    | 2.29                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:484:MET:HG3  | 1:A:488:MET:HE3  | 1.76                     | 0.66              |
| 1:A:132:ILE:HG22 | 1:A:132:ILE:O    | 1.97                     | 0.65              |
| 1:A:232:ARG:O    | 1:A:232:ARG:HD3  | 1.96                     | 0.65              |
| 1:B:546:GLY:HA3  | 1:B:576:LEU:HG   | 1.79                     | 0.65              |
| 1:A:561:THR:C    | 1:A:563:LYS:H    | 2.03                     | 0.65              |
| 1:B:311:LYS:HG3  | 1:B:335:TYR:CE1  | 2.31                     | 0.65              |
| 1:B:441:MET:CE   | 1:B:444:LEU:HD22 | 2.27                     | 0.65              |
| 1:B:561:THR:HG23 | 1:B:562:ALA:N    | 2.11                     | 0.65              |
| 1:B:163:ILE:H    | 1:B:163:ILE:CD1  | 2.09                     | 0.65              |
| 1:A:563:LYS:C    | 1:A:565:ASN:H    | 2.05                     | 0.65              |
| 1:B:563:LYS:C    | 1:B:565:ASN:H    | 2.05                     | 0.65              |
| 1:B:577:THR:CG2  | 1:B:580:GLY:H    | 2.07                     | 0.64              |
| 1:A:307:PHE:CE2  | 1:A:338:GLU:HG3  | 2.32                     | 0.64              |
| 1:A:546:GLY:HA3  | 1:A:576:LEU:HG   | 1.79                     | 0.64              |
| 1:B:484:MET:HG3  | 1:B:488:MET:HE3  | 1.78                     | 0.64              |
| 1:A:84:LEU:HD11  | 1:A:101:ILE:CD1  | 2.28                     | 0.64              |
| 1:A:384:HIS:O    | 1:A:385:MET:HG2  | 1.98                     | 0.64              |
| 1:B:112:PHE:HE1  | 1:B:127:LEU:HD21 | 1.62                     | 0.64              |
| 1:B:81:VAL:HG21  | 1:B:111:LEU:HD13 | 1.80                     | 0.64              |
| 1:B:249:MET:HE3  | 1:B:352:CYS:HB3  | 1.80                     | 0.63              |
| 1:B:22:ASN:O     | 1:B:24:GLU:HB2   | 1.98                     | 0.63              |
| 1:A:62:ARG:HD3   | 1:A:62:ARG:H     | 1.64                     | 0.63              |
| 1:A:249:MET:CE   | 1:A:293:ILE:HD12 | 2.28                     | 0.63              |
| 1:A:561:THR:HG23 | 1:A:562:ALA:N    | 2.14                     | 0.63              |
| 1:A:379:GLU:HG3  | 1:A:380:LYS:N    | 2.12                     | 0.63              |
| 1:B:84:LEU:HD11  | 1:B:101:ILE:CD1  | 2.29                     | 0.63              |
| 1:A:308:ALA:HB1  | 1:B:305:LYS:CB   | 2.29                     | 0.63              |
| 1:B:307:PHE:CE2  | 1:B:338:GLU:HG3  | 2.33                     | 0.62              |
| 1:B:561:THR:HG23 | 1:B:562:ALA:H    | 1.64                     | 0.62              |
| 1:A:564:ASN:HB3  | 1:A:566:TRP:CD1  | 2.34                     | 0.62              |
| 1:B:366:VAL:HG21 | 1:B:391:ILE:HG13 | 1.81                     | 0.62              |
| 1:B:380:LYS:O    | 1:B:381:ILE:HG12 | 1.99                     | 0.62              |
| 1:A:202:VAL:HG21 | 1:A:229:ILE:HD11 | 1.81                     | 0.62              |
| 1:A:93:ASN:N     | 1:A:94:PRO:CD    | 2.62                     | 0.62              |
| 1:A:312:ARG:HE   | 1:B:305:LYS:HD2  | 1.64                     | 0.62              |
| 1:A:112:PHE:HE1  | 1:A:127:LEU:HD21 | 1.64                     | 0.62              |
| 1:B:22:ASN:O     | 1:B:24:GLU:N     | 2.32                     | 0.62              |
| 1:A:81:VAL:HG21  | 1:A:111:LEU:HD13 | 1.79                     | 0.62              |
| 1:A:163:ILE:H    | 1:A:163:ILE:CD1  | 2.09                     | 0.62              |
| 1:B:202:VAL:HG21 | 1:B:229:ILE:HD11 | 1.80                     | 0.62              |
| 1:A:22:ASN:O     | 1:A:24:GLU:HB2   | 2.00                     | 0.62              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:232:ARG:O    | 1:B:232:ARG:HD3  | 1.98                     | 0.62              |
| 1:B:288:MET:HE2  | 1:B:300:VAL:HG23 | 1.81                     | 0.62              |
| 1:B:448:ILE:HG13 | 1:B:449:ILE:H    | 1.64                     | 0.62              |
| 1:B:564:ASN:HB3  | 1:B:566:TRP:CD1  | 2.34                     | 0.61              |
| 1:A:22:ASN:O     | 1:A:24:GLU:N     | 2.33                     | 0.61              |
| 1:A:375:ASP:O    | 1:A:377:ASP:N    | 2.34                     | 0.61              |
| 1:B:152:VAL:HG21 | 1:B:165:ASN:ND2  | 2.15                     | 0.61              |
| 1:B:201:LEU:H    | 1:B:201:LEU:CD2  | 2.13                     | 0.61              |
| 1:A:33:LEU:HD22  | 1:A:33:LEU:H     | 1.66                     | 0.61              |
| 1:A:328:MET:C    | 1:A:330:LYS:H    | 2.08                     | 0.61              |
| 1:A:64:PRO:O     | 1:A:65:LEU:HD23  | 2.01                     | 0.61              |
| 1:B:33:LEU:H     | 1:B:33:LEU:HD22  | 1.65                     | 0.61              |
| 1:B:62:ARG:HD3   | 1:B:62:ARG:H     | 1.65                     | 0.61              |
| 1:B:168:ARG:HG3  | 1:B:168:ARG:HH11 | 1.66                     | 0.61              |
| 1:B:328:MET:C    | 1:B:330:LYS:H    | 2.08                     | 0.61              |
| 1:B:375:ASP:O    | 1:B:377:ASP:N    | 2.33                     | 0.61              |
| 1:A:201:LEU:H    | 1:A:201:LEU:CD2  | 2.14                     | 0.60              |
| 1:B:384:HIS:O    | 1:B:385:MET:HG2  | 2.01                     | 0.60              |
| 1:A:210:ARG:HG3  | 1:A:210:ARG:NH1  | 2.15                     | 0.60              |
| 1:A:382:ARG:CB   | 1:A:386:ARG:HD2  | 2.31                     | 0.60              |
| 1:A:380:LYS:O    | 1:A:381:ILE:HG12 | 2.02                     | 0.60              |
| 1:A:484:MET:CG   | 1:A:488:MET:HE3  | 2.30                     | 0.60              |
| 1:B:263:TYR:CE2  | 1:B:344:THR:HG22 | 2.37                     | 0.60              |
| 1:B:372:MET:HE1  | 1:B:480:TRP:CB   | 2.29                     | 0.60              |
| 1:A:564:ASN:O    | 1:A:565:ASN:HB3  | 2.01                     | 0.60              |
| 1:A:343:SER:OG   | 1:B:339:LEU:HD23 | 2.02                     | 0.60              |
| 1:A:394:ASP:CG   | 1:A:397:ILE:HG12 | 2.26                     | 0.60              |
| 1:A:152:VAL:HG21 | 1:A:165:ASN:ND2  | 2.17                     | 0.60              |
| 1:A:307:PHE:HE2  | 1:A:338:GLU:HG3  | 1.65                     | 0.60              |
| 1:A:347:HIS:CD2  | 1:B:336:GLN:NE2  | 2.70                     | 0.60              |
| 1:A:435:LYS:HD2  | 1:A:436:TRP:CE3  | 2.35                     | 0.59              |
| 1:B:382:ARG:CB   | 1:B:386:ARG:HD2  | 2.31                     | 0.59              |
| 1:B:451:ASP:C    | 1:B:453:GLY:H    | 2.10                     | 0.59              |
| 1:B:484:MET:CG   | 1:B:488:MET:HE3  | 2.32                     | 0.59              |
| 1:B:564:ASN:O    | 1:B:565:ASN:HB3  | 2.02                     | 0.59              |
| 1:A:347:HIS:HD2  | 1:B:336:GLN:NE2  | 2.00                     | 0.59              |
| 1:B:261:TYR:CD2  | 1:B:348:LEU:HD13 | 2.37                     | 0.59              |
| 1:A:62:ARG:NH2   | 1:A:87:ASP:OD2   | 2.35                     | 0.59              |
| 1:A:328:MET:HE3  | 1:B:353:MET:CE   | 2.32                     | 0.59              |
| 1:A:368:GLN:NE2  | 1:A:479:ARG:HB2  | 2.17                     | 0.59              |
| 1:A:329:LEU:HD13 | 1:B:353:MET:HB2  | 1.85                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:384:HIS:O    | 1:A:385:MET:CG   | 2.51                     | 0.59              |
| 1:B:307:PHE:HE2  | 1:B:338:GLU:HG3  | 1.67                     | 0.59              |
| 1:A:451:ASP:C    | 1:A:453:GLY:H    | 2.10                     | 0.59              |
| 1:A:362:LYS:NZ   | 1:A:396:LYS:HD2  | 2.18                     | 0.59              |
| 1:B:362:LYS:NZ   | 1:B:396:LYS:HD2  | 2.17                     | 0.58              |
