



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:55 AM UTC

PDB ID : 4AY5 / pdb\_00004ay5  
Title : Human O-GlcNAc transferase (OGT) in complex with UDP and glycopeptide  
Authors : Schimpl, M.; Zheng, X.; Blair, D.E.; Schuettelkopf, A.W.; Navratilova, I.; Aristotelous, T.; Ferenbach, A.T.; Macnaughtan, M.A.; Borodkin, V.S.; van Aalten, D.M.F.  
Deposited on : 2012-06-18  
Resolution : 3.15 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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                                             |
| Mogul                          | : | 2022.3.0, CSD as543be (2022)                                     |
| Xtriage (Phenix)               | : | 2.0                                                              |
| EDS                            | : | 3.0                                                              |
| Buster-report                  | : | wwPDB partial adaption of 1.1.7 (2018)                           |
| 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                                                             |

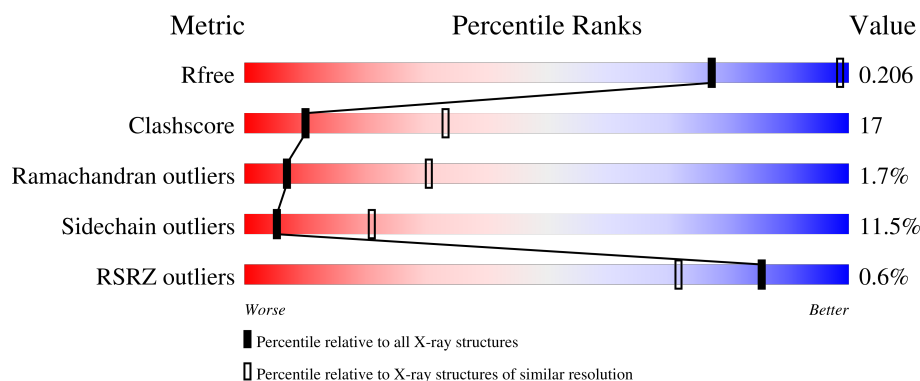
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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                      | 2361 (3.20-3.12)                                      |
| Clashscore            | 190562                      | 2486 (3.20-3.12)                                      |
| Ramachandran outliers | 187476                      | 2405 (3.20-3.12)                                      |
| Sidechain outliers    | 187428                      | 2404 (3.20-3.12)                                      |
| RSRZ outliers         | 180081                      | 2361 (3.20-3.12)                                      |

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     | 723    |                  |
| 1   | B     | 723    |                  |
| 1   | C     | 723    |                  |
| 1   | D     | 723    |                  |

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| Mol | Chain | Length | Quality of chain                                                                        |
|-----|-------|--------|-----------------------------------------------------------------------------------------|
| 2   | I     | 11     | <div> <div>9%</div> <div>27%</div> <div>36%</div> <div>36%</div> </div>                 |
| 2   | J     | 11     | <div> <div>18%</div> <div>18%</div> <div>36%</div> <div>36%</div> <div>9%</div> </div>  |
| 2   | K     | 11     | <div> <div>18%</div> <div>36%</div> <div>18%</div> <div>27%</div> <div>18%</div> </div> |
| 2   | L     | 11     | <div> <div>9%</div> <div>27%</div> <div>36%</div> <div>36%</div> </div>                 |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22524 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 UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT.

| Mol | Chain | Residues | Atoms |      |     |      |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|---------|-------|
| 1   | A     | 698      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5514  | 3499 | 964 | 1013 | 38 |         |         |       |
| 1   | B     | 698      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5514  | 3499 | 964 | 1013 | 38 |         |         |       |
| 1   | C     | 698      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5514  | 3499 | 964 | 1013 | 38 |         |         |       |
| 1   | D     | 698      | Total | C    | N   | O    | S  | 0       | 0       | 0     |
|     |       |          | 5514  | 3499 | 964 | 1013 | 38 |         |         |       |

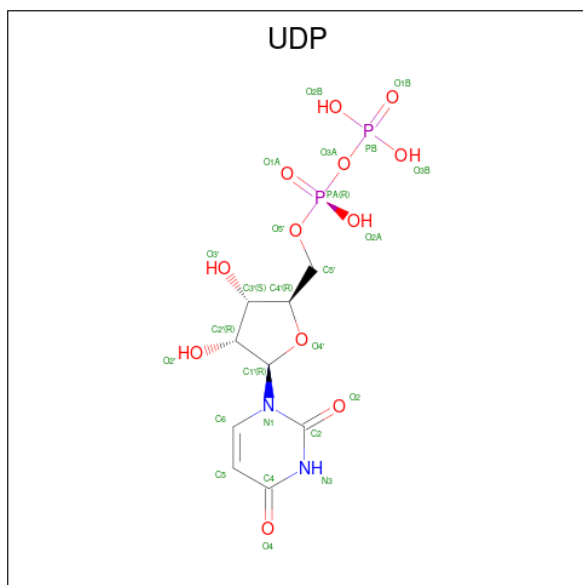
There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 309     | GLY      | -      | expression tag | UNP O15294 |
| A     | 310     | PRO      | -      | expression tag | UNP O15294 |
| A     | 311     | GLY      | -      | expression tag | UNP O15294 |
| A     | 312     | SER      | -      | expression tag | UNP O15294 |
| B     | 309     | GLY      | -      | expression tag | UNP O15294 |
| B     | 310     | PRO      | -      | expression tag | UNP O15294 |
| B     | 311     | GLY      | -      | expression tag | UNP O15294 |
| B     | 312     | SER      | -      | expression tag | UNP O15294 |
| C     | 309     | GLY      | -      | expression tag | UNP O15294 |
| C     | 310     | PRO      | -      | expression tag | UNP O15294 |
| C     | 311     | GLY      | -      | expression tag | UNP O15294 |
| C     | 312     | SER      | -      | expression tag | UNP O15294 |
| D     | 309     | GLY      | -      | expression tag | UNP O15294 |
| D     | 310     | PRO      | -      | expression tag | UNP O15294 |
| D     | 311     | GLY      | -      | expression tag | UNP O15294 |
| D     | 312     | SER      | -      | expression tag | UNP O15294 |

- Molecule 2 is a protein called GTAB1TIDE.

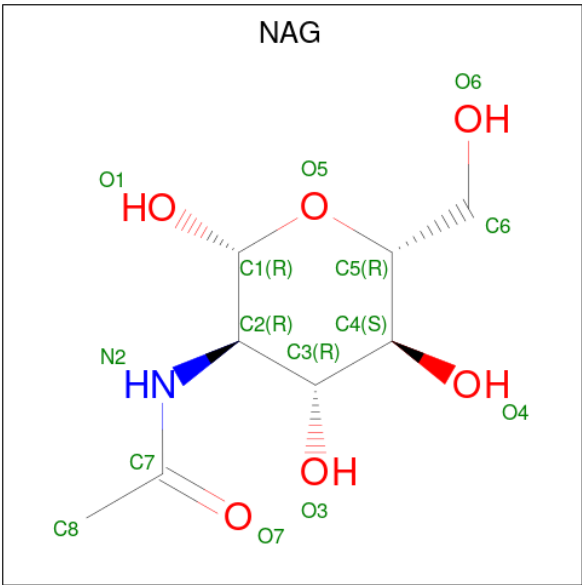
| Mol | Chain | Residues | Atoms |    |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---------|---------|-------|
| 2   | I     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 78    | 49 | 12 | 17 |         |         |       |
| 2   | J     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 78    | 49 | 12 | 17 |         |         |       |
| 2   | K     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 78    | 49 | 12 | 17 |         |         |       |
| 2   | L     | 11       | Total | C  | N  | O  | 0       | 0       | 0     |
|     |       |          | 78    | 49 | 12 | 17 |         |         |       |

- Molecule 3 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



| Mol | Chain | Residues | Atoms |   |   |    |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|----|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 25    | 9 | 2 | 12 | 2 |         |         |
| 3   | B     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 25    | 9 | 2 | 12 | 2 |         |         |
| 3   | C     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 25    | 9 | 2 | 12 | 2 |         |         |
| 3   | D     | 1        | Total | C | N | O  | P | 0       | 0       |
|     |       |          | 25    | 9 | 2 | 12 | 2 |         |         |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).

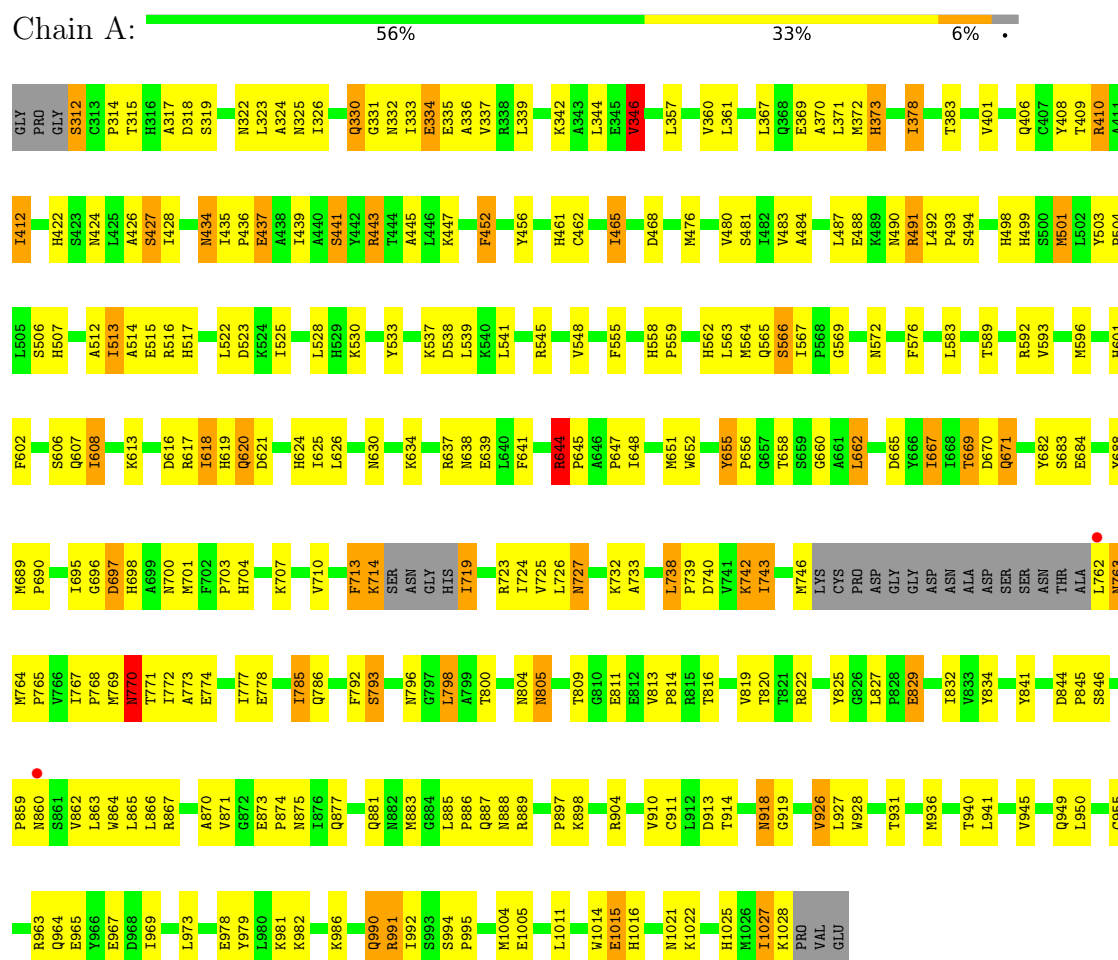


| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | I     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | K     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | L     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

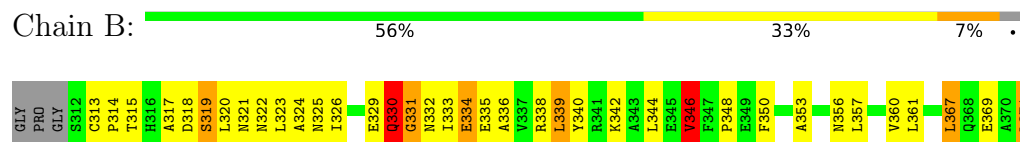
### 3 Residue-property plots

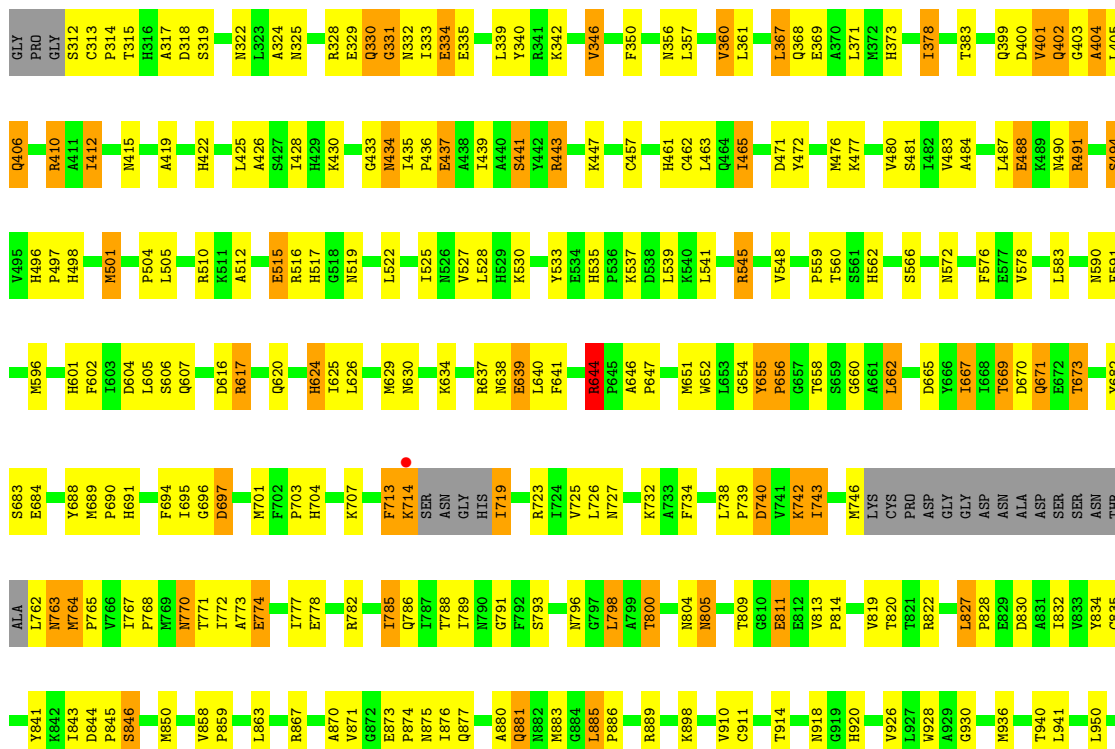
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT



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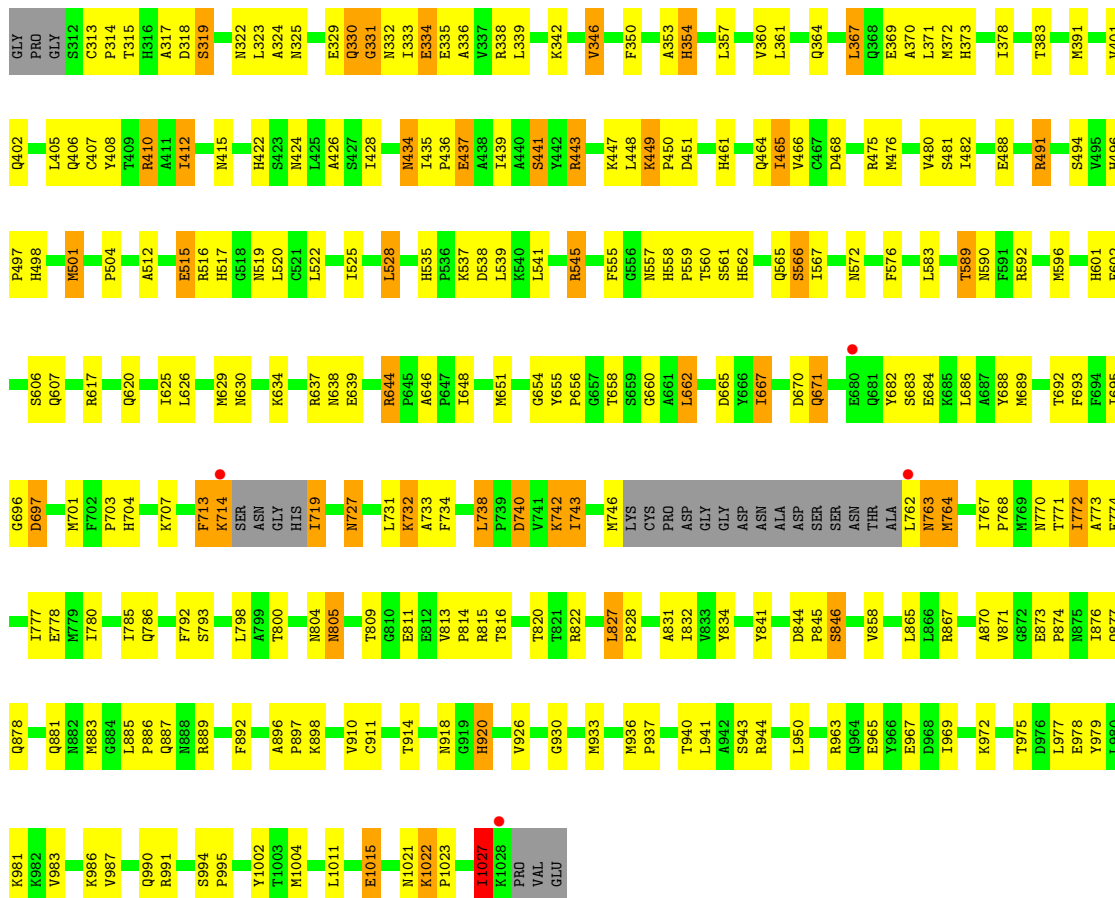




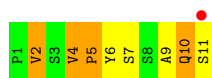
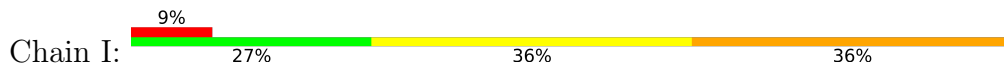




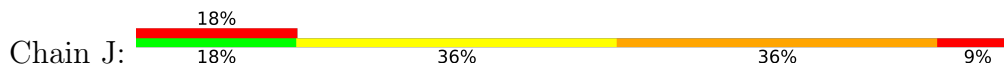
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE--PEPTIDE N-ACETYLGLUCOSAMINYL TRANSFERASE 110 KDA SUBUNIT



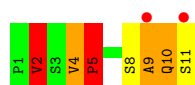
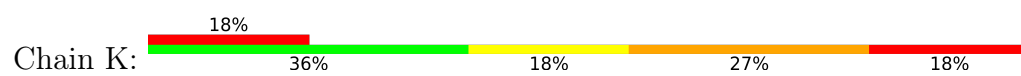
• Molecule 2: GTAB1TIDE



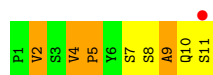
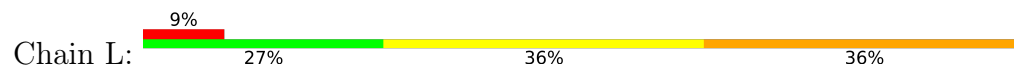
• Molecule 2: GTAB1TIDE



• Molecule 2: GTAB1TIDE



• Molecule 2: GTAB1TIDE



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 3 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 274.17Å 274.17Å 142.15Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 237.44 – 3.15<br>237.44 – 3.15                              | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.6 (237.44-3.15)<br>99.6 (237.44-3.15)                    | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.11                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.06 (at 3.18Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.6.0117                                             | Depositor        |
| R, $R_{free}$                                                           | 0.174 , 0.204<br>0.173 , 0.206                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 502 reflections (0.47%)                                     | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.1                                                        | Xtriage          |
| Anisotropy                                                              | 0.006                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.34 , 61.8                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$ | Xtriage          |
| Estimated twinning fraction                                             | 0.036 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.95                                                        | EDS              |
| Total number of atoms                                                   | 22524                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 60.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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 ⓘ

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

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     | 1.31         | 17/5641 (0.3%)  | 1.36        | 37/7650 (0.5%)   |
| 1   | B     | 1.27         | 8/5641 (0.1%)   | 1.36        | 38/7650 (0.5%)   |
| 1   | C     | 1.29         | 12/5641 (0.2%)  | 1.35        | 42/7650 (0.5%)   |
| 1   | D     | 1.13         | 4/5641 (0.1%)   | 1.26        | 32/7650 (0.4%)   |
| 2   | I     | 1.99         | 1/80 (1.2%)     | 2.16        | 3/109 (2.8%)     |
| 2   | J     | 2.05         | 2/80 (2.5%)     | 2.11        | 3/109 (2.8%)     |
| 2   | K     | 1.96         | 2/80 (2.5%)     | 2.11        | 2/109 (1.8%)     |
| 2   | L     | 1.83         | 1/80 (1.2%)     | 2.05        | 0/109            |
| All | All   | 1.26         | 47/22884 (0.2%) | 1.35        | 157/31036 (0.5%) |

All (47) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 2   | I     | 5    | PRO  | CA-C    | -7.84 | 1.42        | 1.52     |
| 2   | L     | 5    | PRO  | CA-C    | -7.52 | 1.43        | 1.52     |
| 1   | C     | 548  | VAL  | CA-CB   | -7.52 | 1.45        | 1.54     |
| 2   | J     | 5    | PRO  | CA-C    | -7.29 | 1.43        | 1.52     |
| 1   | A     | 499  | HIS  | CG-CD2  | 6.92  | 1.43        | 1.35     |
| 1   | B     | 601  | HIS  | CA-C    | -6.79 | 1.44        | 1.52     |
| 1   | C     | 793  | SER  | CA-C    | -6.66 | 1.44        | 1.52     |
| 1   | A     | 644  | ARG  | C-O     | -6.49 | 1.20        | 1.23     |
| 1   | A     | 461  | HIS  | ND1-CE1 | 6.45  | 1.39        | 1.32     |
| 1   | A     | 499  | HIS  | CE1-NE2 | 6.28  | 1.38        | 1.32     |
| 2   | K     | 5    | PRO  | CA-C    | -6.23 | 1.44        | 1.52     |
| 1   | C     | 517  | HIS  | ND1-CE1 | 6.21  | 1.38        | 1.32     |
| 1   | A     | 931  | THR  | CA-C    | -5.88 | 1.46        | 1.52     |
| 1   | B     | 656  | PRO  | CA-C    | 5.87  | 1.58        | 1.53     |
| 1   | B     | 499  | HIS  | CG-CD2  | 5.76  | 1.42        | 1.35     |
| 2   | K     | 2    | VAL  | N-CA    | 5.73  | 1.53        | 1.46     |
| 1   | A     | 1025 | HIS  | C-O     | -5.73 | 1.16        | 1.23     |
| 1   | C     | 517  | HIS  | CG-CD2  | 5.61  | 1.42        | 1.35     |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | A     | 601  | HIS  | CA-C    | -5.57 | 1.45        | 1.52     |
| 1   | B     | 698  | HIS  | CA-C    | -5.57 | 1.45        | 1.52     |
| 1   | B     | 1025 | HIS  | CG-CD2  | 5.57  | 1.42        | 1.35     |
| 1   | A     | 373  | HIS  | CA-C    | -5.56 | 1.45        | 1.52     |
| 1   | C     | 624  | HIS  | CA-C    | -5.55 | 1.45        | 1.52     |
| 1   | C     | 590  | ASN  | CA-C    | -5.54 | 1.45        | 1.52     |
| 1   | A     | 931  | THR  | N-CA    | -5.52 | 1.41        | 1.46     |
| 1   | C     | 843  | ILE  | C-O     | 5.50  | 1.30        | 1.24     |
| 1   | A     | 1016 | HIS  | CG-CD2  | 5.49  | 1.41        | 1.35     |
| 1   | C     | 652  | TRP  | NE1-CE2 | -5.48 | 1.31        | 1.37     |
| 1   | C     | 691  | HIS  | CA-C    | -5.46 | 1.45        | 1.52     |
| 1   | C     | 601  | HIS  | CA-C    | -5.41 | 1.46        | 1.52     |
| 2   | J     | 2    | VAL  | N-CA    | 5.40  | 1.53        | 1.46     |
| 1   | C     | 461  | HIS  | CG-ND1  | -5.35 | 1.32        | 1.38     |
| 1   | A     | 955  | CYS  | CA-C    | -5.28 | 1.47        | 1.53     |
| 1   | A     | 619  | HIS  | CG-ND1  | -5.28 | 1.32        | 1.38     |
| 1   | A     | 548  | VAL  | CA-CB   | -5.26 | 1.47        | 1.54     |
| 1   | D     | 354  | HIS  | CG-ND1  | -5.19 | 1.32        | 1.38     |
| 1   | B     | 529  | HIS  | CA-C    | -5.17 | 1.46        | 1.53     |
| 1   | B     | 624  | HIS  | CG-ND1  | -5.16 | 1.32        | 1.38     |
| 1   | A     | 517  | HIS  | ND1-CE1 | 5.08  | 1.37        | 1.32     |
| 1   | A     | 652  | TRP  | CA-C    | -5.07 | 1.46        | 1.52     |
| 1   | D     | 601  | HIS  | CA-C    | -5.05 | 1.46        | 1.52     |
| 1   | D     | 920  | HIS  | CG-CD2  | 5.05  | 1.41        | 1.35     |
| 1   | D     | 558  | HIS  | N-CA    | -5.03 | 1.40        | 1.46     |
| 1   | C     | 601  | HIS  | CE1-NE2 | 5.01  | 1.37        | 1.32     |
| 1   | A     | 427  | SER  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | B     | 666  | TYR  | CA-C    | -5.01 | 1.46        | 1.52     |
| 1   | A     | 608  | ILE  | CA-C    | -5.00 | 1.47        | 1.52     |