| 1:A:263:TYR:CE2  | 1:A:344:THR:HG22 | 2.37                     | 0.58              |
| 1:B:467:LYS:HE3  | 1:B:469:ARG:NH1  | 2.18                     | 0.58              |
| 1:A:372:MET:HE1  | 1:A:480:TRP:CB   | 2.31                     | 0.58              |
| 1:B:421:LEU:O    | 1:B:425:VAL:HG23 | 2.03                     | 0.58              |
| 1:A:366:VAL:HG21 | 1:A:391:ILE:HG13 | 1.85                     | 0.58              |
| 1:A:561:THR:HG23 | 1:A:562:ALA:H    | 1.66                     | 0.58              |
| 1:A:163:ILE:HD12 | 1:A:163:ILE:N    | 2.13                     | 0.58              |
| 1:A:330:LYS:O    | 1:A:333:PRO:HD2  | 2.04                     | 0.58              |
| 1:B:163:ILE:HD12 | 1:B:163:ILE:N    | 2.13                     | 0.58              |
| 1:B:416:ILE:C    | 1:B:450:GLN:HB2  | 2.29                     | 0.58              |
| 1:B:30:VAL:O     | 1:B:57:ASP:HA    | 2.04                     | 0.58              |
| 1:A:357:GLN:HE21 | 1:B:325:LEU:CD2  | 2.16                     | 0.58              |
| 1:A:440:ASP:C    | 1:A:442:GLN:N    | 2.61                     | 0.58              |
| 1:B:62:ARG:NH2   | 1:B:87:ASP:OD2   | 2.37                     | 0.58              |
| 1:B:433:GLU:CD   | 1:B:433:GLU:N    | 2.58                     | 0.58              |
| 1:B:394:ASP:CG   | 1:B:397:ILE:HG12 | 2.29                     | 0.57              |
| 1:B:464:HIS:CD2  | 1:B:465:ASN:HD21 | 2.22                     | 0.57              |
| 1:A:311:LYS:HG3  | 1:A:335:TYR:CE1  | 2.34                     | 0.57              |
| 1:A:103:PHE:O    | 1:A:129:GLU:HA   | 2.04                     | 0.57              |
| 1:B:64:PRO:O     | 1:B:65:LEU:HD23  | 2.03                     | 0.57              |
| 1:A:473:HIS:ND1  | 1:A:479:ARG:HG2  | 2.19                     | 0.57              |
| 1:A:483:TYR:O    | 1:A:486:ASP:HB2  | 2.05                     | 0.57              |
| 1:B:61:ARG:HH21  | 1:B:95:GLN:HE22  | 1.52                     | 0.57              |
| 1:B:210:ARG:HG3  | 1:B:210:ARG:NH1  | 2.17                     | 0.57              |
| 1:B:464:HIS:CD2  | 1:B:465:ASN:ND2  | 2.73                     | 0.57              |
| 1:A:433:GLU:CD   | 1:A:433:GLU:N    | 2.62                     | 0.57              |
| 1:B:403:ILE:HG23 | 1:B:438:ILE:CD1  | 2.34                     | 0.57              |
| 1:B:103:PHE:O    | 1:B:129:GLU:HA   | 2.05                     | 0.57              |
| 1:A:416:ILE:C    | 1:A:450:GLN:HB2  | 2.30                     | 0.57              |
| 1:A:421:LEU:O    | 1:A:425:VAL:HG23 | 2.05                     | 0.57              |
| 1:A:403:ILE:HG23 | 1:A:438:ILE:CD1  | 2.33                     | 0.57              |
| 1:B:202:VAL:O    | 1:B:206:LEU:HG   | 2.05                     | 0.57              |
| 1:B:368:GLN:NE2  | 1:B:479:ARG:HB2  | 2.20                     | 0.56              |
| 1:B:435:LYS:HD2  | 1:B:436:TRP:CE3  | 2.39                     | 0.56              |
| 1:B:330:LYS:O    | 1:B:333:PRO:HD2  | 2.05                     | 0.56              |
| 1:B:483:TYR:O    | 1:B:486:ASP:HB2  | 2.05                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:249:MET:SD   | 1:A:293:ILE:HD12 | 2.46                     | 0.56              |
| 1:A:346:LEU:HD11 | 1:B:335:TYR:CE2  | 2.39                     | 0.56              |
| 1:A:357:GLN:NE2  | 1:B:325:LEU:HD23 | 2.20                     | 0.56              |
| 1:A:444:LEU:N    | 1:A:444:LEU:HD12 | 2.20                     | 0.56              |
| 1:A:464:HIS:CD2  | 1:A:465:ASN:ND2  | 2.74                     | 0.56              |
| 1:B:93:ASN:N     | 1:B:94:PRO:CD    | 2.64                     | 0.56              |
| 1:A:261:TYR:CD2  | 1:A:348:LEU:HD13 | 2.41                     | 0.56              |
| 1:A:90:ASN:OD1   | 1:A:91:PRO:O     | 2.23                     | 0.56              |
| 1:B:90:ASN:OD1   | 1:B:91:PRO:O     | 2.24                     | 0.56              |
| 1:A:36:ARG:HD3   | 1:A:135:LEU:HD11 | 1.88                     | 0.56              |
| 1:A:61:ARG:NH2   | 1:A:95:GLN:HE22  | 2.03                     | 0.56              |
| 1:A:288:MET:HE2  | 1:A:300:VAL:HG23 | 1.87                     | 0.56              |
| 1:B:439:ASN:HA   | 1:B:448:ILE:HD11 | 1.87                     | 0.56              |
| 1:A:168:ARG:HG3  | 1:A:168:ARG:HH11 | 1.70                     | 0.56              |
| 1:B:4:LYS:NZ     | 1:B:280:GLU:HG3  | 2.21                     | 0.56              |
| 1:B:241:LEU:HD12 | 1:B:408:LEU:HD11 | 1.88                     | 0.56              |
| 1:B:421:LEU:HD13 | 1:B:421:LEU:C    | 2.31                     | 0.56              |
| 1:A:464:HIS:CD2  | 1:A:465:ASN:HD21 | 2.24                     | 0.55              |
| 1:A:547:ILE:HG23 | 1:A:572:SER:HB2  | 1.88                     | 0.55              |
| 1:B:367:GLU:HG2  | 1:B:408:LEU:HD12 | 1.88                     | 0.55              |
| 1:B:384:HIS:O    | 1:B:385:MET:CG   | 2.54                     | 0.55              |
| 1:A:257:GLU:O    | 1:A:260:VAL:HG12 | 2.07                     | 0.55              |
| 1:A:339:LEU:HD11 | 1:B:304:LEU:CD2  | 2.36                     | 0.55              |
| 1:B:61:ARG:NH2   | 1:B:95:GLN:HE22  | 2.05                     | 0.55              |
| 1:B:473:HIS:ND1  | 1:B:479:ARG:HG2  | 2.21                     | 0.55              |
| 1:A:61:ARG:HH21  | 1:A:95:GLN:HE22  | 1.52                     | 0.55              |
| 1:B:368:GLN:NE2  | 1:B:479:ARG:H    | 2.05                     | 0.55              |
| 1:A:237:ILE:C    | 1:A:239:PRO:HD2  | 2.32                     | 0.55              |
| 1:A:288:MET:HE2  | 1:A:300:VAL:HG22 | 1.87                     | 0.55              |
| 1:B:372:MET:HE1  | 1:B:480:TRP:CA   | 2.37                     | 0.55              |
| 1:A:247:GLN:HG3  | 1:A:285:TRP:HZ2  | 1.72                     | 0.55              |
| 1:A:176:LEU:C    | 1:A:176:LEU:HD13 | 2.30                     | 0.55              |
| 1:B:37:MET:HE1   | 1:B:132:ILE:CD1  | 2.37                     | 0.55              |
| 1:A:238:SER:N    | 1:A:239:PRO:HD2  | 2.22                     | 0.54              |
| 1:A:467:LYS:HE3  | 1:A:469:ARG:NH1  | 2.22                     | 0.54              |
| 1:B:263:TYR:CZ   | 1:B:344:THR:HG22 | 2.42                     | 0.54              |
| 1:B:380:LYS:C    | 1:B:381:ILE:HG12 | 2.31                     | 0.54              |
| 1:B:440:ASP:C    | 1:B:442:GLN:N    | 2.64                     | 0.54              |
| 1:A:105:GLU:OE1  | 1:A:168:ARG:NH2  | 2.41                     | 0.54              |
| 1:A:382:ARG:HG3  | 1:A:382:ARG:HH11 | 1.73                     | 0.54              |
| 1:B:22:ASN:O     | 1:B:23:ALA:C     | 2.50                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:176:LEU:HD13 | 1:B:176:LEU:C    | 2.32                     | 0.54              |
| 1:B:385:MET:O    | 1:B:389:VAL:HG23 | 2.07                     | 0.54              |
| 1:B:444:LEU:HD12 | 1:B:444:LEU:N    | 2.22                     | 0.54              |
| 1:A:95:GLN:O     | 1:A:96:TYR:HB2   | 2.07                     | 0.54              |
| 1:A:296:VAL:O    | 1:A:300:VAL:HG23 | 2.07                     | 0.54              |
| 1:A:380:LYS:C    | 1:A:381:ILE:HG12 | 2.33                     | 0.54              |
| 1:A:22:ASN:O     | 1:A:23:ALA:C     | 2.51                     | 0.54              |
| 1:B:288:MET:HE2  | 1:B:300:VAL:HG22 | 1.89                     | 0.54              |
| 1:B:375:ASP:CG   | 1:B:376:ALA:N    | 2.65                     | 0.54              |
| 1:A:263:TYR:CZ   | 1:A:344:THR:HG22 | 2.43                     | 0.54              |
| 1:A:385:MET:O    | 1:A:389:VAL:HG23 | 2.08                     | 0.54              |
| 1:B:370:LEU:HD11 | 1:B:388:ILE:HD11 | 1.90                     | 0.54              |
| 1:A:279:ASP:OD1  | 1:A:280:GLU:N    | 2.41                     | 0.53              |
| 1:B:95:GLN:O     | 1:B:96:TYR:HB2   | 2.09                     | 0.53              |
| 1:A:439:ASN:HA   | 1:A:448:ILE:HD11 | 1.89                     | 0.53              |
| 1:B:203:GLN:O    | 1:B:206:LEU:HD12 | 2.07                     | 0.53              |
| 1:B:279:ASP:OD1  | 1:B:280:GLU:N    | 2.42                     | 0.53              |
| 1:A:201:LEU:HD22 | 1:A:201:LEU:N    | 2.22                     | 0.53              |
| 1:A:202:VAL:O    | 1:A:206:LEU:HG   | 2.09                     | 0.53              |
| 1:B:382:ARG:HG3  | 1:B:382:ARG:HH11 | 1.73                     | 0.53              |
| 1:B:462:HIS:HB3  | 1:B:464:HIS:CE1  | 2.43                     | 0.53              |
| 1:A:84:LEU:HD11  | 1:A:101:ILE:HD13 | 1.90                     | 0.53              |
| 1:B:134:PHE:C    | 1:B:134:PHE:CD2  | 2.87                     | 0.53              |
| 1:B:561:THR:C    | 1:B:563:LYS:N    | 2.63                     | 0.53              |
| 1:A:332:MET:HB3  | 1:A:333:PRO:HD3  | 1.91                     | 0.53              |
| 1:A:421:LEU:C    | 1:A:421:LEU:HD13 | 2.34                     | 0.53              |
| 1:A:561:THR:C    | 1:A:563:LYS:N    | 2.66                     | 0.53              |
| 1:B:249:MET:CE   | 1:B:293:ILE:HD12 | 2.38                     | 0.53              |
| 1:A:368:GLN:NE2  | 1:A:479:ARG:H    | 2.06                     | 0.53              |
| 1:A:375:ASP:CG   | 1:A:376:ALA:N    | 2.66                     | 0.53              |
| 1:A:451:ASP:O    | 1:A:453:GLY:N    | 2.42                     | 0.53              |
| 1:B:451:ASP:O    | 1:B:453:GLY:N    | 2.42                     | 0.53              |
| 1:A:37:MET:HE1   | 1:A:132:ILE:HD12 | 1.90                     | 0.53              |
| 1:A:456:LYS:HD3  | 1:A:457:ILE:N    | 2.24                     | 0.53              |
| 1:B:134:PHE:HE1  | 1:B:176:LEU:HA   | 1.71                     | 0.53              |
| 1:A:347:HIS:CD2  | 1:B:336:GLN:HE21 | 2.26                     | 0.53              |
| 1:A:369:ASP:CG   | 1:A:375:ASP:HB2  | 2.34                     | 0.53              |
| 1:B:209:TYR:HB3  | 1:B:216:MET:CE   | 2.28                     | 0.53              |
| 1:A:95:GLN:O     | 1:A:96:TYR:CB    | 2.57                     | 0.52              |
| 1:B:95:GLN:O     | 1:B:96:TYR:CB    | 2.57                     | 0.52              |
| 1:A:36:ARG:HD3   | 1:A:135:LEU:CD1  | 2.39                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:249:MET:SD   | 1:B:293:ILE:HD12 | 2.50                     | 0.52              |
| 1:B:456:LYS:HD3  | 1:B:457:ILE:N    | 2.24                     | 0.52              |
| 1:A:249:MET:HE2  | 1:A:293:ILE:HD12 | 1.91                     | 0.52              |
| 1:B:447:PRO:HG3  | 1:B:457:ILE:HB   | 1.91                     | 0.52              |
| 1:A:30:VAL:O     | 1:A:57:ASP:HA    | 2.10                     | 0.52              |
| 1:A:304:LEU:O    | 1:A:307:PHE:HB3  | 2.10                     | 0.52              |
| 1:A:365:LYS:HB2  | 1:A:477:MET:HE1  | 1.90                     | 0.52              |
| 1:B:242:HIS:ND1  | 1:B:404:ARG:NH1  | 2.58                     | 0.52              |
| 1:B:332:MET:HB3  | 1:B:333:PRO:HD3  | 1.92                     | 0.52              |
| 1:A:76:PRO:HG2   | 1:A:105:GLU:O    | 2.09                     | 0.52              |
| 1:A:232:ARG:NH2  | 1:A:551:GLU:OE1  | 2.43                     | 0.52              |
| 1:A:232:ARG:HH22 | 1:A:551:GLU:CD   | 2.17                     | 0.52              |
| 1:A:447:PRO:HG3  | 1:A:457:ILE:HB   | 1.92                     | 0.52              |
| 1:B:84:LEU:HD11  | 1:B:101:ILE:HD11 | 1.92                     | 0.52              |
| 1:B:369:ASP:CG   | 1:B:375:ASP:HB2  | 2.35                     | 0.52              |
| 1:A:588:ILE:HD12 | 1:A:588:ILE:C    | 2.35                     | 0.52              |
| 1:B:201:LEU:HD22 | 1:B:201:LEU:N    | 2.22                     | 0.52              |
| 1:B:46:GLU:O     | 1:B:50:GLU:HG2   | 2.10                     | 0.51              |
| 1:A:203:GLN:O    | 1:A:206:LEU:HD12 | 2.10                     | 0.51              |
| 1:A:416:ILE:HG13 | 1:A:420:ASN:HB2  | 1.93                     | 0.51              |
| 1:B:536:GLY:HA3  | 1:B:537:PRO:C    | 2.34                     | 0.51              |
| 1:A:84:LEU:HD11  | 1:A:101:ILE:HD11 | 1.93                     | 0.51              |
| 1:A:247:GLN:HG3  | 1:A:285:TRP:CZ2  | 2.44                     | 0.51              |
| 1:A:198:PHE:CD1  | 1:A:229:ILE:HD13 | 2.45                     | 0.51              |
| 1:B:54:LEU:CD2   | 1:B:55:VAL:N     | 2.69                     | 0.51              |
| 1:B:198:PHE:CD1  | 1:B:229:ILE:HD13 | 2.44                     | 0.51              |
| 1:A:33:LEU:O     | 1:A:36:ARG:HB2   | 2.11                     | 0.51              |
| 1:A:372:MET:HE1  | 1:A:480:TRP:CA   | 2.41                     | 0.51              |
| 1:B:7:VAL:HB     | 1:B:41:CYS:SG    | 2.51                     | 0.51              |
| 1:B:140:GLN:C    | 1:B:141:ILE:HD12 | 2.36                     | 0.51              |
| 1:B:547:ILE:HG23 | 1:B:572:SER:HB2  | 1.91                     | 0.51              |
| 1:A:241:LEU:HD12 | 1:A:408:LEU:HD11 | 1.92                     | 0.51              |
| 1:B:123:PHE:HD1  | 1:B:123:PHE:H    | 1.58                     | 0.51              |
| 1:B:247:GLN:HG3  | 1:B:285:TRP:HZ2  | 1.74                     | 0.51              |
| 1:B:380:LYS:O    | 1:B:381:ILE:CG2  | 2.56                     | 0.51              |
| 1:A:462:HIS:HB3  | 1:A:464:HIS:CE1  | 2.45                     | 0.51              |
| 1:A:536:GLY:HA3  | 1:A:537:PRO:C    | 2.34                     | 0.51              |
| 1:B:26:LYS:HD3   | 1:B:69:GLU:HB2   | 1.92                     | 0.51              |
| 1:B:365:LYS:HB2  | 1:B:477:MET:HE1  | 1.92                     | 0.51              |
| 1:B:238:SER:N    | 1:B:239:PRO:HD2  | 2.25                     | 0.51              |
| 1:B:263:TYR:OH   | 1:B:344:THR:HG22 | 2.10                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:105:GLU:O    | 1:A:106:ALA:C    | 2.54                     | 0.51              |
| 1:B:289:ARG:HG2  | 1:B:290:HIS:N    | 2.25                     | 0.51              |
| 1:B:304:LEU:O    | 1:B:307:PHE:HB3  | 2.10                     | 0.51              |
| 1:A:46:GLU:O     | 1:A:50:GLU:HG2   | 2.11                     | 0.50              |
| 1:A:135:LEU:C    | 1:A:135:LEU:HD23 | 2.35                     | 0.50              |
| 1:A:379:GLU:CG   | 1:A:380:LYS:H    | 2.19                     | 0.50              |
| 1:B:437:ILE:HD11 | 1:B:586:ARG:HD2  | 1.93                     | 0.50              |
| 1:A:54:LEU:CD2   | 1:A:55:VAL:N     | 2.73                     | 0.50              |
| 1:A:123:PHE:CD1  | 1:A:123:PHE:N    | 2.78                     | 0.50              |
| 1:A:335:TYR:CE2  | 1:B:346:LEU:HD11 | 2.46                     | 0.50              |
| 1:A:436:TRP:CE3  | 1:A:436:TRP:HA   | 2.46                     | 0.50              |
| 1:B:84:LEU:HD11  | 1:B:101:ILE:HD13 | 1.93                     | 0.50              |
| 1:B:89:GLN:HE21  | 1:B:89:GLN:CA    | 2.04                     | 0.50              |
| 1:A:370:LEU:HD11 | 1:A:388:ILE:HD11 | 1.93                     | 0.50              |
| 1:B:559:THR:HG23 | 1:B:567:GLU:HA   | 1.93                     | 0.50              |
| 1:A:440:ASP:C    | 1:A:442:GLN:H    | 2.18                     | 0.50              |
| 1:B:232:ARG:HH22 | 1:B:551:GLU:CD   | 2.20                     | 0.50              |