All (157) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 827 | LEU  | CA-C-N  | 8.05  | 128.36      | 119.90   |
| 1   | C     | 827 | LEU  | C-N-CA  | 8.05  | 128.36      | 119.90   |
| 1   | A     | 785 | ILE  | CB-CA-C | -7.41 | 102.31      | 112.02   |
| 1   | C     | 785 | ILE  | CB-CA-C | -7.33 | 102.59      | 111.97   |
| 1   | A     | 655 | TYR  | CA-C-N  | 7.17  | 128.80      | 119.84   |
| 1   | A     | 655 | TYR  | C-N-CA  | 7.17  | 128.80      | 119.84   |
| 1   | A     | 883 | MET  | N-CA-C  | -7.13 | 104.18      | 113.17   |
| 1   | A     | 606 | SER  | N-CA-C  | -7.08 | 103.90      | 112.54   |
| 1   | C     | 740 | ASP  | N-CA-C  | 7.08  | 121.42      | 111.30   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | B     | 876  | ILE  | N-CA-C   | -7.04 | 103.91      | 110.53   |
| 1   | D     | 572  | ASN  | CA-C-N   | 7.02  | 126.72      | 119.56   |
| 1   | D     | 572  | ASN  | C-N-CA   | 7.02  | 126.72      | 119.56   |
| 1   | B     | 564  | MET  | N-CA-C   | 7.02  | 122.02      | 113.17   |
| 1   | B     | 567  | ILE  | N-CA-C   | 7.02  | 120.78      | 112.35   |
| 1   | D     | 1021 | ASN  | N-CA-C   | 7.01  | 120.90      | 110.52   |
| 1   | D     | 767  | ILE  | CA-C-N   | 6.86  | 127.31      | 120.52   |
| 1   | D     | 767  | ILE  | C-N-CA   | 6.86  | 127.31      | 120.52   |
| 1   | D     | 827  | LEU  | CA-C-N   | 6.69  | 126.93      | 119.90   |
| 1   | D     | 827  | LEU  | C-N-CA   | 6.69  | 126.93      | 119.90   |
| 1   | C     | 1021 | ASN  | N-CA-C   | 6.64  | 120.88      | 110.32   |
| 1   | C     | 378  | ILE  | CB-CA-C  | -6.63 | 103.39      | 111.88   |
| 1   | B     | 827  | LEU  | CA-C-N   | 6.62  | 126.86      | 119.90   |
| 1   | B     | 827  | LEU  | C-N-CA   | 6.62  | 126.86      | 119.90   |
| 1   | A     | 378  | ILE  | CB-CA-C  | -6.52 | 103.53      | 111.88   |
| 1   | B     | 346  | VAL  | CB-CA-C  | -6.46 | 103.55      | 112.02   |
| 1   | B     | 785  | ILE  | CB-CA-C  | -6.44 | 103.72      | 111.97   |
| 1   | A     | 798  | LEU  | N-CA-C   | -6.43 | 106.01      | 114.31   |
| 1   | D     | 465  | ILE  | CB-CA-C  | -6.38 | 101.92      | 112.26   |
| 1   | A     | 767  | ILE  | CA-C-N   | 6.38  | 126.83      | 120.52   |
| 1   | A     | 767  | ILE  | C-N-CA   | 6.38  | 126.83      | 120.52   |
| 1   | C     | 883  | MET  | N-CA-C   | -6.34 | 105.30      | 113.16   |
| 1   | A     | 513  | ILE  | N-CA-C   | -6.26 | 104.53      | 110.42   |
| 1   | A     | 991  | ARG  | CG-CD-NE | -6.24 | 98.28       | 112.00   |
| 1   | A     | 589  | THR  | N-CA-C   | 6.23  | 118.34      | 110.24   |
| 1   | C     | 591  | PHE  | N-CA-C   | -6.22 | 104.42      | 111.14   |
| 1   | D     | 566  | SER  | CA-C-N   | 6.22  | 126.40      | 120.43   |
| 1   | D     | 566  | SER  | C-N-CA   | 6.22  | 126.40      | 120.43   |
| 1   | A     | 992  | ILE  | CB-CA-C  | -6.20 | 103.92      | 112.04   |
| 1   | C     | 655  | TYR  | CA-C-N   | 6.20  | 127.58      | 119.84   |
| 1   | C     | 655  | TYR  | C-N-CA   | 6.20  | 127.58      | 119.84   |
| 1   | C     | 578  | VAL  | N-CA-C   | 6.17  | 117.01      | 107.99   |
| 1   | B     | 433  | GLY  | CA-C-N   | -6.15 | 113.37      | 122.41   |
| 1   | B     | 433  | GLY  | C-N-CA   | -6.15 | 113.37      | 122.41   |
| 1   | B     | 606  | SER  | N-CA-C   | -6.13 | 105.65      | 113.01   |
| 1   | B     | 373  | HIS  | N-CA-C   | 6.12  | 117.74      | 111.14   |
| 1   | B     | 740  | ASP  | N-CA-C   | 6.11  | 120.04      | 111.30   |
| 1   | B     | 738  | LEU  | CA-C-N   | 6.10  | 125.32      | 118.97   |
| 1   | B     | 738  | LEU  | C-N-CA   | 6.10  | 125.32      | 118.97   |
| 1   | D     | 738  | LEU  | CA-C-N   | 6.06  | 125.27      | 118.97   |
| 1   | D     | 738  | LEU  | C-N-CA   | 6.06  | 125.27      | 118.97   |
| 1   | C     | 859  | PRO  | CA-C-N   | -6.04 | 111.87      | 122.62   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | C     | 859 | PRO  | C-N-CA  | -6.04 | 111.87      | 122.62   |
| 1   | B     | 883 | MET  | N-CA-C  | -6.02 | 105.70      | 113.16   |
| 1   | D     | 567 | ILE  | N-CA-C  | 5.98  | 120.15      | 112.67   |
| 1   | B     | 339 | LEU  | N-CA-C  | 5.97  | 117.48      | 110.97   |
| 1   | C     | 767 | ILE  | CA-C-N  | 5.95  | 125.92      | 120.21   |
| 1   | C     | 767 | ILE  | C-N-CA  | 5.95  | 125.92      | 120.21   |
| 1   | B     | 378 | ILE  | CB-CA-C | -5.93 | 104.13      | 112.14   |
| 2   | J     | 10  | GLN  | CA-C-N  | 5.93  | 132.37      | 121.70   |
| 2   | J     | 10  | GLN  | C-N-CA  | 5.93  | 132.37      | 121.70   |
| 1   | B     | 380 | ILE  | N-CA-C  | 5.88  | 116.62      | 110.62   |
| 2   | I     | 10  | GLN  | CA-C-N  | 5.88  | 132.28      | 121.70   |
| 2   | I     | 10  | GLN  | C-N-CA  | 5.88  | 132.28      | 121.70   |
| 1   | B     | 654 | GLY  | N-CA-C  | 5.87  | 119.59      | 112.49   |
| 1   | A     | 572 | ASN  | CA-C-N  | 5.87  | 125.73      | 119.28   |
| 1   | A     | 572 | ASN  | C-N-CA  | 5.87  | 125.73      | 119.28   |
| 1   | A     | 346 | VAL  | CB-CA-C | -5.84 | 104.50      | 111.97   |
| 1   | D     | 798 | LEU  | N-CA-C  | -5.80 | 106.82      | 114.31   |
| 1   | A     | 465 | ILE  | CB-CA-C | -5.80 | 102.71      | 112.16   |
| 1   | C     | 606 | SER  | N-CA-C  | -5.80 | 105.31      | 112.38   |
| 1   | B     | 376 | GLU  | N-CA-C  | 5.77  | 118.03      | 111.11   |
| 1   | B     | 655 | TYR  | CA-C-N  | 5.77  | 129.10      | 120.96   |
| 1   | B     | 655 | TYR  | C-N-CA  | 5.77  | 129.10      | 120.96   |
| 1   | B     | 902 | VAL  | O-C-N   | 5.77  | 127.90      | 121.90   |
| 1   | C     | 885 | LEU  | CA-C-N  | 5.74  | 125.76      | 119.90   |
| 1   | C     | 885 | LEU  | C-N-CA  | 5.74  | 125.76      | 119.90   |
| 1   | D     | 313 | CYS  | N-CA-C  | 5.72  | 122.45      | 109.81   |
| 1   | D     | 589 | THR  | N-CA-C  | 5.69  | 117.63      | 110.24   |
| 1   | B     | 737 | SER  | N-CA-C  | -5.64 | 105.65      | 112.54   |
| 1   | A     | 452 | PHE  | CA-C-N  | 5.64  | 124.83      | 118.97   |
| 1   | A     | 452 | PHE  | C-N-CA  | 5.64  | 124.83      | 118.97   |
| 2   | K     | 10  | GLN  | CA-C-N  | 5.63  | 131.84      | 121.70   |
| 2   | K     | 10  | GLN  | C-N-CA  | 5.63  | 131.84      | 121.70   |
| 1   | C     | 876 | ILE  | N-CA-C  | -5.62 | 105.25      | 110.53   |
| 2   | I     | 6   | TYR  | N-CA-CB | -5.61 | 101.95      | 111.31   |
| 1   | B     | 572 | ASN  | CA-C-O  | 5.60  | 122.93      | 119.29   |
| 1   | C     | 625 | ILE  | N-CA-C  | 5.60  | 115.93      | 107.75   |
| 1   | D     | 535 | HIS  | N-CA-C  | 5.60  | 117.13      | 110.07   |
| 1   | A     | 875 | ASN  | N-CA-C  | 5.60  | 117.38      | 111.28   |
| 1   | D     | 448 | LEU  | CA-C-N  | -5.59 | 116.11      | 122.26   |
| 1   | D     | 448 | LEU  | C-N-CA  | -5.59 | 116.11      | 122.26   |
| 1   | D     | 449 | LYS  | O-C-N   | 5.58  | 124.62      | 121.27   |
| 1   | A     | 593 | VAL  | N-CA-C  | 5.58  | 116.22      | 110.36   |

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| Mol | Chain | Res  | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|---------|-------|-------------|----------|
| 1   | C     | 433  | GLY  | CA-C-N  | -5.55 | 113.18      | 122.17   |
| 1   | C     | 433  | GLY  | C-N-CA  | -5.55 | 113.18      | 122.17   |
| 1   | A     | 738  | LEU  | CA-C-N  | 5.54  | 124.73      | 118.97   |
| 1   | A     | 738  | LEU  | C-N-CA  | 5.54  | 124.73      | 118.97   |
| 1   | A     | 566  | SER  | CA-C-N  | 5.53  | 124.75      | 120.33   |
| 1   | A     | 566  | SER  | C-N-CA  | 5.53  | 124.75      | 120.33   |
| 1   | B     | 313  | CYS  | N-CA-C  | 5.52  | 122.00      | 109.81   |
| 1   | D     | 693  | PHE  | N-CA-C  | -5.51 | 106.40      | 113.23   |
| 1   | B     | 553  | SER  | N-CA-C  | -5.50 | 106.41      | 113.02   |
| 1   | D     | 364  | GLN  | N-CA-C  | -5.50 | 106.34      | 113.16   |
| 1   | C     | 419  | ALA  | N-CA-C  | 5.46  | 117.31      | 111.36   |
| 1   | C     | 465  | ILE  | CB-CA-C | -5.45 | 103.43      | 112.26   |
| 1   | A     | 928  | TRP  | N-CA-C  | -5.43 | 105.39      | 112.23   |
| 1   | D     | 606  | SER  | N-CA-C  | -5.42 | 105.92      | 112.54   |
| 1   | B     | 448  | LEU  | N-CA-C  | 5.41  | 117.17      | 111.28   |
| 1   | C     | 811  | GLU  | N-CA-C  | 5.40  | 117.92      | 111.71   |
| 1   | D     | 1027 | ILE  | CB-CA-C | 5.39  | 118.39      | 112.19   |
| 1   | B     | 566  | SER  | CA-C-N  | 5.39  | 124.64      | 120.33   |
| 1   | B     | 566  | SER  | C-N-CA  | 5.39  | 124.64      | 120.33   |
| 1   | D     | 740  | ASP  | N-CA-C  | 5.38  | 119.00      | 111.30   |
| 2   | J     | 6    | TYR  | N-CA-CB | -5.37 | 102.35      | 111.31   |
| 1   | C     | 404  | ALA  | N-CA-C  | -5.36 | 104.84      | 111.33   |
| 1   | C     | 644  | ARG  | N-CA-CB | -5.35 | 105.73      | 111.66   |
| 1   | C     | 875  | ASN  | N-CA-C  | 5.33  | 117.09      | 111.28   |
| 1   | C     | 646  | ALA  | CA-C-N  | 5.32  | 124.95      | 119.05   |
| 1   | C     | 646  | ALA  | C-N-CA  | 5.32  | 124.95      | 119.05   |
| 1   | A     | 992  | ILE  | N-CA-C  | 5.32  | 115.98      | 110.82   |
| 1   | B     | 466  | VAL  | N-CA-C  | -5.29 | 107.14      | 112.17   |
| 1   | A     | 490  | ASN  | N-CA-C  | 5.28  | 118.72      | 111.54   |
| 1   | B     | 548  | VAL  | N-CA-CB | -5.27 | 104.82      | 111.46   |
| 1   | D     | 466  | VAL  | N-CA-C  | -5.27 | 107.17      | 112.17   |
| 1   | C     | 800  | THR  | N-CA-CB | 5.25  | 117.77      | 109.94   |
| 1   | C     | 535  | HIS  | N-CA-C  | 5.22  | 116.64      | 110.07   |
| 1   | C     | 313  | CYS  | N-CA-C  | 5.21  | 120.08      | 109.60   |
| 1   | C     | 410  | ARG  | N-CA-CB | 5.21  | 117.78      | 110.12   |
| 1   | C     | 572  | ASN  | CA-C-N  | 5.21  | 124.88      | 119.56   |
| 1   | C     | 572  | ASN  | C-N-CA  | 5.21  | 124.88      | 119.56   |
| 1   | A     | 569  | GLY  | N-CA-C  | 5.21  | 120.19      | 113.27   |
| 1   | C     | 673  | THR  | N-CA-C  | -5.20 | 105.29      | 111.69   |
| 1   | A     | 337  | VAL  | CB-CA-C | -5.19 | 105.24      | 111.88   |
| 1   | A     | 618  | ILE  | N-CA-C  | -5.19 | 106.02      | 110.74   |
| 1   | C     | 798  | LEU  | N-CA-C  | -5.17 | 107.64      | 114.31   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 1   | D     | 876  | ILE  | N-CA-C   | -5.13 | 105.71      | 110.53   |
| 1   | B     | 432  | SER  | CA-C-N   | -5.12 | 115.39      | 122.86   |
| 1   | B     | 432  | SER  | C-N-CA   | -5.12 | 115.39      | 122.86   |
| 1   | A     | 919  | GLY  | N-CA-C   | -5.11 | 103.88      | 111.03   |
| 1   | C     | 782  | ARG  | N-CA-C   | -5.11 | 107.02      | 113.20   |
| 1   | B     | 380  | ILE  | CB-CA-C  | -5.10 | 105.26      | 112.14   |
| 1   | A     | 913  | ASP  | N-CA-C   | 5.08  | 117.59      | 109.96   |
| 1   | D     | 482  | ILE  | CB-CA-C  | -5.08 | 105.28      | 112.14   |
| 1   | C     | 996  | LEU  | O-C-N    | 5.08  | 127.58      | 122.09   |
| 1   | D     | 646  | ALA  | CA-C-N   | 5.08  | 124.68      | 119.05   |
| 1   | D     | 646  | ALA  | C-N-CA   | 5.08  | 124.68      | 119.05   |
| 1   | C     | 881  | GLN  | CA-CB-CG | -5.07 | 103.95      | 114.10   |
| 1   | D     | 883  | MET  | N-CA-C   | -5.07 | 106.87      | 113.16   |
| 1   | A     | 445  | ALA  | N-CA-C   | -5.07 | 105.65      | 111.07   |
| 1   | C     | 785  | ILE  | N-CA-C   | 5.06  | 115.28      | 110.42   |
| 1   | A     | 567  | ILE  | N-CA-C   | 5.04  | 118.40      | 112.35   |
| 1   | B     | 530  | LYS  | CA-C-N   | 5.04  | 123.28      | 119.66   |
| 1   | B     | 530  | LYS  | C-N-CA   | 5.04  | 123.28      | 119.66   |
| 1   | D     | 410  | ARG  | N-CA-CB  | 5.03  | 117.97      | 110.22   |
| 1   | B     | 798  | LEU  | N-CA-C   | -5.02 | 107.83      | 114.31   |
| 1   | A     | 1021 | ASN  | N-CA-C   | 5.02  | 117.94      | 110.52   |
| 1   | A     | 410  | ARG  | N-CA-CB  | 5.02  | 117.58      | 110.16   |