| 1:B:588:ILE:C    | 1:B:588:ILE:HD12 | 2.36                     | 0.50              |
| 1:A:263:TYR:OH   | 1:A:344:THR:HG22 | 2.12                     | 0.50              |
| 1:B:123:PHE:CD1  | 1:B:123:PHE:N    | 2.78                     | 0.50              |
| 1:B:379:GLU:CG   | 1:B:380:LYS:H    | 2.17                     | 0.50              |
| 1:A:74:ILE:HD12  | 1:A:80:SER:HB3   | 1.94                     | 0.50              |
| 1:A:437:ILE:HD11 | 1:A:586:ARG:HD2  | 1.93                     | 0.50              |
| 1:B:59:ASN:O     | 1:B:60:ARG:C     | 2.55                     | 0.50              |
| 1:A:363:LEU:HD23 | 1:A:391:ILE:HD12 | 1.94                     | 0.50              |
| 1:A:451:ASP:C    | 1:A:453:GLY:N    | 2.70                     | 0.50              |
| 1:A:484:MET:SD   | 1:A:488:MET:HE3  | 2.52                     | 0.50              |
| 1:B:105:GLU:O    | 1:B:106:ALA:C    | 2.53                     | 0.50              |
| 1:B:168:ARG:HG3  | 1:B:168:ARG:NH1  | 2.27                     | 0.50              |
| 1:B:232:ARG:NH2  | 1:B:551:GLU:OE1  | 2.45                     | 0.50              |
| 1:B:257:GLU:O    | 1:B:260:VAL:HG12 | 2.11                     | 0.50              |
| 1:A:56:GLU:OE1   | 1:A:62:ARG:HG3   | 2.12                     | 0.49              |
| 1:A:232:ARG:HD3  | 1:A:232:ARG:C    | 2.36                     | 0.49              |
| 1:A:289:ARG:HG2  | 1:A:290:HIS:N    | 2.25                     | 0.49              |
| 1:A:310:GLU:O    | 1:A:311:LYS:HD2  | 2.12                     | 0.49              |
| 1:B:142:PHE:CE1  | 1:B:571:GLY:HA3  | 2.46                     | 0.49              |
| 1:B:416:ILE:HG13 | 1:B:420:ASN:HB2  | 1.92                     | 0.49              |
| 1:B:436:TRP:CE3  | 1:B:436:TRP:HA   | 2.47                     | 0.49              |
| 1:A:35:MET:HE2   | 1:A:39:SER:HB3   | 1.92                     | 0.49              |
| 1:A:30:VAL:HG21  | 1:A:35:MET:SD    | 2.52                     | 0.49              |
| 1:A:82:LYS:HA    | 1:A:85:MET:CE    | 2.42                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:310:GLU:O    | 1:B:311:LYS:HD2  | 2.12                     | 0.49              |
| 1:B:451:ASP:C    | 1:B:453:GLY:N    | 2.70                     | 0.49              |
| 1:B:540:ILE:CD1  | 1:B:569:ILE:HB   | 2.38                     | 0.49              |
| 1:A:135:LEU:HD23 | 1:A:136:PRO:N    | 2.28                     | 0.49              |
| 1:A:163:ILE:HB   | 1:A:164:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:386:ARG:HG2  | 1:A:387:ASN:N    | 2.28                     | 0.49              |
| 1:B:375:ASP:HA   | 1:B:479:ARG:HH12 | 1.77                     | 0.49              |
| 1:B:237:ILE:C    | 1:B:239:PRO:HD2  | 2.38                     | 0.49              |
| 1:A:142:PHE:CE1  | 1:A:571:GLY:HA3  | 2.47                     | 0.49              |
| 1:B:4:LYS:HZ2    | 1:B:280:GLU:HG3  | 1.77                     | 0.49              |
| 1:B:163:ILE:HB   | 1:B:164:PRO:HD3  | 1.94                     | 0.49              |
| 1:A:440:ASP:O    | 1:A:442:GLN:N    | 2.45                     | 0.49              |
| 1:A:279:ASP:CG   | 1:A:281:LYS:HE2  | 2.38                     | 0.48              |
| 1:A:287:GLU:O    | 1:A:287:GLU:HG2  | 2.14                     | 0.48              |
| 1:B:497:ASP:OD2  | 1:B:500:HIS:HB2  | 2.12                     | 0.48              |
| 1:A:488:MET:O    | 1:A:492:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:389:VAL:HB   | 1:B:390:PRO:HD3  | 1.96                     | 0.48              |
| 1:B:577:THR:O    | 1:B:578:PRO:C    | 2.55                     | 0.48              |
| 1:A:123:PHE:HD1  | 1:A:123:PHE:H    | 1.58                     | 0.48              |
| 1:A:357:GLN:HE21 | 1:B:325:LEU:HD23 | 1.78                     | 0.48              |
| 1:A:389:VAL:HB   | 1:A:390:PRO:HD3  | 1.96                     | 0.48              |
| 1:B:30:VAL:HG21  | 1:B:35:MET:SD    | 2.53                     | 0.48              |
| 1:B:141:ILE:HA   | 1:B:570:LEU:O    | 2.14                     | 0.48              |
| 1:A:577:THR:O    | 1:A:578:PRO:C    | 2.57                     | 0.48              |
| 1:B:257:GLU:O    | 1:B:258:ASN:C    | 2.57                     | 0.48              |
| 1:A:367:GLU:HG2  | 1:A:408:LEU:HD12 | 1.95                     | 0.48              |
| 1:A:441:MET:HA   | 1:A:441:MET:HE3  | 1.96                     | 0.48              |
| 1:B:368:GLN:HE21 | 1:B:479:ARG:HB2  | 1.77                     | 0.48              |
| 1:B:403:ILE:HG23 | 1:B:438:ILE:HD11 | 1.95                     | 0.48              |
| 1:A:59:ASN:O     | 1:A:60:ARG:C     | 2.57                     | 0.48              |
| 1:A:257:GLU:O    | 1:A:258:ASN:C    | 2.56                     | 0.48              |
| 1:A:368:GLN:HE21 | 1:A:479:ARG:HB2  | 1.78                     | 0.48              |
| 1:A:559:THR:HG23 | 1:A:567:GLU:HA   | 1.95                     | 0.48              |
| 1:B:383:ASP:O    | 1:B:384:HIS:HB2  | 2.14                     | 0.48              |
| 1:B:436:TRP:HA   | 1:B:436:TRP:HE3  | 1.79                     | 0.48              |
| 1:B:441:MET:HE3  | 1:B:441:MET:HA   | 1.96                     | 0.48              |
| 1:B:561:THR:O    | 1:B:563:LYS:HG3  | 2.13                     | 0.48              |
| 1:A:4:LYS:HZ3    | 1:A:280:GLU:HG3  | 1.78                     | 0.48              |
| 1:A:82:LYS:HA    | 1:A:85:MET:HE2   | 1.94                     | 0.48              |
| 1:A:564:ASN:O    | 1:A:565:ASN:CB   | 2.61                     | 0.48              |
| 1:B:171:GLU:HA   | 1:B:205:LYS:HG2  | 1.95                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:386:ARG:HG2  | 1:B:387:ASN:N    | 2.27                     | 0.48              |
| 1:B:563:LYS:C    | 1:B:565:ASN:N    | 2.69                     | 0.48              |
| 1:A:44:MET:O     | 1:A:45:HIS:C     | 2.57                     | 0.48              |
| 1:A:436:TRP:HA   | 1:A:436:TRP:HE3  | 1.79                     | 0.48              |
| 1:B:344:THR:O    | 1:B:348:LEU:N    | 2.47                     | 0.48              |
| 1:B:363:LEU:HD23 | 1:B:391:ILE:HD12 | 1.96                     | 0.48              |
| 1:A:35:MET:HE3   | 1:A:35:MET:O     | 2.13                     | 0.47              |
| 1:A:140:GLN:C    | 1:A:141:ILE:HD12 | 2.39                     | 0.47              |
| 1:B:37:MET:HE1   | 1:B:132:ILE:HD13 | 1.96                     | 0.47              |
| 1:B:228:LEU:HD23 | 1:B:229:ILE:N    | 2.29                     | 0.47              |
| 1:B:305:LYS:C    | 1:B:307:PHE:N    | 2.72                     | 0.47              |
| 1:A:242:HIS:CE1  | 1:A:404:ARG:CZ   | 2.96                     | 0.47              |
| 1:A:436:TRP:O    | 1:A:437:ILE:C    | 2.56                     | 0.47              |
| 1:B:26:LYS:HG2   | 1:B:69:GLU:HB2   | 1.96                     | 0.47              |
| 1:B:35:MET:HE2   | 1:B:39:SER:HB3   | 1.96                     | 0.47              |
| 1:B:296:VAL:O    | 1:B:297:SER:C    | 2.55                     | 0.47              |
| 1:A:367:GLU:HG3  | 1:A:405:ILE:CD1  | 2.45                     | 0.47              |
| 1:A:403:ILE:HG23 | 1:A:438:ILE:HD11 | 1.96                     | 0.47              |
| 1:B:564:ASN:O    | 1:B:565:ASN:CB   | 2.62                     | 0.47              |
| 1:A:3:LEU:HD11   | 1:A:134:PHE:CZ   | 2.49                     | 0.47              |
| 1:A:171:GLU:HA   | 1:A:205:LYS:HG2  | 1.95                     | 0.47              |
| 1:A:344:THR:O    | 1:A:348:LEU:N    | 2.45                     | 0.47              |
| 1:B:33:LEU:HD12  | 1:B:135:LEU:HD11 | 1.97                     | 0.47              |