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     | 5514  | 0        | 5489     | 193     | 0            |
| 1   | B     | 5514  | 0        | 5489     | 212     | 0            |
| 1   | C     | 5514  | 0        | 5489     | 190     | 0            |
| 1   | D     | 5514  | 0        | 5489     | 178     | 0            |
| 2   | I     | 78    | 0        | 75       | 4       | 0            |
| 2   | J     | 78    | 0        | 75       | 5       | 0            |
| 2   | K     | 78    | 0        | 75       | 4       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | L     | 78    | 0        | 75       | 5       | 0            |
| 3   | A     | 25    | 0        | 11       | 2       | 0            |
| 3   | B     | 25    | 0        | 11       | 2       | 0            |
| 3   | C     | 25    | 0        | 11       | 2       | 0            |
| 3   | D     | 25    | 0        | 11       | 3       | 0            |
| 4   | I     | 14    | 0        | 13       | 0       | 0            |
| 4   | J     | 14    | 0        | 13       | 0       | 0            |
| 4   | K     | 14    | 0        | 13       | 0       | 0            |
| 4   | L     | 14    | 0        | 13       | 0       | 0            |
| All | All   | 22524 | 0        | 22352    | 778     | 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 17.

All (778) 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:443:ARG:HG2  | 1:A:443:ARG:HH11 | 1.26                     | 1.01              |
| 1:A:773:ALA:O    | 1:A:777:ILE:HG22 | 1.61                     | 1.00              |
| 1:D:713:PHE:H    | 1:D:713:PHE:HD1  | 1.03                     | 0.99              |
| 1:A:713:PHE:HD1  | 1:A:713:PHE:H    | 1.02                     | 0.96              |
| 1:B:662:LEU:HD12 | 1:B:662:LEU:H    | 1.30                     | 0.95              |
| 1:C:443:ARG:HH11 | 1:C:443:ARG:HG2  | 1.30                     | 0.95              |
| 1:B:713:PHE:HD1  | 1:B:713:PHE:H    | 1.00                     | 0.95              |
| 1:B:671:GLN:HG2  | 1:B:688:TYR:CE2  | 2.05                     | 0.92              |
| 1:C:713:PHE:HD1  | 1:C:713:PHE:H    | 1.00                     | 0.91              |
| 1:D:773:ALA:O    | 1:D:777:ILE:HG22 | 1.71                     | 0.91              |
| 1:D:443:ARG:HG2  | 1:D:443:ARG:HH11 | 1.34                     | 0.91              |
| 1:B:443:ARG:HG2  | 1:B:443:ARG:HH11 | 1.37                     | 0.90              |
| 1:A:994:SER:HB2  | 1:A:995:PRO:HD3  | 1.54                     | 0.89              |
| 1:B:644:ARG:HH11 | 1:B:644:ARG:CG   | 1.85                     | 0.89              |
| 1:D:671:GLN:HG2  | 1:D:688:TYR:CE2  | 2.08                     | 0.88              |
| 1:D:805:ASN:H    | 1:D:805:ASN:HD22 | 1.19                     | 0.87              |
| 1:C:773:ALA:O    | 1:C:777:ILE:HG22 | 1.73                     | 0.87              |
| 1:D:644:ARG:CG   | 1:D:644:ARG:HH11 | 1.89                     | 0.85              |
| 1:D:662:LEU:H    | 1:D:662:LEU:HD12 | 1.40                     | 0.85              |
| 1:B:773:ALA:O    | 1:B:777:ILE:HG22 | 1.77                     | 0.84              |
| 1:C:671:GLN:HG2  | 1:C:688:TYR:CE2  | 2.13                     | 0.84              |
| 1:A:1015:GLU:OE1 | 1:A:1015:GLU:HA  | 1.78                     | 0.83              |
| 1:A:662:LEU:HD12 | 1:A:662:LEU:H    | 1.42                     | 0.83              |
| 1:B:994:SER:HB2  | 1:B:995:PRO:CD   | 2.10                     | 0.82              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:714:LYS:HZ3  | 1:B:719:ILE:N    | 1.77                     | 0.82              |
| 1:A:714:LYS:HZ3  | 1:A:719:ILE:N    | 1.77                     | 0.81              |
| 1:C:994:SER:HB2  | 1:C:995:PRO:CD   | 2.12                     | 0.80              |
| 1:C:662:LEU:HD12 | 1:C:662:LEU:H    | 1.47                     | 0.80              |
| 1:D:443:ARG:HH11 | 1:D:443:ARG:CG   | 1.93                     | 0.80              |
| 1:C:1015:GLU:HA  | 1:C:1015:GLU:OE1 | 1.82                     | 0.79              |
| 1:D:994:SER:HB2  | 1:D:995:PRO:HD3  | 1.65                     | 0.78              |
| 1:B:994:SER:HB2  | 1:B:995:PRO:HD3  | 1.65                     | 0.78              |
| 1:B:317:ALA:HB2  | 1:B:346:VAL:HB   | 1.64                     | 0.78              |
| 1:C:443:ARG:HH11 | 1:C:443:ARG:CG   | 1.97                     | 0.78              |
| 1:C:805:ASN:HD22 | 1:C:805:ASN:H    | 1.30                     | 0.77              |
| 1:C:644:ARG:HH11 | 1:C:644:ARG:CG   | 1.96                     | 0.77              |
| 1:B:443:ARG:HH11 | 1:B:443:ARG:CG   | 1.98                     | 0.76              |
| 1:C:740:ASP:HB2  | 1:C:768:PRO:HG3  | 1.67                     | 0.76              |
| 1:B:476:MET:O    | 1:B:480:VAL:HG23 | 1.86                     | 0.76              |
| 1:B:367:LEU:N    | 1:B:367:LEU:HD23 | 2.01                     | 0.75              |
| 1:A:740:ASP:HB2  | 1:A:768:PRO:HG3  | 1.69                     | 0.74              |
| 1:A:426:ALA:HB2  | 1:A:441:SER:HB3  | 1.70                     | 0.74              |
| 1:D:740:ASP:HB2  | 1:D:768:PRO:HG3  | 1.70                     | 0.74              |
| 1:B:809:THR:OG1  | 1:B:811:GLU:HG3  | 1.88                     | 0.73              |
| 1:A:713:PHE:CD1  | 1:A:713:PHE:N    | 2.56                     | 0.73              |
| 3:D:1201:UDP:O2  | 2:L:4:VAL:HG11   | 1.89                     | 0.73              |
| 1:A:644:ARG:CG   | 1:A:644:ARG:HH11 | 2.01                     | 0.73              |
| 1:D:707:LYS:HE2  | 1:D:762:LEU:HD22 | 1.72                     | 0.72              |
| 1:B:644:ARG:HH11 | 1:B:644:ARG:HG2  | 1.55                     | 0.72              |
| 1:D:361:LEU:HD13 | 1:D:369:GLU:HG2  | 1.70                     | 0.72              |
| 1:D:713:PHE:CD1  | 1:D:713:PHE:N    | 2.58                     | 0.72              |
| 1:A:671:GLN:HG2  | 1:A:688:TYR:CE2  | 2.26                     | 0.71              |
| 1:D:1015:GLU:OE1 | 1:D:1015:GLU:HA  | 1.88                     | 0.71              |
| 1:B:1015:GLU:OE1 | 1:B:1015:GLU:HA  | 1.89                     | 0.71              |
| 1:B:367:LEU:HD23 | 1:B:367:LEU:H    | 1.54                     | 0.71              |
| 1:A:844:ASP:HB2  | 1:A:845:PRO:HD2  | 1.72                     | 0.71              |
| 1:C:713:PHE:CD1  | 1:C:713:PHE:N    | 2.55                     | 0.70              |
| 1:B:426:ALA:HB2  | 1:B:441:SER:HB3  | 1.73                     | 0.70              |
| 1:B:662:LEU:H    | 1:B:662:LEU:CD1  | 2.03                     | 0.70              |
| 1:C:809:THR:OG1  | 1:C:811:GLU:HG3  | 1.92                     | 0.70              |
| 1:D:476:MET:O    | 1:D:480:VAL:HG23 | 1.91                     | 0.70              |
| 1:D:644:ARG:HH11 | 1:D:644:ARG:HG3  | 1.55                     | 0.70              |
| 3:C:1201:UDP:O2  | 2:K:4:VAL:HG11   | 1.92                     | 0.70              |
| 1:A:667:ILE:HG22 | 1:A:684:GLU:HB2  | 1.73                     | 0.69              |
| 1:B:644:ARG:NH1  | 1:B:644:ARG:HG3  | 2.06                     | 0.69              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:994:SER:HB2  | 1:A:995:PRO:CD   | 2.22                     | 0.69              |
| 1:B:704:HIS:CD2  | 1:B:814:PRO:HG2  | 2.28                     | 0.69              |
| 1:D:994:SER:HB2  | 1:D:995:PRO:CD   | 2.22                     | 0.68              |
| 1:B:434:ASN:HB2  | 1:B:437:GLU:CG   | 2.23                     | 0.68              |
| 1:D:426:ALA:HB2  | 1:D:441:SER:HB3  | 1.75                     | 0.68              |
| 1:A:607:GLN:OE1  | 1:A:607:GLN:HA   | 1.92                     | 0.68              |
| 1:A:859:PRO:HG2  | 1:B:1016:HIS:ND1 | 2.09                     | 0.68              |
| 1:B:350:PHE:CD1  | 1:B:350:PHE:C    | 2.72                     | 0.68              |
| 1:A:669:THR:OG1  | 1:A:670:ASP:N    | 2.24                     | 0.67              |
| 1:A:793:SER:HB2  | 1:A:816:THR:HG22 | 1.76                     | 0.67              |
| 1:D:644:ARG:HG3  | 1:D:644:ARG:NH1  | 2.06                     | 0.67              |
| 1:B:324:ALA:HB2  | 1:B:339:LEU:HB2  | 1.77                     | 0.67              |
| 1:A:434:ASN:HB2  | 1:A:437:GLU:CG   | 2.24                     | 0.67              |
| 1:B:361:LEU:HD13 | 1:B:369:GLU:HG2  | 1.76                     | 0.67              |
| 2:I:4:VAL:HG12   | 2:I:5:PRO:HD2    | 1.76                     | 0.67              |
| 1:D:793:SER:HB2  | 1:D:816:THR:HG22 | 1.76                     | 0.67              |
| 1:A:707:LYS:HE2  | 1:A:762:LEU:HD22 | 1.77                     | 0.67              |
| 1:B:805:ASN:H    | 1:B:805:ASN:HD22 | 1.43                     | 0.66              |
| 1:A:443:ARG:HH11 | 1:A:443:ARG:CG   | 2.04                     | 0.66              |
| 1:C:714:LYS:HZ3  | 1:C:719:ILE:N    | 1.94                     | 0.66              |
| 1:D:805:ASN:H    | 1:D:805:ASN:ND2  | 1.87                     | 0.66              |
| 1:A:714:LYS:NZ   | 1:A:719:ILE:N    | 2.43                     | 0.66              |
| 1:B:660:GLY:HA2  | 1:B:683:SER:HB3  | 1.78                     | 0.66              |
| 1:A:918:ASN:N    | 1:A:918:ASN:HD22 | 1.92                     | 0.65              |
| 1:B:350:PHE:C    | 1:B:350:PHE:HD1  | 2.05                     | 0.65              |
| 1:B:746:MET:HG3  | 1:B:763:ASN:HA   | 1.78                     | 0.65              |
| 1:A:877:GLN:OE1  | 1:A:877:GLN:HA   | 1.95                     | 0.65              |
| 1:B:793:SER:HB2  | 1:B:816:THR:HG22 | 1.80                     | 0.64              |
| 1:D:877:GLN:HA   | 1:D:877:GLN:OE1  | 1.98                     | 0.64              |
| 1:B:963:ARG:O    | 1:B:967:GLU:HG3  | 1.98                     | 0.64              |
| 1:C:361:LEU:HD13 | 1:C:369:GLU:HG2  | 1.79                     | 0.64              |
| 1:C:994:SER:HB2  | 1:C:995:PRO:HD3  | 1.80                     | 0.64              |
| 1:A:476:MET:O    | 1:A:480:VAL:HG23 | 1.99                     | 0.63              |
| 1:D:805:ASN:ND2  | 1:D:805:ASN:N    | 2.45                     | 0.63              |
| 1:B:671:GLN:HG2  | 1:B:688:TYR:HE2  | 1.63                     | 0.63              |
| 1:B:644:ARG:HH11 | 1:B:644:ARG:HG3  | 1.58                     | 0.63              |
| 1:D:746:MET:HG3  | 1:D:763:ASN:HA   | 1.81                     | 0.63              |
| 1:B:658:THR:HB   | 1:B:682:TYR:HA   | 1.81                     | 0.63              |
| 1:C:644:ARG:HH11 | 1:C:644:ARG:HG3  | 1.64                     | 0.63              |
| 1:D:498:HIS:O    | 1:D:501:MET:HE3  | 2.00                     | 0.62              |
| 1:B:583:LEU:HD22 | 1:B:637:ARG:HD3  | 1.82                     | 0.62              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:638:ASN:O    | 1:C:639:GLU:C     | 2.43                     | 0.62              |
| 1:D:324:ALA:HB2  | 1:D:339:LEU:HB2   | 1.82                     | 0.62              |
| 1:A:743:ILE:O    | 1:A:743:ILE:HG22  | 2.00                     | 0.62              |