| 1:B:484:MET:O    | 1:B:488:MET:HG3  | 2.13                     | 0.47              |
| 1:A:484:MET:O    | 1:A:488:MET:HG3  | 2.14                     | 0.47              |
| 1:B:90:ASN:OD1   | 1:B:90:ASN:C     | 2.58                     | 0.47              |
| 1:B:425:VAL:HG11 | 1:B:435:LYS:HG2  | 1.96                     | 0.47              |
| 1:A:222:LYS:O    | 1:A:223:ASP:HB3  | 2.15                     | 0.47              |
| 1:A:380:LYS:HB2  | 1:A:381:ILE:H    | 1.56                     | 0.47              |
| 1:A:403:ILE:HG23 | 1:A:438:ILE:HD13 | 1.96                     | 0.47              |
| 1:A:561:THR:CG2  | 1:A:562:ALA:H    | 2.26                     | 0.47              |
| 1:A:563:LYS:C    | 1:A:565:ASN:N    | 2.69                     | 0.47              |
| 1:B:56:GLU:OE1   | 1:B:62:ARG:HG3   | 2.15                     | 0.47              |
| 1:B:82:LYS:HA    | 1:B:85:MET:HE2   | 1.96                     | 0.47              |
| 1:B:222:LYS:O    | 1:B:223:ASP:HB3  | 2.13                     | 0.47              |
| 1:B:383:ASP:OD1  | 1:B:413:LYS:NZ   | 2.47                     | 0.47              |
| 1:A:26:LYS:HD3   | 1:A:69:GLU:HB2   | 1.96                     | 0.47              |
| 1:B:27:VAL:HG11  | 1:B:65:LEU:HD12  | 1.97                     | 0.47              |
| 1:B:285:TRP:O    | 1:B:289:ARG:HD2  | 2.14                     | 0.47              |
| 1:B:586:ARG:HH11 | 1:B:586:ARG:HG2  | 1.80                     | 0.47              |
| 1:A:152:VAL:HG11 | 1:A:165:ASN:HD22 | 1.80                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:44:MET:O     | 1:B:45:HIS:C     | 2.56                     | 0.47              |
| 1:B:82:LYS:HA    | 1:B:85:MET:CE    | 2.45                     | 0.47              |
| 1:B:279:ASP:CG   | 1:B:281:LYS:HE2  | 2.40                     | 0.47              |
| 1:A:263:TYR:CZ   | 1:A:274:LYS:HG2  | 2.50                     | 0.46              |
| 1:B:76:PRO:HG2   | 1:B:105:GLU:O    | 2.15                     | 0.46              |
| 1:A:346:LEU:HD11 | 1:B:335:TYR:HE2  | 1.81                     | 0.46              |
| 1:B:39:SER:HB2   | 1:B:281:LYS:NZ   | 2.30                     | 0.46              |
| 1:B:211:ALA:C    | 1:B:213:ASP:H    | 2.23                     | 0.46              |
| 1:B:287:GLU:O    | 1:B:287:GLU:HG2  | 2.15                     | 0.46              |
| 1:A:37:MET:HE1   | 1:A:132:ILE:CD1  | 2.46                     | 0.46              |
| 1:A:279:ASP:HB3  | 1:A:281:LYS:HG2  | 1.98                     | 0.46              |
| 1:A:328:MET:C    | 1:A:330:LYS:N    | 2.72                     | 0.46              |
| 1:A:383:ASP:O    | 1:A:384:HIS:HB2  | 2.15                     | 0.46              |
| 1:B:92:ASP:O     | 1:B:93:ASN:HB2   | 2.15                     | 0.46              |
| 1:B:247:GLN:HG3  | 1:B:285:TRP:CZ2  | 2.49                     | 0.46              |
| 1:B:386:ARG:O    | 1:B:387:ASN:C    | 2.58                     | 0.46              |
| 1:A:81:VAL:O     | 1:A:85:MET:HG3   | 2.15                     | 0.46              |
| 1:A:180:LEU:O    | 1:A:222:LYS:NZ   | 2.48                     | 0.46              |
| 1:B:33:LEU:O     | 1:B:36:ARG:HB2   | 2.15                     | 0.46              |
| 1:B:440:ASP:C    | 1:B:442:GLN:H    | 2.23                     | 0.46              |
| 1:B:81:VAL:O     | 1:B:85:MET:HG3   | 2.16                     | 0.46              |
| 1:A:7:VAL:HB     | 1:A:41:CYS:SG    | 2.56                     | 0.46              |
| 1:A:425:VAL:HG11 | 1:A:435:LYS:HG2  | 1.98                     | 0.46              |
| 1:B:74:ILE:HD12  | 1:B:80:SER:HB3   | 1.97                     | 0.46              |
| 1:A:94:PRO:HG3   | 1:A:123:PHE:HE2  | 1.81                     | 0.46              |
| 1:A:312:ARG:NH1  | 1:A:312:ARG:HB2  | 2.31                     | 0.46              |
| 1:A:383:ASP:O    | 1:A:383:ASP:OD1  | 2.34                     | 0.46              |
| 1:A:384:HIS:O    | 1:A:385:MET:SD   | 2.74                     | 0.46              |
| 1:B:261:TYR:CE2  | 1:B:348:LEU:HD13 | 2.50                     | 0.46              |
| 1:A:168:ARG:HG3  | 1:A:168:ARG:NH1  | 2.29                     | 0.46              |
| 1:A:295:VAL:O    | 1:A:298:GLN:HB3  | 2.16                     | 0.46              |
| 1:B:305:LYS:O    | 1:B:307:PHE:N    | 2.49                     | 0.46              |
| 1:B:362:LYS:HZ1  | 1:B:396:LYS:HD2  | 1.80                     | 0.46              |
| 1:B:388:ILE:O    | 1:B:392:LEU:HD13 | 2.16                     | 0.46              |
| 1:B:393:LEU:O    | 1:B:394:ASP:C    | 2.59                     | 0.46              |
| 1:A:386:ARG:C    | 1:A:388:ILE:N    | 2.73                     | 0.46              |
| 1:B:327:GLN:CD   | 1:B:327:GLN:N    | 2.74                     | 0.46              |
| 1:A:211:ALA:C    | 1:A:213:ASP:H    | 2.24                     | 0.46              |
| 1:A:372:MET:CA   | 1:A:372:MET:HE2  | 2.46                     | 0.46              |
| 1:A:577:THR:HG22 | 1:A:580:GLY:CA   | 2.46                     | 0.46              |
| 1:A:296:VAL:O    | 1:A:297:SER:C    | 2.58                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:394:ASP:OD1  | 1:A:396:LYS:HB3  | 2.17                     | 0.45              |
| 1:B:178:ALA:O    | 1:B:180:LEU:N    | 2.49                     | 0.45              |
| 1:B:436:TRP:O    | 1:B:437:ILE:C    | 2.59                     | 0.45              |
| 1:A:372:MET:CE   | 1:A:480:TRP:HB2  | 2.40                     | 0.45              |
| 1:A:388:ILE:O    | 1:A:392:LEU:HD13 | 2.17                     | 0.45              |
| 1:B:180:LEU:O    | 1:B:222:LYS:NZ   | 2.50                     | 0.45              |
| 1:B:372:MET:CE   | 1:B:480:TRP:HB2  | 2.40                     | 0.45              |
| 1:B:577:THR:HG22 | 1:B:580:GLY:CA   | 2.46                     | 0.45              |
| 1:A:3:LEU:HD11   | 1:A:134:PHE:CE2  | 2.52                     | 0.45              |
| 1:A:92:ASP:O     | 1:A:93:ASN:HB2   | 2.16                     | 0.45              |
| 1:A:209:TYR:HB3  | 1:A:216:MET:CE   | 2.28                     | 0.45              |
| 1:A:249:MET:SD   | 1:A:293:ILE:CD1  | 3.05                     | 0.45              |
| 1:A:383:ASP:OD1  | 1:A:413:LYS:NZ   | 2.48                     | 0.45              |
| 1:B:35:MET:HE3   | 1:B:35:MET:O     | 2.16                     | 0.45              |
| 1:B:242:HIS:CE1  | 1:B:404:ARG:CZ   | 2.99                     | 0.45              |
| 1:B:394:ASP:OD1  | 1:B:396:LYS:HB3  | 2.15                     | 0.45              |
| 1:A:103:PHE:HB2  | 1:A:129:GLU:HB3  | 1.99                     | 0.45              |
| 1:A:242:HIS:ND1  | 1:A:404:ARG:NH1  | 2.64                     | 0.45              |
| 1:B:328:MET:C    | 1:B:330:LYS:N    | 2.72                     | 0.45              |
| 1:B:386:ARG:C    | 1:B:388:ILE:N    | 2.73                     | 0.45              |
| 1:A:212:ASP:O    | 1:A:213:ASP:HB2  | 2.17                     | 0.45              |
| 1:A:285:TRP:O    | 1:A:289:ARG:HD2  | 2.15                     | 0.45              |
| 1:A:561:THR:O    | 1:A:563:LYS:HG3  | 2.16                     | 0.45              |
| 1:A:573:THR:OG1  | 1:A:574:HIS:HD2  | 2.00                     | 0.45              |
| 1:B:384:HIS:HA   | 1:B:409:TYR:OH   | 2.17                     | 0.45              |
| 1:B:484:MET:SD   | 1:B:488:MET:HE3  | 2.56                     | 0.45              |
| 1:A:7:VAL:CG1    | 1:A:37:MET:HE3   | 2.47                     | 0.45              |
| 1:B:372:MET:C    | 1:B:374:THR:H    | 2.24                     | 0.45              |
| 1:B:403:ILE:HG23 | 1:B:438:ILE:HD13 | 1.98                     | 0.45              |