| 1:B:714:LYS:NZ   | 1:B:719:ILE:N     | 2.47                     | 0.62              |
| 1:B:740:ASP:HB2  | 1:B:768:PRO:HG3   | 1.81                     | 0.62              |
| 1:C:324:ALA:HB2  | 1:C:339:LEU:HB2   | 1.80                     | 0.62              |
| 1:A:768:PRO:HG2  | 1:A:770:ASN:OD1   | 1.98                     | 0.61              |
| 1:A:644:ARG:HH11 | 1:A:644:ARG:HG2   | 1.65                     | 0.61              |
| 1:B:644:ARG:CG   | 1:B:644:ARG:NH1   | 2.50                     | 0.61              |
| 1:C:335:GLU:OE1  | 1:C:335:GLU:HA    | 1.99                     | 0.61              |
| 1:C:660:GLY:HA2  | 1:C:683:SER:HB3   | 1.82                     | 0.61              |
| 1:A:965:GLU:O    | 1:A:969:ILE:HG13  | 2.00                     | 0.61              |
| 1:C:805:ASN:HD22 | 1:C:805:ASN:N     | 1.98                     | 0.61              |
| 1:B:695:ILE:HG13 | 1:B:696:GLY:N     | 2.15                     | 0.61              |
| 1:A:867:ARG:HB3  | 1:A:870:ALA:HA    | 1.82                     | 0.61              |
| 1:C:426:ALA:HB2  | 1:C:441:SER:HB3   | 1.83                     | 0.61              |
| 1:C:671:GLN:HG2  | 1:C:688:TYR:HE2   | 1.65                     | 0.61              |
| 1:D:714:LYS:HZ3  | 1:D:719:ILE:N     | 1.99                     | 0.61              |
| 1:A:498:HIS:O    | 1:A:501:MET:HE3   | 2.00                     | 0.61              |
| 1:B:688:TYR:CD2  | 1:B:1027:ILE:HG22 | 2.36                     | 0.61              |
| 1:C:322:ASN:HA   | 1:C:325:ASN:HD22  | 1.65                     | 0.61              |
| 1:C:867:ARG:HB3  | 1:C:870:ALA:HA    | 1.83                     | 0.61              |
| 1:D:434:ASN:HB2  | 1:D:437:GLU:CG    | 2.31                     | 0.60              |
| 1:B:994:SER:CB   | 1:B:995:PRO:CD    | 2.77                     | 0.60              |
| 1:C:746:MET:HG3  | 1:C:763:ASN:HA    | 1.83                     | 0.60              |
| 1:A:881:GLN:HG3  | 1:A:885:LEU:O     | 2.00                     | 0.60              |
| 1:C:941:LEU:C    | 1:C:941:LEU:HD23  | 2.26                     | 0.60              |
| 1:D:844:ASP:HB2  | 1:D:845:PRO:HD2   | 1.83                     | 0.60              |
| 1:C:367:LEU:HD23 | 1:C:367:LEU:N     | 2.17                     | 0.60              |
| 3:B:1201:UDP:O2  | 2:J:4:VAL:HG11    | 2.02                     | 0.60              |
| 1:D:324:ALA:HA   | 1:D:339:LEU:HD12  | 1.84                     | 0.60              |
| 1:D:357:LEU:HD23 | 1:D:373:HIS:CE1   | 2.36                     | 0.60              |
| 1:A:361:LEU:HD13 | 1:A:369:GLU:HG2   | 1.82                     | 0.60              |
| 1:C:695:ILE:HG13 | 1:C:696:GLY:N     | 2.17                     | 0.60              |
| 1:D:671:GLN:HG2  | 1:D:688:TYR:HE2   | 1.65                     | 0.59              |
| 1:B:426:ALA:HB2  | 1:B:441:SER:CB    | 2.32                     | 0.59              |
| 1:A:335:GLU:HA   | 1:A:335:GLU:OE1   | 2.02                     | 0.59              |
| 1:A:822:ARG:HB3  | 1:A:827:LEU:HB2   | 1.84                     | 0.59              |
| 1:B:324:ALA:HB2  | 1:B:339:LEU:CB    | 2.32                     | 0.59              |
| 1:C:644:ARG:HG3  | 1:C:644:ARG:NH1   | 2.15                     | 0.59              |
| 1:A:324:ALA:HB2  | 1:A:339:LEU:HB2   | 1.83                     | 0.59              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:314:PRO:O    | 1:C:318:ASP:HB2  | 2.03                     | 0.59              |
| 1:D:805:ASN:HD22 | 1:D:805:ASN:N    | 1.94                     | 0.59              |
| 1:C:329:GLU:OE1  | 1:C:329:GLU:HA   | 2.02                     | 0.59              |
| 1:C:986:LYS:O    | 1:C:990:GLN:HG2  | 2.03                     | 0.59              |
| 1:A:703:PRO:HD2  | 1:A:813:VAL:HG22 | 1.85                     | 0.59              |
| 1:B:844:ASP:HB2  | 1:B:845:PRO:CD   | 2.33                     | 0.59              |
| 1:C:435:ILE:HB   | 1:C:436:PRO:HD3  | 1.84                     | 0.59              |
| 1:A:583:LEU:HD22 | 1:A:637:ARG:HD3  | 1.85                     | 0.59              |
| 1:A:644:ARG:CG   | 1:A:644:ARG:NH1  | 2.63                     | 0.59              |
| 1:C:476:MET:O    | 1:C:480:VAL:HG23 | 2.02                     | 0.59              |
| 1:C:644:ARG:CG   | 1:C:644:ARG:NH1  | 2.61                     | 0.59              |
| 1:A:785:ILE:HG22 | 1:A:786:GLN:HG2  | 1.85                     | 0.59              |
| 1:D:408:TYR:CE1  | 1:D:424:ASN:HB3  | 2.38                     | 0.59              |
| 1:A:994:SER:CB   | 1:A:995:PRO:HD3  | 2.30                     | 0.58              |
| 1:A:695:ILE:HG13 | 1:A:696:GLY:N    | 2.18                     | 0.58              |
| 1:C:638:ASN:O    | 1:C:641:PHE:N    | 2.36                     | 0.58              |
| 1:A:805:ASN:HD22 | 1:A:805:ASN:H    | 1.49                     | 0.58              |
| 1:D:350:PHE:CD1  | 1:D:350:PHE:C    | 2.81                     | 0.58              |
| 1:C:317:ALA:HB2  | 1:C:346:VAL:HB   | 1.85                     | 0.58              |
| 1:D:963:ARG:O    | 1:D:967:GLU:HG3  | 2.03                     | 0.58              |
| 2:J:4:VAL:HG12   | 2:J:5:PRO:HD2    | 1.84                     | 0.58              |
| 1:A:314:PRO:O    | 1:A:318:ASP:HB2  | 2.03                     | 0.58              |
| 1:A:844:ASP:HB2  | 1:A:845:PRO:CD   | 2.33                     | 0.58              |
| 1:C:805:ASN:H    | 1:C:805:ASN:ND2  | 2.01                     | 0.58              |
| 1:C:877:GLN:OE1  | 1:C:877:GLN:HA   | 2.04                     | 0.58              |
| 1:D:644:ARG:HH11 | 1:D:644:ARG:HG2  | 1.65                     | 0.58              |
| 1:B:318:ASP:O    | 1:B:322:ASN:ND2  | 2.36                     | 0.57              |
| 1:C:805:ASN:N    | 1:C:805:ASN:ND2  | 2.52                     | 0.57              |
| 1:D:660:GLY:HA2  | 1:D:683:SER:HB3  | 1.85                     | 0.57              |
| 1:A:941:LEU:C    | 1:A:941:LEU:HD23 | 2.30                     | 0.57              |
| 1:B:324:ALA:HA   | 1:B:339:LEU:HD12 | 1.87                     | 0.57              |
| 1:A:994:SER:CB   | 1:A:995:PRO:CD   | 2.81                     | 0.57              |
| 1:B:434:ASN:HB2  | 1:B:437:GLU:HG2  | 1.87                     | 0.57              |
| 1:B:435:ILE:HB   | 1:B:436:PRO:HD3  | 1.86                     | 0.57              |
| 1:A:660:GLY:HA2  | 1:A:683:SER:HB3  | 1.85                     | 0.57              |
| 1:D:846:SER:HB2  | 1:D:963:ARG:HH21 | 1.69                     | 0.57              |
| 1:C:994:SER:HB2  | 1:C:995:PRO:HD2  | 1.86                     | 0.56              |
| 1:B:498:HIS:O    | 1:B:501:MET:HE3  | 2.06                     | 0.56              |
| 1:D:944:ARG:HG2  | 1:D:944:ARG:HH11 | 1.70                     | 0.56              |
| 1:A:330:GLN:O    | 1:A:332:ASN:N    | 2.39                     | 0.56              |
| 1:B:844:ASP:HB2  | 1:B:845:PRO:HD2  | 1.86                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:415:ASN:OD1  | 1:D:415:ASN:C    | 2.47                     | 0.56              |
| 1:D:525:ILE:HA   | 1:D:528:LEU:HD12 | 1.87                     | 0.56              |
| 1:A:435:ILE:HB   | 1:A:436:PRO:HD3  | 1.86                     | 0.56              |
| 1:D:704:HIS:CD2  | 1:D:814:PRO:HG2  | 2.40                     | 0.56              |
| 1:A:809:THR:OG1  | 1:A:811:GLU:HG3  | 2.05                     | 0.56              |
| 1:A:860:ASN:HB2  | 1:B:1016:HIS:HE1 | 1.70                     | 0.56              |
| 1:A:1015:GLU:OE1 | 1:A:1015:GLU:CA  | 2.53                     | 0.56              |
| 1:C:704:HIS:O    | 1:C:727:ASN:HB3  | 2.05                     | 0.56              |
| 1:D:350:PHE:C    | 1:D:350:PHE:HD1  | 2.14                     | 0.56              |
| 1:D:367:LEU:N    | 1:D:367:LEU:HD23 | 2.20                     | 0.56              |
| 1:B:321:ASN:HD21 | 1:B:356:ASN:HD22 | 1.53                     | 0.56              |
| 1:B:986:LYS:O    | 1:B:990:GLN:HG2  | 2.06                     | 0.55              |
| 1:C:443:ARG:CG   | 1:C:443:ARG:NH1  | 2.63                     | 0.55              |
| 1:A:324:ALA:HA   | 1:A:339:LEU:HD12 | 1.88                     | 0.55              |
| 1:A:607:GLN:OE1  | 1:A:607:GLN:CA   | 2.54                     | 0.55              |
| 1:A:859:PRO:HG2  | 1:B:1016:HIS:CE1 | 2.41                     | 0.55              |
| 1:A:1004:MET:HE1 | 1:D:792:PHE:CE1  | 2.41                     | 0.55              |
| 1:D:314:PRO:O    | 1:D:318:ASP:HB2  | 2.05                     | 0.55              |
| 1:A:608:ILE:HG22 | 1:A:608:ILE:O    | 2.05                     | 0.55              |
| 1:D:333:ILE:O    | 1:D:334:GLU:C    | 2.49                     | 0.55              |
| 1:B:322:ASN:HA   | 1:B:325:ASN:HD22 | 1.71                     | 0.55              |
| 1:C:886:PRO:HG2  | 1:C:889:ARG:HG2  | 1.87                     | 0.55              |
| 1:D:317:ALA:HB2  | 1:D:346:VAL:HB   | 1.88                     | 0.55              |
| 1:D:994:SER:CB   | 1:D:995:PRO:CD   | 2.84                     | 0.55              |
| 1:A:333:ILE:O    | 1:A:334:GLU:C    | 2.49                     | 0.55              |
| 2:J:8:SER:O      | 2:J:9:ALA:O      | 2.25                     | 0.55              |
| 1:C:525:ILE:HA   | 1:C:528:LEU:HD12 | 1.89                     | 0.55              |
| 1:C:669:THR:OG1  | 1:C:670:ASP:N    | 2.34                     | 0.55              |
| 1:D:583:LEU:HD22 | 1:D:637:ARG:HD3  | 1.88                     | 0.55              |
| 1:D:809:THR:OG1  | 1:D:811:GLU:HG3  | 2.06                     | 0.55              |
| 1:C:496:HIS:CG   | 1:C:497:PRO:HD2  | 2.41                     | 0.55              |
| 1:C:434:ASN:HB2  | 1:C:437:GLU:CG   | 2.37                     | 0.55              |
| 1:C:624:HIS:O    | 1:C:647:PRO:HG2  | 2.07                     | 0.54              |
| 1:A:719:ILE:CG2  | 1:A:719:ILE:O    | 2.55                     | 0.54              |
| 1:B:1002:TYR:CD1 | 1:B:1002:TYR:C   | 2.85                     | 0.54              |
| 1:D:335:GLU:HA   | 1:D:335:GLU:OE1  | 2.07                     | 0.54              |
| 1:D:443:ARG:CG   | 1:D:443:ARG:NH1  | 2.61                     | 0.54              |
| 2:L:4:VAL:HG12   | 2:L:5:PRO:HD2    | 1.89                     | 0.54              |
| 1:B:877:GLN:HA   | 1:B:877:GLN:OE1  | 2.07                     | 0.54              |
| 1:A:689:MET:HE1  | 1:A:1005:GLU:HB2 | 1.90                     | 0.54              |
| 1:D:443:ARG:HG2  | 1:D:443:ARG:NH1  | 2.13                     | 0.54              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:D:607:GLN:HA   | 1:D:607:GLN:OE1   | 2.06                     | 0.54              |
| 1:B:443:ARG:CG   | 1:B:443:ARG:NH1   | 2.65                     | 0.54              |
| 1:B:873:GLU:N    | 1:B:874:PRO:HD2   | 2.23                     | 0.54              |
| 2:K:4:VAL:HG12   | 2:K:5:PRO:HD2     | 1.90                     | 0.54              |
| 1:B:329:GLU:OE1  | 1:B:329:GLU:HA    | 2.06                     | 0.54              |
| 1:D:662:LEU:H    | 1:D:662:LEU:CD1   | 2.16                     | 0.54              |
| 1:A:707:LYS:HE2  | 1:A:762:LEU:CD2   | 2.38                     | 0.53              |
| 1:B:333:ILE:O    | 1:B:334:GLU:C     | 2.51                     | 0.53              |
| 1:B:512:ALA:O    | 1:B:516:ARG:HG2   | 2.08                     | 0.53              |
| 1:B:713:PHE:CD1  | 1:B:713:PHE:N     | 2.55                     | 0.53              |
| 1:D:658:THR:HB   | 1:D:682:TYR:HA    | 1.90                     | 0.53              |
| 1:A:424:ASN:O    | 1:A:427:SER:HB2   | 2.09                     | 0.53              |
| 1:C:785:ILE:HG22 | 1:C:786:GLN:HG2   | 1.91                     | 0.53              |
| 1:D:772:ILE:O    | 1:D:773:ALA:C     | 2.51                     | 0.53              |
| 1:A:644:ARG:NH1  | 1:A:644:ARG:HG3   | 2.24                     | 0.53              |
| 1:B:977:LEU:HD23 | 1:B:977:LEU:N     | 2.24                     | 0.53              |
| 1:C:498:HIS:O    | 1:C:501:MET:HE3   | 2.09                     | 0.53              |
| 1:C:994:SER:CB   | 1:C:995:PRO:CD    | 2.79                     | 0.53              |
| 1:D:986:LYS:O    | 1:D:990:GLN:HG2   | 2.09                     | 0.53              |
| 1:A:746:MET:HG3  | 1:A:763:ASN:HA    | 1.90                     | 0.53              |
| 1:B:719:ILE:O    | 1:B:719:ILE:CG2   | 2.57                     | 0.53              |
| 1:C:324:ALA:HB2  | 1:C:339:LEU:CB    | 2.38                     | 0.53              |
| 1:A:625:ILE:HG12 | 1:A:648:ILE:HB    | 1.90                     | 0.53              |
| 1:C:644:ARG:HH11 | 1:C:644:ARG:HG2   | 1.70                     | 0.52              |
| 1:C:707:LYS:HE2  | 1:C:762:LEU:HD22  | 1.91                     | 0.52              |
| 1:D:772:ILE:HD12 | 1:D:772:ILE:H     | 1.75                     | 0.52              |
| 1:B:525:ILE:HA   | 1:B:528:LEU:HD12  | 1.92                     | 0.52              |
| 1:C:873:GLU:N    | 1:C:874:PRO:HD2   | 2.23                     | 0.52              |
| 1:B:805:ASN:HD22 | 1:B:805:ASN:N     | 2.06                     | 0.52              |
| 1:A:332:ASN:HD21 | 1:A:335:GLU:HB2   | 1.75                     | 0.52              |
| 1:C:333:ILE:O    | 1:C:334:GLU:C     | 2.53                     | 0.52              |
| 1:D:941:LEU:C    | 1:D:941:LEU:HD23  | 2.35                     | 0.52              |
| 1:A:834:TYR:O    | 1:A:863:LEU:HD12  | 2.08                     | 0.52              |
| 1:B:881:GLN:HG3  | 1:B:885:LEU:O     | 2.10                     | 0.52              |
| 1:C:918:ASN:HD22 | 1:C:918:ASN:N     | 2.08                     | 0.52              |
| 1:D:545:ARG:NH1  | 1:D:576:PHE:O     | 2.43                     | 0.52              |
| 1:A:563:LEU:HA   | 1:A:696:GLY:HA2   | 1.92                     | 0.52              |
| 1:C:658:THR:HB   | 1:C:682:TYR:HA    | 1.92                     | 0.52              |
| 1:C:726:LEU:HD22 | 1:C:819:VAL:HG22  | 1.91                     | 0.52              |
| 1:C:920:HIS:HB2  | 3:C:1201:UDP:O2B  | 2.09                     | 0.52              |
| 1:D:688:TYR:CD2  | 1:D:1027:ILE:HG22 | 2.45                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:318:ASP:O    | 1:A:322:ASN:ND2  | 2.43                     | 0.51              |
| 1:A:443:ARG:HG2  | 1:A:443:ARG:NH1  | 2.06                     | 0.51              |
| 1:A:658:THR:HB   | 1:A:682:TYR:HA   | 1.90                     | 0.51              |
| 1:A:725:VAL:C    | 1:A:726:LEU:HD23 | 2.35                     | 0.51              |
| 1:B:314:PRO:O    | 1:B:318:ASP:HB2  | 2.10                     | 0.51              |
| 1:B:772:ILE:HD12 | 1:B:772:ILE:H    | 1.76                     | 0.51              |
| 1:B:329:GLU:C    | 1:B:331:GLY:H    | 2.19                     | 0.51              |
| 1:B:335:GLU:OE1  | 1:B:335:GLU:HA   | 2.11                     | 0.51              |
| 1:B:415:ASN:OD1  | 1:B:415:ASN:C    | 2.51                     | 0.51              |
| 1:D:844:ASP:HB2  | 1:D:845:PRO:CD   | 2.40                     | 0.51              |
| 1:A:644:ARG:N    | 1:A:645:PRO:HD3  | 2.25                     | 0.51              |
| 1:A:772:ILE:O    | 1:A:773:ALA:C    | 2.50                     | 0.51              |
| 3:A:1201:UDP:O2  | 2:I:4:VAL:HG11   | 2.10                     | 0.51              |
| 1:C:515:GLU:HA   | 1:C:660:GLY:O    | 2.11                     | 0.51              |
| 1:D:557:ASN:O    | 2:L:5:PRO:HG3    | 2.11                     | 0.51              |
| 1:A:624:HIS:O    | 1:A:647:PRO:HG2  | 2.10                     | 0.51              |
| 1:C:350:PHE:CD1  | 1:C:350:PHE:C    | 2.86                     | 0.51              |
| 1:D:590:ASN:HD22 | 1:D:811:GLU:HB3  | 1.76                     | 0.51              |
| 1:B:344:LEU:HD21 | 1:B:353:ALA:HB3  | 1.93                     | 0.51              |
| 1:D:519:ASN:HA   | 1:D:522:LEU:HD12 | 1.92                     | 0.51              |
| 1:D:743:ILE:HG22 | 1:D:743:ILE:O    | 2.10                     | 0.51              |
| 1:A:725:VAL:O    | 1:A:726:LEU:HD23 | 2.11                     | 0.50              |
| 1:D:667:ILE:HG22 | 1:D:684:GLU:HB2  | 1.93                     | 0.50              |
| 1:D:703:PRO:HD2  | 1:D:813:VAL:HG22 | 1.93                     | 0.50              |
| 1:D:881:GLN:HG3  | 1:D:885:LEU:O    | 2.11                     | 0.50              |
| 1:C:719:ILE:CG2  | 1:C:719:ILE:O    | 2.59                     | 0.50              |
| 1:A:963:ARG:O    | 1:A:967:GLU:HG3  | 2.12                     | 0.50              |
| 1:B:662:LEU:HD12 | 1:B:662:LEU:N    | 2.13                     | 0.50              |
| 1:D:426:ALA:HB2  | 1:D:441:SER:CB   | 2.38                     | 0.50              |
| 1:B:457:CYS:SG   | 1:B:494:SER:HB3  | 2.51                     | 0.50              |
| 1:D:731:LEU:O    | 1:D:734:PHE:HB3  | 2.11                     | 0.50              |
| 1:D:822:ARG:HB3  | 1:D:827:LEU:HB2  | 1.93                     | 0.50              |
| 1:A:434:ASN:HB2  | 1:A:437:GLU:HG2  | 1.91                     | 0.50              |
| 1:B:822:ARG:HB3  | 1:B:827:LEU:HB2  | 1.94                     | 0.50              |
| 1:B:367:LEU:N    | 1:B:367:LEU:CD2  | 2.74                     | 0.50              |
| 1:B:805:ASN:N    | 1:B:805:ASN:ND2  | 2.59                     | 0.50              |
| 1:C:788:THR:O    | 1:C:789:ILE:HG13 | 2.11                     | 0.50              |
| 1:C:318:ASP:O    | 1:C:322:ASN:ND2  | 2.45                     | 0.50              |
| 1:D:318:ASP:O    | 1:D:322:ASN:ND2  | 2.45                     | 0.50              |
| 1:D:515:GLU:HA   | 1:D:660:GLY:O    | 2.11                     | 0.50              |
| 1:A:638:ASN:O    | 1:A:639:GLU:C    | 2.54                     | 0.50              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:742:LYS:HE3  | 1:D:768:PRO:HB3  | 1.94                     | 0.50              |
| 1:A:465:ILE:HA   | 1:A:841:TYR:HB3  | 1.94                     | 0.50              |
| 1:A:555:PHE:O    | 1:A:592:ARG:HD3  | 2.11                     | 0.50              |
| 1:A:566:SER:HB2  | 1:A:697:ASP:OD1  | 2.12                     | 0.50              |
| 1:A:825:TYR:CE2  | 1:A:904:ARG:HD2  | 2.46                     | 0.50              |
| 1:D:435:ILE:HB   | 1:D:436:PRO:HD3  | 1.93                     | 0.50              |
| 1:A:559:PRO:HA   | 1:A:562:HIS:ND1  | 2.27                     | 0.49              |
| 1:C:673:THR:HG22 | 1:C:941:LEU:HG   | 1.93                     | 0.49              |
| 1:D:512:ALA:O    | 1:D:516:ARG:HG2  | 2.12                     | 0.49              |
| 1:A:324:ALA:HB2  | 1:A:339:LEU:CB   | 2.42                     | 0.49              |
| 1:C:704:HIS:CD2  | 1:C:814:PRO:HG2  | 2.47                     | 0.49              |
| 1:C:835:CYS:SG   | 1:C:911:CYS:HB2  | 2.53                     | 0.49              |
| 1:D:324:ALA:HB2  | 1:D:339:LEU:CB   | 2.41                     | 0.49              |
| 1:A:911:CYS:HB2  | 1:A:926:VAL:HG21 | 1.94                     | 0.49              |
| 1:D:468:ASP:O    | 1:D:475:ARG:NH2  | 2.39                     | 0.49              |
| 1:A:539:LEU:HD21 | 1:A:1014:TRP:CE2 | 2.48                     | 0.49              |
| 1:B:742:LYS:HE3  | 1:B:768:PRO:HB3  | 1.93                     | 0.49              |
| 1:B:762:LEU:O    | 1:B:763:ASN:HB3  | 2.11                     | 0.49              |
| 1:C:689:MET:HB3  | 1:C:690:PRO:HD2  | 1.95                     | 0.49              |
| 1:C:742:LYS:HE3  | 1:C:768:PRO:HB3  | 1.95                     | 0.49              |
| 1:D:704:HIS:O    | 1:D:727:ASN:HB3  | 2.13                     | 0.49              |
| 1:B:576:PHE:CE2  | 1:B:1007:GLU:HG2 | 2.48                     | 0.49              |
| 1:B:707:LYS:HE2  | 1:B:762:LEU:HD22 | 1.95                     | 0.49              |
| 1:C:437:GLU:CD   | 1:C:437:GLU:H    | 2.19                     | 0.49              |
| 1:A:644:ARG:HH22 | 1:A:665:ASP:CG   | 2.20                     | 0.49              |
| 1:B:967:GLU:O    | 1:B:971:VAL:HG23 | 2.13                     | 0.49              |
| 1:C:834:TYR:HA   | 1:C:910:VAL:O    | 2.13                     | 0.49              |
| 1:D:342:LYS:O    | 1:D:346:VAL:HG23 | 2.13                     | 0.49              |
| 1:A:738:LEU:HD22 | 1:A:739:PRO:HD2  | 1.93                     | 0.49              |
| 1:B:940:THR:O    | 1:B:941:LEU:C    | 2.56                     | 0.49              |
| 1:C:457:CYS:SG   | 1:C:494:SER:HB3  | 2.52                     | 0.49              |
| 1:D:322:ASN:HA   | 1:D:325:ASN:HD22 | 1.76                     | 0.49              |
| 1:D:465:ILE:O    | 1:D:465:ILE:HG22 | 2.12                     | 0.49              |
| 1:D:707:LYS:HE2  | 1:D:762:LEU:CD2  | 2.42                     | 0.49              |
| 1:D:873:GLU:N    | 1:D:874:PRO:HD2  | 2.26                     | 0.49              |
| 1:D:1002:TYR:CD1 | 1:D:1002:TYR:C   | 2.91                     | 0.49              |
| 1:B:703:PRO:HD2  | 1:B:813:VAL:HG22 | 1.94                     | 0.49              |
| 1:D:468:ASP:C    | 1:D:468:ASP:OD1  | 2.54                     | 0.49              |
| 1:A:492:LEU:HD12 | 1:A:493:PRO:HD2  | 1.95                     | 0.48              |
| 1:B:342:LYS:O    | 1:B:346:VAL:HG23 | 2.12                     | 0.48              |
| 1:C:350:PHE:C    | 1:C:350:PHE:HD1  | 2.21                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:714:LYS:NZ   | 1:C:719:ILE:N    | 2.60                     | 0.48              |
| 1:D:319:SER:O    | 1:D:323:LEU:HG   | 2.13                     | 0.48              |
| 1:D:562:HIS:ND1  | 1:D:898:LYS:HE2  | 2.28                     | 0.48              |
| 1:A:408:TYR:CE1  | 1:A:424:ASN:HB3  | 2.48                     | 0.48              |
| 1:A:864:TRP:O    | 1:A:865:LEU:HD23 | 2.13                     | 0.48              |
| 1:C:412:ILE:HD13 | 1:C:422:HIS:CE1  | 2.48                     | 0.48              |