| 1:B:445:GLY:O    | 1:B:457:ILE:HG21 | 2.17                     | 0.45              |
| 1:A:145:ASP:OD1  | 1:A:145:ASP:O    | 2.35                     | 0.45              |
| 1:A:305:LYS:C    | 1:A:307:PHE:N    | 2.74                     | 0.45              |
| 1:B:360:VAL:O    | 1:B:361:ASP:C    | 2.58                     | 0.45              |
| 1:B:492:VAL:C    | 1:B:494:ASP:H    | 2.24                     | 0.45              |
| 1:A:327:GLN:N    | 1:A:327:GLN:CD   | 2.75                     | 0.45              |
| 1:B:152:VAL:HG11 | 1:B:165:ASN:HD22 | 1.82                     | 0.45              |
| 1:B:293:ILE:HD13 | 1:B:293:ILE:H    | 1.81                     | 0.45              |
| 1:B:383:ASP:O    | 1:B:383:ASP:OD1  | 2.35                     | 0.45              |
| 1:A:228:LEU:HD23 | 1:A:229:ILE:N    | 2.32                     | 0.45              |
| 1:A:588:ILE:HG13 | 1:A:589:SER:N    | 2.31                     | 0.45              |
| 1:B:232:ARG:HD3  | 1:B:232:ARG:C    | 2.40                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:279:ASP:HB3  | 1:B:281:LYS:HG2  | 1.99                     | 0.45              |
| 1:B:299:ASN:N    | 1:B:299:ASN:HD22 | 2.14                     | 0.45              |
| 1:B:588:ILE:HG13 | 1:B:589:SER:N    | 2.32                     | 0.45              |
| 1:A:393:LEU:O    | 1:A:394:ASP:C    | 2.60                     | 0.44              |
| 1:A:386:ARG:O    | 1:A:387:ASN:C    | 2.60                     | 0.44              |
| 1:B:440:ASP:O    | 1:B:442:GLN:N    | 2.51                     | 0.44              |
| 1:B:297:SER:OG   | 1:B:353:MET:HE1  | 2.17                     | 0.44              |
| 1:B:573:THR:OG1  | 1:B:574:HIS:HD2  | 2.00                     | 0.44              |
| 1:A:305:LYS:O    | 1:A:306:GLN:C    | 2.61                     | 0.44              |
| 1:A:380:LYS:O    | 1:A:381:ILE:CG2  | 2.58                     | 0.44              |
| 1:A:384:HIS:HA   | 1:A:409:TYR:OH   | 2.17                     | 0.44              |
| 1:B:12:MET:O     | 1:B:17:LEU:HD23  | 2.18                     | 0.44              |
| 1:B:7:VAL:CG1    | 1:B:37:MET:HE3   | 2.46                     | 0.44              |
| 1:B:312:ARG:NH1  | 1:B:312:ARG:HB2  | 2.33                     | 0.44              |
| 1:A:12:MET:O     | 1:A:17:LEU:HD23  | 2.18                     | 0.44              |
| 1:A:362:LYS:HZ1  | 1:A:396:LYS:HD2  | 1.81                     | 0.44              |
| 1:A:372:MET:C    | 1:A:374:THR:H    | 2.24                     | 0.44              |
| 1:A:375:ASP:O    | 1:A:378:GLY:N    | 2.51                     | 0.44              |
| 1:B:11:ILE:O     | 1:B:15:VAL:HB    | 2.18                     | 0.44              |
| 1:B:561:THR:CG2  | 1:B:562:ALA:H    | 2.24                     | 0.44              |
| 1:A:297:SER:OG   | 1:A:353:MET:HE1  | 2.18                     | 0.44              |
| 1:A:358:GLN:O    | 1:A:396:LYS:HD3  | 2.18                     | 0.44              |
| 1:A:368:GLN:O    | 1:A:372:MET:HB2  | 2.18                     | 0.44              |
| 1:B:193:ASP:C    | 1:B:195:ASN:N    | 2.76                     | 0.44              |
| 1:B:305:LYS:O    | 1:B:306:GLN:C    | 2.61                     | 0.44              |
| 1:B:343:SER:O    | 1:B:347:HIS:HB2  | 2.17                     | 0.44              |
| 1:B:367:GLU:HG3  | 1:B:405:ILE:CD1  | 2.48                     | 0.44              |
| 1:A:305:LYS:HB3  | 1:B:308:ALA:HB1  | 1.99                     | 0.44              |
| 1:B:358:GLN:O    | 1:B:396:LYS:HD3  | 2.18                     | 0.44              |
| 1:A:178:ALA:O    | 1:A:180:LEU:N    | 2.51                     | 0.44              |
| 1:A:305:LYS:O    | 1:A:307:PHE:N    | 2.51                     | 0.44              |
| 1:A:445:GLY:O    | 1:A:457:ILE:HG21 | 2.17                     | 0.44              |
| 1:B:103:PHE:HB2  | 1:B:129:GLU:HB3  | 2.00                     | 0.44              |
| 1:A:249:MET:HE1  | 1:A:293:ILE:HG21 | 2.00                     | 0.43              |
| 1:A:493:GLU:OE1  | 1:A:495:LYS:HD3  | 2.18                     | 0.43              |
| 1:B:26:LYS:CD    | 1:B:69:GLU:HB2   | 2.49                     | 0.43              |
| 1:B:503:PHE:O    | 1:B:504:LEU:C    | 2.62                     | 0.43              |
| 1:A:63:GLU:HA    | 1:A:64:PRO:HD3   | 1.81                     | 0.43              |
| 1:A:141:ILE:HA   | 1:A:570:LEU:O    | 2.18                     | 0.43              |
| 1:B:212:ASP:O    | 1:B:213:ASP:HB2  | 2.18                     | 0.43              |
| 1:B:296:VAL:O    | 1:B:300:VAL:HG23 | 2.18                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:234:PHE:HZ   | 1:A:484:MET:HE2  | 1.83                     | 0.43              |
| 1:A:335:TYR:CZ   | 1:B:301:THR:HG22 | 2.54                     | 0.43              |
| 1:B:129:GLU:CD   | 1:B:129:GLU:O    | 2.61                     | 0.43              |
| 1:B:245:THR:O    | 1:B:246:PHE:C    | 2.60                     | 0.43              |
| 1:B:488:MET:O    | 1:B:492:VAL:HG23 | 2.19                     | 0.43              |
| 1:A:126:THR:HG22 | 1:A:127:LEU:N    | 2.34                     | 0.43              |
| 1:A:261:TYR:CE2  | 1:A:348:LEU:HD13 | 2.53                     | 0.43              |
| 1:A:466:ARG:O    | 1:A:467:LYS:C    | 2.61                     | 0.43              |
| 1:B:304:LEU:HA   | 1:B:342:TYR:CE2  | 2.54                     | 0.43              |
| 1:B:410:ILE:HD11 | 1:B:421:LEU:HD23 | 1.99                     | 0.43              |
| 1:A:193:ASP:C    | 1:A:195:ASN:N    | 2.77                     | 0.43              |
| 1:A:325:LEU:HD23 | 1:A:325:LEU:O    | 2.19                     | 0.43              |
| 1:B:3:LEU:HA     | 1:B:180:LEU:HD21 | 2.01                     | 0.43              |
| 1:A:312:ARG:CB   | 1:A:312:ARG:HH11 | 2.32                     | 0.42              |
| 1:B:305:LYS:O    | 1:B:308:ALA:N    | 2.52                     | 0.42              |
| 1:B:561:THR:O    | 1:B:563:LYS:N    | 2.52                     | 0.42              |
| 1:A:75:THR:OG1   | 1:A:77:THR:HG23  | 2.18                     | 0.42              |
| 1:B:388:ILE:C    | 1:B:392:LEU:HD13 | 2.44                     | 0.42              |
| 1:A:245:THR:O    | 1:A:246:PHE:C    | 2.61                     | 0.42              |
| 1:A:343:SER:O    | 1:A:347:HIS:HB2  | 2.19                     | 0.42              |
| 1:A:410:ILE:HD11 | 1:A:421:LEU:HD23 | 2.01                     | 0.42              |
| 1:A:305:LYS:O    | 1:A:308:ALA:N    | 2.53                     | 0.42              |
| 1:A:305:LYS:HE3  | 1:A:305:LYS:HB2  | 1.89                     | 0.42              |
| 1:B:244:LEU:O    | 1:B:293:ILE:CD1  | 2.67                     | 0.42              |
| 1:B:493:GLU:OE1  | 1:B:495:LYS:HD3  | 2.18                     | 0.42              |
| 1:A:11:ILE:O     | 1:A:15:VAL:HB    | 2.19                     | 0.42              |
| 1:A:141:ILE:HG12 | 1:A:552:MET:HG2  | 2.00                     | 0.42              |
| 1:A:392:LEU:O    | 1:A:402:LYS:HE2  | 2.18                     | 0.42              |
| 1:B:75:THR:HA    | 1:B:76:PRO:HD3   | 1.86                     | 0.42              |
| 1:B:387:ASN:C    | 1:B:390:PRO:HD2  | 2.44                     | 0.42              |
| 1:B:388:ILE:HG22 | 1:B:392:LEU:HD13 | 2.01                     | 0.42              |
| 1:A:90:ASN:OD1   | 1:A:90:ASN:C     | 2.63                     | 0.42              |
| 1:A:227:LEU:C    | 1:A:227:LEU:HD23 | 2.44                     | 0.42              |
| 1:A:444:LEU:N    | 1:A:444:LEU:CD1  | 2.83                     | 0.42              |