| 1:B:846:SER:HB2  | 1:B:963:ARG:HH21 | 1.77                     | 0.48              |
| 1:B:941:LEU:C    | 1:B:941:LEU:HD23 | 2.39                     | 0.48              |
| 1:D:329:GLU:HA   | 1:D:329:GLU:OE1  | 2.12                     | 0.48              |
| 1:B:559:PRO:O    | 1:B:560:THR:C    | 2.55                     | 0.48              |
| 1:B:719:ILE:O    | 1:B:719:ILE:HG22 | 2.13                     | 0.48              |
| 1:C:434:ASN:HB2  | 1:C:437:GLU:HG2  | 1.95                     | 0.48              |
| 1:C:1000:LYS:O   | 1:C:1004:MET:HG3 | 2.13                     | 0.48              |
| 1:B:667:ILE:HG22 | 1:B:684:GLU:HB2  | 1.94                     | 0.48              |
| 1:A:796:ASN:O    | 1:A:798:LEU:N    | 2.44                     | 0.48              |
| 1:C:607:GLN:OE1  | 1:C:607:GLN:HA   | 2.13                     | 0.48              |
| 1:C:956:LEU:H    | 1:C:956:LEU:HD12 | 1.78                     | 0.48              |
| 1:A:312:SER:O    | 1:A:314:PRO:HD3  | 2.14                     | 0.48              |
| 1:B:340:TYR:CZ   | 1:B:356:ASN:HB3  | 2.48                     | 0.48              |
| 1:B:822:ARG:NH2  | 1:B:909:ASP:OD2  | 2.45                     | 0.48              |
| 3:D:1201:UDP:O2A | 2:L:7:SER:HB2    | 2.14                     | 0.48              |
| 1:A:697:ASP:HB3  | 1:A:701:MET:HG3  | 1.95                     | 0.48              |
| 1:B:881:GLN:NE2  | 1:B:887:GLN:HA   | 2.28                     | 0.48              |
| 1:D:330:GLN:O    | 1:D:332:ASN:N    | 2.46                     | 0.48              |
| 1:A:704:HIS:O    | 1:A:727:ASN:HB3  | 2.14                     | 0.47              |
| 1:B:519:ASN:HA   | 1:B:522:LEU:HD12 | 1.95                     | 0.47              |
| 1:C:510:ARG:NH1  | 1:C:510:ARG:HG3  | 2.28                     | 0.47              |
| 1:D:815:ARG:NH1  | 1:D:815:ARG:HG3  | 2.29                     | 0.47              |
| 1:A:785:ILE:CG2  | 1:A:786:GLN:HG2  | 2.45                     | 0.47              |
| 1:B:697:ASP:HB3  | 1:B:701:MET:HG3  | 1.96                     | 0.47              |
| 1:D:638:ASN:O    | 1:D:639:GLU:C    | 2.57                     | 0.47              |
| 1:D:697:ASP:HB3  | 1:D:701:MET:HG3  | 1.95                     | 0.47              |
| 1:A:860:ASN:HB2  | 1:B:1016:HIS:CE1 | 2.49                     | 0.47              |
| 1:D:660:GLY:HA2  | 1:D:683:SER:CB   | 2.43                     | 0.47              |
| 1:D:714:LYS:NZ   | 1:D:719:ILE:N    | 2.63                     | 0.47              |
| 1:D:937:PRO:HA   | 1:D:943:SER:O    | 2.15                     | 0.47              |
| 1:A:443:ARG:CG   | 1:A:443:ARG:NH1  | 2.70                     | 0.47              |
| 1:B:1004:MET:HE3 | 1:C:791:GLY:C    | 2.39                     | 0.47              |
| 1:C:342:LYS:O    | 1:C:346:VAL:HG23 | 2.15                     | 0.47              |
| 1:A:805:ASN:HD22 | 1:A:805:ASN:N    | 2.13                     | 0.47              |
| 1:D:525:ILE:O    | 1:D:528:LEU:HB2  | 2.13                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:A:545:ARG:NH1  | 1:A:576:PHE:O     | 2.47                     | 0.47              |
| 1:A:688:TYR:CD2  | 1:A:1027:ILE:HG22 | 2.49                     | 0.47              |
| 1:B:616:ASP:O    | 1:B:620:GLN:HB2   | 2.15                     | 0.47              |
| 1:B:669:THR:OG1  | 1:B:670:ASP:N     | 2.47                     | 0.47              |
| 1:C:743:ILE:O    | 1:C:743:ILE:HG22  | 2.14                     | 0.47              |
| 1:D:465:ILE:O    | 1:D:465:ILE:CG2   | 2.58                     | 0.47              |
| 1:D:566:SER:HB2  | 1:D:697:ASP:OD1   | 2.14                     | 0.47              |
| 1:A:408:TYR:O    | 1:A:412:ILE:HG13  | 2.15                     | 0.47              |
| 1:B:435:ILE:N    | 1:B:436:PRO:CD    | 2.77                     | 0.47              |
| 1:C:324:ALA:HA   | 1:C:339:LEU:HD12  | 1.95                     | 0.47              |
| 1:C:443:ARG:HG2  | 1:C:443:ARG:NH1   | 2.11                     | 0.47              |
| 1:A:613:LYS:O    | 1:A:616:ASP:HB2   | 2.14                     | 0.47              |
| 1:B:468:ASP:O    | 1:B:475:ARG:NH2   | 2.35                     | 0.47              |
| 1:B:660:GLY:HA2  | 1:B:683:SER:CB    | 2.44                     | 0.47              |
| 1:C:688:TYR:CD2  | 1:C:1027:ILE:HG22 | 2.50                     | 0.47              |
| 1:C:734:PHE:HE1  | 1:C:789:ILE:HG22  | 1.80                     | 0.47              |
| 1:B:695:ILE:HB   | 1:B:1002:TYR:CE2  | 2.50                     | 0.47              |
| 1:C:604:ASP:OD1  | 1:C:604:ASP:C     | 2.54                     | 0.47              |
| 1:C:804:ASN:OD1  | 1:C:804:ASN:C     | 2.58                     | 0.47              |
| 1:B:319:SER:HA   | 1:B:322:ASN:HD22  | 1.79                     | 0.46              |
| 1:C:764:MET:HA   | 1:C:765:PRO:HD2   | 1.79                     | 0.46              |
| 1:C:844:ASP:HB2  | 1:C:845:PRO:HD2   | 1.95                     | 0.46              |
| 1:A:596:MET:HG2  | 1:A:602:PHE:CG    | 2.50                     | 0.46              |
| 1:B:695:ILE:HG13 | 1:B:696:GLY:H     | 1.79                     | 0.46              |
| 1:B:713:PHE:HD1  | 1:B:713:PHE:N     | 1.83                     | 0.46              |
| 3:B:1201:UDP:O2A | 2:J:7:SER:HB2     | 2.14                     | 0.46              |
| 1:A:638:ASN:O    | 1:A:641:PHE:N     | 2.48                     | 0.46              |
| 1:C:465:ILE:O    | 1:C:465:ILE:CG2   | 2.63                     | 0.46              |
| 1:C:512:ALA:O    | 1:C:516:ARG:HG2   | 2.15                     | 0.46              |
| 2:I:4:VAL:CG1    | 2:I:5:PRO:HD2     | 2.43                     | 0.46              |
| 1:D:785:ILE:HG22 | 1:D:786:GLN:HG2   | 1.96                     | 0.46              |
| 1:A:342:LYS:O    | 1:A:346:VAL:HG23  | 2.15                     | 0.46              |
| 1:D:896:ALA:HB1  | 1:D:897:PRO:HD2   | 1.97                     | 0.46              |
| 1:D:911:CYS:O    | 1:D:933:MET:HA    | 2.16                     | 0.46              |
| 1:A:501:MET:HE3  | 1:A:501:MET:HB3   | 1.76                     | 0.46              |
| 1:B:357:LEU:HD23 | 1:B:373:HIS:CE1   | 2.51                     | 0.46              |
| 1:D:335:GLU:O    | 1:D:336:ALA:C     | 2.57                     | 0.46              |
| 1:D:629:MET:O    | 1:D:654:GLY:HA3   | 2.16                     | 0.46              |
| 1:A:426:ALA:HB2  | 1:A:441:SER:CB    | 2.40                     | 0.46              |
| 1:A:719:ILE:O    | 1:A:719:ILE:HG22  | 2.16                     | 0.46              |
| 1:B:604:ASP:C    | 1:B:604:ASP:OD1   | 2.59                     | 0.46              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:C:530:LYS:HE2   | 1:C:533:TYR:OH   | 2.16                     | 0.46              |
| 1:A:428:ILE:HG23  | 1:A:428:ILE:HD12 | 1.43                     | 0.46              |
| 1:A:538:ASP:C     | 1:A:539:LEU:HD23 | 2.40                     | 0.46              |
| 1:A:655:TYR:HA    | 1:A:656:PRO:HD3  | 1.70                     | 0.46              |
| 1:A:940:THR:O     | 1:A:941:LEU:C    | 2.59                     | 0.46              |
| 1:A:969:ILE:O     | 1:A:973:LEU:HD12 | 2.16                     | 0.46              |
| 1:B:330:GLN:H     | 1:B:330:GLN:HG3  | 1.58                     | 0.46              |
| 1:B:496:HIS:CG    | 1:B:497:PRO:HD2  | 2.51                     | 0.46              |
| 1:C:583:LEU:HD22  | 1:C:637:ARG:HD3  | 1.98                     | 0.46              |
| 1:C:651:MET:HE3   | 1:C:651:MET:HB3  | 1.72                     | 0.46              |
| 1:A:512:ALA:O     | 1:A:516:ARG:HG2  | 2.16                     | 0.46              |
| 1:B:461:HIS:O     | 1:B:465:ILE:HG13 | 2.15                     | 0.46              |
| 1:C:519:ASN:HA    | 1:C:522:LEU:HD12 | 1.97                     | 0.46              |
| 2:K:8:SER:O       | 2:K:9:ALA:O      | 2.34                     | 0.46              |
| 1:B:629:MET:O     | 1:B:654:GLY:HA3  | 2.16                     | 0.46              |
| 1:D:1011:LEU:HD23 | 1:D:1011:LEU:HA  | 1.72                     | 0.46              |
| 1:B:562:HIS:ND1   | 1:B:898:LYS:HE2  | 2.31                     | 0.45              |
| 1:C:357:LEU:HD23  | 1:C:373:HIS:CE1  | 2.51                     | 0.45              |
| 1:C:402:GLN:HE21  | 1:C:406:GLN:NE2  | 2.14                     | 0.45              |
| 1:C:772:ILE:O     | 1:C:773:ALA:C    | 2.57                     | 0.45              |
| 1:D:940:THR:O     | 1:D:941:LEU:C    | 2.59                     | 0.45              |
| 1:A:796:ASN:C     | 1:A:798:LEU:H    | 2.24                     | 0.45              |
| 1:A:950:LEU:HD23  | 1:A:950:LEU:HA   | 1.67                     | 0.45              |
| 1:B:607:GLN:HA    | 1:B:607:GLN:OE1  | 2.16                     | 0.45              |
| 1:C:330:GLN:O     | 1:C:332:ASN:N    | 2.49                     | 0.45              |
| 1:C:703:PRO:HD2   | 1:C:813:VAL:HG22 | 1.98                     | 0.45              |
| 1:C:844:ASP:HB2   | 1:C:845:PRO:CD   | 2.46                     | 0.45              |
| 1:D:434:ASN:HB2   | 1:D:437:GLU:HG2  | 1.96                     | 0.45              |
| 1:A:689:MET:HB3   | 1:A:690:PRO:HD2  | 1.98                     | 0.45              |
| 1:C:545:ARG:NH1   | 1:C:576:PHE:O    | 2.49                     | 0.45              |
| 1:C:965:GLU:O     | 1:C:969:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:651:MET:HE3   | 1:A:651:MET:HB3  | 1.77                     | 0.45              |
| 1:A:979:TYR:O     | 1:A:982:LYS:HB3  | 2.16                     | 0.45              |
| 1:B:994:SER:CB    | 1:B:995:PRO:HD3  | 2.36                     | 0.45              |
| 1:D:496:HIS:CG    | 1:D:497:PRO:HD2  | 2.51                     | 0.45              |
| 1:D:644:ARG:HH22  | 1:D:665:ASP:CG   | 2.25                     | 0.45              |
| 1:A:462:CYS:O     | 1:A:465:ILE:HB   | 2.15                     | 0.45              |
| 1:A:525:ILE:HA    | 1:A:528:LEU:HD12 | 1.98                     | 0.45              |
| 1:A:918:ASN:N     | 1:A:918:ASN:ND2  | 2.62                     | 0.45              |
| 1:B:644:ARG:HH22  | 1:B:665:ASP:CG   | 2.24                     | 0.45              |
| 1:D:555:PHE:O     | 1:D:592:ARG:HD3  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:330:GLN:O    | 1:B:332:ASN:N    | 2.49                     | 0.45              |
| 1:B:704:HIS:NE2  | 1:B:814:PRO:HG2  | 2.32                     | 0.45              |
| 1:C:425:LEU:O    | 1:C:426:ALA:C    | 2.59                     | 0.45              |
| 1:C:963:ARG:O    | 1:C:967:GLU:HG3  | 2.16                     | 0.45              |
| 1:D:559:PRO:O    | 1:D:560:THR:C    | 2.57                     | 0.45              |
| 1:A:330:GLN:C    | 1:A:332:ASN:H    | 2.25                     | 0.45              |
| 1:A:468:ASP:OD1  | 1:A:468:ASP:C    | 2.60                     | 0.45              |
| 1:B:617:ARG:HA   | 1:B:617:ARG:HD2  | 1.79                     | 0.45              |