| 1:A:497:ASP:OD2  | 1:A:500:HIS:HB2  | 2.19                     | 0.42              |
| 1:B:33:LEU:HD22  | 1:B:33:LEU:N     | 2.33                     | 0.42              |
| 1:B:245:THR:HG21 | 1:B:553:ARG:HH21 | 1.85                     | 0.42              |
| 1:B:249:MET:HE2  | 1:B:293:ILE:HD12 | 2.00                     | 0.42              |
| 1:B:372:MET:HE1  | 1:B:480:TRP:HA   | 2.01                     | 0.42              |
| 1:B:384:HIS:O    | 1:B:385:MET:SD   | 2.77                     | 0.42              |
| 1:A:27:VAL:HG11  | 1:A:65:LEU:HD12  | 2.00                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:440:ASP:O    | 1:A:441:MET:C    | 2.61                     | 0.42              |
| 1:B:65:LEU:N     | 1:B:66:PRO:HD3   | 2.33                     | 0.42              |
| 1:B:330:LYS:C    | 1:B:332:MET:H    | 2.27                     | 0.42              |
| 1:B:383:ASP:O    | 1:B:384:HIS:CB   | 2.67                     | 0.42              |
| 1:B:145:ASP:OD1  | 1:B:145:ASP:O    | 2.36                     | 0.42              |
| 1:B:308:ALA:C    | 1:B:310:GLU:N    | 2.78                     | 0.42              |
| 1:B:395:GLN:HA   | 1:B:395:GLN:OE1  | 2.20                     | 0.42              |
| 1:A:21:LYS:NZ    | 1:A:21:LYS:HB3   | 2.35                     | 0.42              |
| 1:A:89:GLN:HE21  | 1:A:89:GLN:CA    | 2.04                     | 0.42              |
| 1:A:406:ILE:O    | 1:A:409:TYR:HB3  | 2.20                     | 0.42              |
| 1:A:562:ALA:O    | 1:A:563:LYS:C    | 2.63                     | 0.42              |
| 1:B:93:ASN:OD1   | 1:B:93:ASN:O     | 2.38                     | 0.42              |
| 1:B:295:VAL:O    | 1:B:298:GLN:HB3  | 2.20                     | 0.42              |
| 1:B:308:ALA:C    | 1:B:310:GLU:H    | 2.27                     | 0.42              |
| 1:B:407:LEU:O    | 1:B:411:ILE:HG13 | 2.20                     | 0.42              |
| 1:A:223:ASP:OD1  | 1:A:223:ASP:C    | 2.62                     | 0.41              |
| 1:A:559:THR:O    | 1:A:563:LYS:HE3  | 2.20                     | 0.41              |
| 1:B:244:LEU:C    | 1:B:293:ILE:HD11 | 2.45                     | 0.41              |
| 1:A:6:ALA:HB1    | 1:A:179:THR:HG22 | 2.02                     | 0.41              |
| 1:A:31:ASP:H     | 1:A:34:SER:HG    | 1.65                     | 0.41              |
| 1:B:94:PRO:HG3   | 1:B:123:PHE:HE2  | 1.84                     | 0.41              |
| 1:B:178:ALA:C    | 1:B:180:LEU:N    | 2.77                     | 0.41              |
| 1:A:65:LEU:N     | 1:A:66:PRO:HD3   | 2.35                     | 0.41              |
| 1:A:386:ARG:CG   | 1:A:387:ASN:N    | 2.83                     | 0.41              |
| 1:B:249:MET:HE2  | 1:B:352:CYS:HB3  | 1.99                     | 0.41              |
| 1:A:257:GLU:O    | 1:A:260:VAL:CG1  | 2.68                     | 0.41              |
| 1:A:293:ILE:H    | 1:A:293:ILE:HD13 | 1.85                     | 0.41              |
| 1:A:330:LYS:C    | 1:A:332:MET:H    | 2.28                     | 0.41              |
| 1:A:370:LEU:HD13 | 1:A:409:TYR:HA   | 2.02                     | 0.41              |
| 1:B:312:ARG:CB   | 1:B:312:ARG:HH11 | 2.33                     | 0.41              |
| 1:B:372:MET:CA   | 1:B:372:MET:HE2  | 2.50                     | 0.41              |
| 1:B:379:GLU:C    | 1:B:380:LYS:HG3  | 2.45                     | 0.41              |
| 1:B:386:ARG:CG   | 1:B:387:ASN:N    | 2.82                     | 0.41              |
| 1:B:227:LEU:HD23 | 1:B:227:LEU:C    | 2.46                     | 0.41              |
| 1:A:492:VAL:C    | 1:A:494:ASP:H    | 2.27                     | 0.41              |
| 1:B:21:LYS:NZ    | 1:B:21:LYS:HB3   | 2.36                     | 0.41              |
| 1:B:219:GLY:O    | 1:B:220:PRO:C    | 2.63                     | 0.41              |
| 1:B:362:LYS:HZ3  | 1:B:396:LYS:HD2  | 1.86                     | 0.41              |
| 1:B:561:THR:OG1  | 1:B:562:ALA:N    | 2.53                     | 0.41              |
| 1:B:562:ALA:O    | 1:B:563:LYS:C    | 2.63                     | 0.41              |
| 1:A:178:ALA:C    | 1:A:180:LEU:N    | 2.79                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:304:LEU:HA   | 1:A:342:TYR:CE2  | 2.56                     | 0.41              |
| 1:A:360:VAL:O    | 1:A:361:ASP:C    | 2.62                     | 0.41              |
| 1:A:436:TRP:HA   | 1:A:439:ASN:HD22 | 1.86                     | 0.41              |
| 1:A:561:THR:OG1  | 1:A:562:ALA:N    | 2.53                     | 0.41              |
| 1:B:263:TYR:CZ   | 1:B:274:LYS:HG2  | 2.55                     | 0.41              |
| 1:B:392:LEU:O    | 1:B:402:LYS:HE2  | 2.20                     | 0.41              |
| 1:B:559:THR:O    | 1:B:563:LYS:HE3  | 2.21                     | 0.41              |
| 1:A:4:LYS:NZ     | 1:A:280:GLU:HG3  | 2.36                     | 0.41              |
| 1:A:33:LEU:HD22  | 1:A:33:LEU:N     | 2.33                     | 0.41              |
| 1:A:58:ILE:HG13  | 1:A:83:CYS:HB3   | 2.03                     | 0.41              |
| 1:A:133:ALA:HB3  | 1:A:172:GLN:HA   | 2.02                     | 0.41              |
| 1:A:171:GLU:CA   | 1:A:205:LYS:HG2  | 2.51                     | 0.41              |
| 1:A:219:GLY:O    | 1:A:220:PRO:C    | 2.64                     | 0.41              |
| 1:A:357:GLN:NE2  | 1:B:325:LEU:CD2  | 2.81                     | 0.41              |
| 1:A:362:LYS:HZ2  | 1:A:396:LYS:HD2  | 1.85                     | 0.41              |
| 1:B:63:GLU:HA    | 1:B:64:PRO:HD3   | 1.80                     | 0.41              |
| 1:B:126:THR:HG22 | 1:B:127:LEU:N    | 2.35                     | 0.41              |
| 1:B:163:ILE:N    | 1:B:164:PRO:CD   | 2.84                     | 0.41              |
| 1:B:228:LEU:C    | 1:B:228:LEU:CD2  | 2.94                     | 0.41              |
| 1:B:244:LEU:CA   | 1:B:293:ILE:HD11 | 2.51                     | 0.41              |
| 1:B:274:LYS:HG3  | 1:B:275:GLU:N    | 2.36                     | 0.41              |
| 1:B:325:LEU:HD23 | 1:B:325:LEU:O    | 2.21                     | 0.41              |
| 1:B:492:VAL:HG13 | 1:B:566:TRP:CG   | 2.56                     | 0.41              |
| 1:A:249:MET:HE2  | 1:A:352:CYS:HB3  | 2.02                     | 0.41              |
| 1:A:419:GLU:O    | 1:A:420:ASN:C    | 2.64                     | 0.41              |
| 1:B:134:PHE:HE2  | 1:B:136:PRO:HG3  | 1.85                     | 0.41              |
| 1:B:440:ASP:O    | 1:B:441:MET:C    | 2.64                     | 0.41              |
| 1:A:228:LEU:CD2  | 1:A:228:LEU:C    | 2.94                     | 0.40              |
| 1:A:308:ALA:C    | 1:A:310:GLU:H    | 2.29                     | 0.40              |
| 1:A:383:ASP:O    | 1:A:384:HIS:CB   | 2.68                     | 0.40              |
| 1:B:150:PHE:CD1  | 1:B:150:PHE:C    | 2.99                     | 0.40              |
| 1:B:179:THR:O    | 1:B:179:THR:HG22 | 2.21                     | 0.40              |
| 1:B:242:HIS:CE1  | 1:B:404:ARG:NH1  | 2.89                     | 0.40              |
| 1:B:375:ASP:OD1  | 1:B:375:ASP:C    | 2.63                     | 0.40              |
| 1:A:93:ASN:OD1   | 1:A:93:ASN:O     | 2.38                     | 0.40              |
| 1:A:388:ILE:C    | 1:A:392:LEU:HD13 | 2.46                     | 0.40              |
| 1:B:359:HIS:HB3  | 1:B:396:LYS:HD3  | 2.03                     | 0.40              |
| 1:A:227:LEU:C    | 1:A:227:LEU:CD2  | 2.95                     | 0.40              |
| 1:A:367:GLU:HG3  | 1:A:405:ILE:HD11 | 2.03                     | 0.40              |
| 1:B:436:TRP:HA   | 1:B:439:ASN:HD22 | 1.86                     | 0.40              |
| 1:A:26:LYS:HG2   | 1:A:69:GLU:HB2   | 2.02                     | 0.40              |

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| Atom-1        | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|---------------|---------------|--------------------------|-------------------|
| 1:A:293:ILE:O | 1:A:294:ALA:C | 2.64                     | 0.40              |
| 1:B:292:HIS:O | 1:B:293:ILE:C | 2.64                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 1   | A     | 535/591 (90%)   | 424 (79%) | 85 (16%)  | 26 (5%)  | 1           | 13 |
| 1   | B     | 535/591 (90%)   | 423 (79%) | 83 (16%)  | 29 (5%)  | 1           | 12 |
| All | All   | 1070/1182 (90%) | 847 (79%) | 168 (16%) | 55 (5%)  | 1           | 13 |

All (55) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 23  | ALA  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 220 | PRO  |
| 1   | A     | 223 | ASP  |
| 1   | A     | 376 | ALA  |
| 1   | A     | 379 | GLU  |
| 1   | A     | 381 | ILE  |
| 1   | A     | 385 | MET  |
| 1   | A     | 387 | ASN  |
| 1   | A     | 450 | GLN  |
| 1   | B     | 23  | ALA  |
| 1   | B     | 93  | ASN  |
| 1   | B     | 220 | PRO  |
| 1   | B     | 223 | ASP  |
| 1   | B     | 376 | ALA  |
| 1   | B     | 379 | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 381 | ILE  |
| 1   | B     | 385 | MET  |
| 1   | B     | 387 | ASN  |
| 1   | B     | 450 | GLN  |
| 1   | A     | 22  | ASN  |
| 1   | A     | 222 | LYS  |
| 1   | A     | 296 | VAL  |
| 1   | A     | 359 | HIS  |
| 1   | A     | 384 | HIS  |
| 1   | A     | 452 | GLY  |
| 1   | B     | 22  | ASN  |
| 1   | B     | 222 | LYS  |
| 1   | B     | 296 | VAL  |
| 1   | B     | 359 | HIS  |
| 1   | B     | 384 | HIS  |
| 1   | B     | 452 | GLY  |
| 1   | A     | 96  | TYR  |
| 1   | A     | 219 | GLY  |
| 1   | B     | 219 | GLY  |
| 1   | B     | 386 | ARG  |
| 1   | A     | 179 | THR  |
| 1   | A     | 212 | ASP  |
| 1   | A     | 386 | ARG  |
| 1   | B     | 96  | TYR  |
| 1   | B     | 179 | THR  |
| 1   | B     | 212 | ASP  |
| 1   | B     | 562 | ALA  |
| 1   | A     | 394 | ASP  |
| 1   | A     | 562 | ALA  |
| 1   | B     | 32  | GLN  |
| 1   | B     | 298 | GLN  |
| 1   | B     | 306 | GLN  |
| 1   | A     | 388 | ILE  |
| 1   | B     | 394 | ASP  |
| 1   | B     | 388 | ILE  |
| 1   | A     | 213 | ASP  |
| 1   | A     | 91  | PRO  |
| 1   | B     | 91  | PRO  |
| 1   | B     | 213 | ASP  |

### 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     | 485/523 (93%)  | 440 (91%) | 45 (9%)  | 8           | 33 |
| 1   | B     | 485/523 (93%)  | 437 (90%) | 48 (10%) | 7           | 31 |
| All | All   | 970/1046 (93%) | 877 (90%) | 93 (10%) | 8           | 32 |

All (93) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 4   | LYS  |
| 1   | A     | 5   | THR  |
| 1   | A     | 21  | LYS  |
| 1   | A     | 25  | TRP  |
| 1   | A     | 42  | CYS  |
| 1   | A     | 60  | ARG  |
| 1   | A     | 84  | LEU  |
| 1   | A     | 89  | GLN  |
| 1   | A     | 111 | LEU  |
| 1   | A     | 115 | LEU  |
| 1   | A     | 140 | GLN  |
| 1   | A     | 163 | ILE  |
| 1   | A     | 193 | ASP  |
| 1   | A     | 201 | LEU  |
| 1   | A     | 220 | PRO  |
| 1   | A     | 227 | LEU  |
| 1   | A     | 228 | LEU  |
| 1   | A     | 232 | ARG  |
| 1   | A     | 241 | LEU  |
| 1   | A     | 243 | GLU  |
| 1   | A     | 244 | LEU  |
| 1   | A     | 260 | VAL  |
| 1   | A     | 289 | ARG  |
| 1   | A     | 293 | ILE  |
| 1   | A     | 330 | LYS  |
| 1   | A     | 332 | MET  |
| 1   | A     | 354 | LYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 358 | GLN  |
| 1   | A     | 375 | ASP  |
| 1   | A     | 380 | LYS  |
| 1   | A     | 382 | ARG  |
| 1   | A     | 384 | HIS  |
| 1   | A     | 395 | GLN  |
| 1   | A     | 405 | ILE  |
| 1   | A     | 436 | TRP  |
| 1   | A     | 456 | LYS  |
| 1   | A     | 497 | ASP  |
| 1   | A     | 504 | LEU  |
| 1   | A     | 544 | VAL  |
| 1   | A     | 563 | LYS  |
| 1   | A     | 574 | HIS  |
| 1   | A     | 577 | THR  |
| 1   | A     | 582 | LEU  |
| 1   | A     | 585 | LEU  |
| 1   | A     | 588 | ILE  |
| 1   | B     | 4   | LYS  |
| 1   | B     | 5   | THR  |
| 1   | B     | 21  | LYS  |
| 1   | B     | 25  | TRP  |
| 1   | B     | 42  | CYS  |
| 1   | B     | 60  | ARG  |
| 1   | B     | 84  | LEU  |
| 1   | B     | 89  | GLN  |
| 1   | B     | 111 | LEU  |
| 1   | B     | 115 | LEU  |
| 1   | B     | 123 | PHE  |
| 1   | B     | 131 | ASN  |
| 1   | B     | 135 | LEU  |
| 1   | B     | 140 | GLN  |
| 1   | B     | 193 | ASP  |
| 1   | B     | 201 | LEU  |
| 1   | B     | 220 | PRO  |
| 1   | B     | 228 | LEU  |
| 1   | B     | 232 | ARG  |
| 1   | B     | 241 | LEU  |
| 1   | B     | 243 | GLU  |
| 1   | B     | 244 | LEU  |
| 1   | B     | 246 | PHE  |
| 1   | B     | 260 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 289 | ARG  |
| 1   | B     | 293 | ILE  |
| 1   | B     | 330 | LYS  |
| 1   | B     | 332 | MET  |
| 1   | B     | 354 | LYS  |
| 1   | B     | 358 | GLN  |
| 1   | B     | 375 | ASP  |
| 1   | B     | 380 | LYS  |
| 1   | B     | 382 | ARG  |
| 1   | B     | 384 | HIS  |
| 1   | B     | 395 | GLN  |
| 1   | B     | 405 | ILE  |
| 1   | B     | 436 | TRP  |
| 1   | B     | 456 | LYS  |
| 1   | B     | 497 | ASP  |
| 1   | B     | 504 | LEU  |
| 1   | B     | 544 | VAL  |
| 1   | B     | 563 | LYS  |
| 1   | B     | 574 | HIS  |
| 1   | B     | 577 | THR  |
| 1   | B     | 578 | PRO  |
| 1   | B     | 582 | LEU  |
| 1   | B     | 585 | LEU  |
| 1   | B     | 588 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 89  | GLN  |
| 1   | A     | 93  | ASN  |
| 1   | A     | 95  | GLN  |
| 1   | A     | 140 | GLN  |
| 1   | A     | 151 | GLN  |
| 1   | A     | 165 | ASN  |
| 1   | A     | 247 | GLN  |
| 1   | A     | 258 | ASN  |
| 1   | A     | 299 | ASN  |
| 1   | A     | 347 | HIS  |
| 1   | A     | 357 | GLN  |
| 1   | A     | 359 | HIS  |
| 1   | A     | 368 | GLN  |
| 1   | A     | 387 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 439 | ASN  |
| 1   | A     | 442 | GLN  |
| 1   | A     | 462 | HIS  |
| 1   | A     | 464 | HIS  |
| 1   | A     | 465 | ASN  |
| 1   | A     | 560 | GLN  |
| 1   | A     | 574 | HIS  |
| 1   | B     | 89  | GLN  |
| 1   | B     | 93  | ASN  |
| 1   | B     | 95  | GLN  |
| 1   | B     | 151 | GLN  |
| 1   | B     | 165 | ASN  |
| 1   | B     | 247 | GLN  |
| 1   | B     | 258 | ASN  |
| 1   | B     | 299 | ASN  |
| 1   | B     | 336 | GLN  |
| 1   | B     | 347 | HIS  |
| 1   | B     | 357 | GLN  |
| 1   | B     | 359 | HIS  |
| 1   | B     | 368 | GLN  |
| 1   | B     | 387 | ASN  |
| 1   | B     | 439 | ASN  |
| 1   | B     | 442 | GLN  |
| 1   | B     | 462 | HIS  |
| 1   | B     | 464 | HIS  |
| 1   | B     | 465 | ASN  |
| 1   | B     | 560 | GLN  |
| 1   | B     | 574 | 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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     | 543/591 (91%)   | -0.15  | 7 (1%) 75 55  | 30, 63, 104, 131      | 1 (0%) |
| 1   | B     | 543/591 (91%)   | -0.22  | 6 (1%) 78 61  | 28, 65, 105, 131      | 1 (0%) |
| All | All   | 1086/1182 (91%) | -0.18  | 13 (1%) 76 58 | 28, 64, 105, 131      | 2 (0%) |

All (13) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | A     | 507 | GLY  | 4.9  |
| 1   | A     | 506 | GLY  | 4.5  |
| 1   | A     | 377 | ASP  | 3.8  |
| 1   | B     | 506 | GLY  | 3.6  |
| 1   | B     | 89  | GLN  | 3.6  |
| 1   | A     | 381 | ILE  | 3.0  |
| 1   | A     | 380 | LYS  | 2.8  |
| 1   | B     | 110 | GLU  | 2.6  |
| 1   | A     | 89  | GLN  | 2.2  |
| 1   | B     | 327 | GLN  | 2.1  |
| 1   | B     | 375 | ASP  | 2.1  |
| 1   | A     | 384 | HIS  | 2.1  |
| 1   | B     | 31  | ASP  | 2.1  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.