| 1:B:1004:MET:HE3 | 1:C:791:GLY:O    | 2.16                     | 0.45              |
| 1:C:401:VAL:O    | 1:C:402:GLN:C    | 2.59                     | 0.45              |
| 1:C:704:HIS:N    | 1:C:704:HIS:ND1  | 2.61                     | 0.45              |
| 1:D:412:ILE:HD13 | 1:D:422:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:723:ARG:O    | 1:A:724:ILE:HG13 | 2.16                     | 0.45              |
| 1:A:885:LEU:HA   | 1:A:886:PRO:HD2  | 1.79                     | 0.45              |
| 1:B:468:ASP:C    | 1:B:468:ASP:OD1  | 2.58                     | 0.45              |
| 1:B:553:SER:HA   | 1:B:583:LEU:HB2  | 1.99                     | 0.45              |
| 1:B:704:HIS:O    | 1:B:727:ASN:HB3  | 2.16                     | 0.45              |
| 1:C:596:MET:HG2  | 1:C:602:PHE:CG   | 2.51                     | 0.45              |
| 1:D:655:TYR:HA   | 1:D:656:PRO:HD3  | 1.74                     | 0.45              |
| 1:C:1022:LYS:O   | 1:C:1023:PRO:C   | 2.59                     | 0.45              |
| 1:D:617:ARG:HA   | 1:D:617:ARG:HD2  | 1.77                     | 0.45              |
| 1:A:412:ILE:HD13 | 1:A:422:HIS:CE1  | 2.52                     | 0.45              |
| 1:A:503:TYR:HB3  | 1:A:504:PRO:HD2  | 1.99                     | 0.45              |
| 1:B:638:ASN:O    | 1:B:639:GLU:C    | 2.58                     | 0.45              |
| 1:B:936:MET:HE3  | 1:B:962:ASN:HA   | 1.99                     | 0.45              |
| 1:C:605:LEU:C    | 1:C:607:GLN:N    | 2.73                     | 0.45              |
| 1:D:846:SER:HB2  | 1:D:963:ARG:NH2  | 2.30                     | 0.45              |
| 1:D:867:ARG:HB3  | 1:D:870:ALA:HA   | 1.98                     | 0.45              |
| 1:A:772:ILE:HD12 | 1:A:772:ILE:H    | 1.81                     | 0.44              |
| 1:D:596:MET:HG2  | 1:D:602:PHE:CG   | 2.51                     | 0.44              |
| 1:D:695:ILE:HG13 | 1:D:696:GLY:N    | 2.31                     | 0.44              |
| 1:D:774:GLU:HA   | 1:D:777:ILE:CG2  | 2.48                     | 0.44              |
| 1:A:829:GLU:H    | 1:A:829:GLU:HG2  | 1.56                     | 0.44              |
| 1:B:371:LEU:HD12 | 1:B:371:LEU:C    | 2.42                     | 0.44              |
| 1:A:726:LEU:HD22 | 1:A:819:VAL:HG22 | 1.97                     | 0.44              |
| 1:B:686:LEU:N    | 1:B:686:LEU:HD23 | 2.33                     | 0.44              |
| 1:B:815:ARG:NH1  | 1:B:815:ARG:HG3  | 2.32                     | 0.44              |
| 1:C:596:MET:HG2  | 1:C:602:PHE:CD1  | 2.52                     | 0.44              |
| 1:C:1002:TYR:CD1 | 1:C:1002:TYR:C   | 2.95                     | 0.44              |
| 1:D:972:LYS:HG2  | 1:D:979:TYR:CD2  | 2.52                     | 0.44              |
| 1:B:557:ASN:HB2  | 1:B:589:THR:HG21 | 2.00                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:564:MET:O    | 1:B:565:GLN:C    | 2.59                     | 0.44              |
| 1:B:918:ASN:N    | 1:B:918:ASN:HD22 | 2.13                     | 0.44              |
| 1:C:487:LEU:O    | 1:C:516:ARG:NH2  | 2.49                     | 0.44              |
| 1:C:846:SER:HB2  | 1:C:963:ARG:HH21 | 1.81                     | 0.44              |
| 1:D:369:GLU:O    | 1:D:370:ALA:C    | 2.60                     | 0.44              |
| 1:B:320:LEU:HA   | 1:B:323:LEU:HD12 | 1.98                     | 0.44              |
| 1:B:764:MET:HA   | 1:B:765:PRO:HD2  | 1.82                     | 0.44              |
| 1:B:770:ASN:OD1  | 1:B:770:ASN:N    | 2.48                     | 0.44              |
| 1:C:1015:GLU:OE1 | 1:C:1015:GLU:CA  | 2.56                     | 0.44              |
| 1:B:412:ILE:HD13 | 1:B:422:HIS:CE1  | 2.53                     | 0.44              |
| 1:B:695:ILE:HD13 | 1:B:1002:TYR:CD2 | 2.53                     | 0.44              |
| 1:D:896:ALA:HB1  | 1:D:897:PRO:CD   | 2.47                     | 0.44              |
| 2:J:4:VAL:CG1    | 2:J:5:PRO:HD2    | 2.48                     | 0.44              |
| 1:A:369:GLU:O    | 1:A:370:ALA:C    | 2.61                     | 0.44              |
| 1:A:558:HIS:CG   | 1:A:559:PRO:HD2  | 2.53                     | 0.44              |
| 1:A:859:PRO:CG   | 1:B:1016:HIS:ND1 | 2.80                     | 0.44              |
| 1:B:877:GLN:O    | 1:B:880:ALA:HB3  | 2.18                     | 0.44              |
| 1:C:430:LYS:HE2  | 1:C:462:CYS:SG   | 2.58                     | 0.44              |
| 1:D:918:ASN:N    | 1:D:918:ASN:HD22 | 2.16                     | 0.44              |
| 1:B:520:LEU:HD23 | 1:B:520:LEU:HA   | 1.73                     | 0.44              |
| 1:C:725:VAL:O    | 1:C:726:LEU:HD23 | 2.17                     | 0.44              |
| 1:D:461:HIS:O    | 1:D:464:GLN:HB3  | 2.18                     | 0.44              |
| 1:B:558:HIS:O    | 1:B:559:PRO:C    | 2.59                     | 0.44              |
| 1:B:731:LEU:O    | 1:B:734:PHE:HB3  | 2.17                     | 0.44              |
| 1:B:1000:LYS:O   | 1:B:1004:MET:HG3 | 2.17                     | 0.44              |
| 1:C:827:LEU:HA   | 1:C:828:PRO:HD2  | 1.78                     | 0.44              |
| 1:C:990:GLN:CA   | 1:C:990:GLN:HE21 | 2.29                     | 0.44              |
| 1:B:443:ARG:HG2  | 1:B:443:ARG:NH1  | 2.16                     | 0.43              |
| 1:B:511:LYS:O    | 1:B:515:GLU:HB2  | 2.18                     | 0.43              |
| 1:B:743:ILE:HG22 | 1:B:743:ILE:O    | 2.18                     | 0.43              |
| 1:B:867:ARG:HB3  | 1:B:870:ALA:HA   | 1.99                     | 0.43              |
| 1:D:865:LEU:O    | 1:D:892:PHE:HA   | 2.18                     | 0.43              |
| 1:A:322:ASN:HA   | 1:A:325:ASN:HD22 | 1.83                     | 0.43              |
| 1:A:704:HIS:CD2  | 1:A:814:PRO:HG2  | 2.53                     | 0.43              |
| 1:B:596:MET:HG2  | 1:B:602:PHE:CG   | 2.53                     | 0.43              |
| 1:D:491:ARG:HD2  | 1:D:491:ARG:HA   | 1.74                     | 0.43              |
| 1:A:487:LEU:O    | 1:A:516:ARG:NH2  | 2.50                     | 0.43              |
| 1:A:506:SER:O    | 1:A:507:HIS:C    | 2.60                     | 0.43              |
| 1:A:539:LEU:HD23 | 1:A:539:LEU:N    | 2.32                     | 0.43              |
| 1:A:618:ILE:O    | 1:A:621:ASP:N    | 2.43                     | 0.43              |
| 1:C:738:LEU:HA   | 1:C:739:PRO:HD2  | 1.79                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:C:834:TYR:O    | 1:C:863:LEU:HD12  | 2.18                     | 0.43              |
| 1:C:877:GLN:O    | 1:C:880:ALA:HB3   | 2.18                     | 0.43              |
| 1:B:796:ASN:O    | 1:B:798:LEU:N     | 2.50                     | 0.43              |
| 1:B:911:CYS:HB2  | 1:B:926:VAL:HG21  | 2.00                     | 0.43              |
| 1:C:533:TYR:OH   | 1:C:616:ASP:OD1   | 2.33                     | 0.43              |
| 1:C:562:HIS:ND1  | 1:C:898:LYS:HE2   | 2.34                     | 0.43              |
| 1:A:564:MET:O    | 1:A:565:GLN:C     | 2.62                     | 0.43              |
| 1:B:398:MET:O    | 1:B:399:GLN:HB2   | 2.18                     | 0.43              |
| 1:B:535:HIS:HB3  | 1:B:647:PRO:HD3   | 1.99                     | 0.43              |
| 1:C:629:MET:O    | 1:C:654:GLY:HA3   | 2.17                     | 0.43              |
| 1:C:789:ILE:C    | 1:C:791:GLY:N     | 2.74                     | 0.43              |
| 1:C:822:ARG:HB3  | 1:C:827:LEU:HB2   | 2.01                     | 0.43              |
| 1:C:885:LEU:HA   | 1:C:886:PRO:HD2   | 1.72                     | 0.43              |
| 1:D:686:LEU:N    | 1:D:686:LEU:HD23  | 2.34                     | 0.43              |
| 1:D:780:ILE:HD12 | 1:D:780:ILE:HG23  | 1.73                     | 0.43              |
| 1:A:335:GLU:O    | 1:A:336:ALA:C     | 2.62                     | 0.43              |
| 1:A:357:LEU:HD23 | 1:A:373:HIS:CE1   | 2.53                     | 0.43              |
| 3:A:1201:UDP:O2A | 2:I:7:SER:HB2     | 2.18                     | 0.43              |
| 1:B:850:MET:HE2  | 1:B:963:ARG:HE    | 1.83                     | 0.43              |
| 1:D:858:VAL:HG22 | 1:D:975:THR:HG23  | 2.00                     | 0.43              |
| 1:A:317:ALA:HB2  | 1:A:346:VAL:HB    | 2.00                     | 0.43              |
| 1:A:860:ASN:OD1  | 1:B:1024:ASP:HB2  | 2.19                     | 0.43              |
| 1:A:945:VAL:O    | 1:A:949:GLN:HG3   | 2.19                     | 0.43              |
| 1:A:1011:LEU:HA  | 1:A:1011:LEU:HD23 | 1.60                     | 0.43              |
| 1:B:439:ILE:O    | 1:B:440:ALA:C     | 2.62                     | 0.43              |
| 1:C:329:GLU:C    | 1:C:331:GLY:H     | 2.25                     | 0.43              |
| 1:C:340:TYR:CZ   | 1:C:356:ASN:HB3   | 2.54                     | 0.43              |
| 1:C:465:ILE:O    | 1:C:465:ILE:HG22  | 2.18                     | 0.43              |
| 1:C:940:THR:O    | 1:C:941:LEU:C     | 2.61                     | 0.43              |
| 1:D:965:GLU:O    | 1:D:969:ILE:HG13  | 2.19                     | 0.43              |
| 1:C:644:ARG:HH22 | 1:C:665:ASP:CG    | 2.27                     | 0.43              |
| 1:C:667:ILE:HG22 | 1:C:684:GLU:HB2   | 2.01                     | 0.43              |
| 1:C:858:VAL:HG22 | 1:C:975:THR:HG23  | 2.01                     | 0.43              |
| 1:D:590:ASN:ND2  | 1:D:811:GLU:HB3   | 2.32                     | 0.43              |
| 1:A:617:ARG:HA   | 1:A:617:ARG:HD2   | 1.86                     | 0.43              |
| 1:A:805:ASN:N    | 1:A:805:ASN:ND2   | 2.67                     | 0.43              |
| 1:B:371:LEU:HD12 | 1:B:371:LEU:O     | 2.18                     | 0.43              |
| 1:B:399:GLN:OE1  | 1:B:399:GLN:HA    | 2.19                     | 0.43              |
| 1:B:408:TYR:CE1  | 1:B:424:ASN:HB3   | 2.53                     | 0.43              |
| 1:B:566:SER:HB2  | 1:B:697:ASP:OD1   | 2.19                     | 0.43              |
| 1:B:710:VAL:HG12 | 1:B:724:ILE:O     | 2.19                     | 0.43              |

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| Atom-1            | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:B:936:MET:HB2   | 1:B:966:TYR:CD2   | 2.54                     | 0.43              |
| 1:B:937:PRO:HB2   | 1:B:944:ARG:NH1   | 2.34                     | 0.43              |
| 1:C:1011:LEU:HD23 | 1:C:1011:LEU:HA   | 1.65                     | 0.43              |
| 1:D:367:LEU:HD23  | 1:D:367:LEU:H     | 1.83                     | 0.43              |
| 1:D:437:GLU:CD    | 1:D:437:GLU:H     | 2.26                     | 0.43              |
| 1:D:834:TYR:HA    | 1:D:910:VAL:O     | 2.19                     | 0.43              |
| 1:A:859:PRO:O     | 1:B:1024:ASP:OD2  | 2.36                     | 0.43              |
| 1:A:897:PRO:O     | 1:A:898:LYS:C     | 2.61                     | 0.43              |
| 1:A:963:ARG:O     | 1:A:964:GLN:C     | 2.62                     | 0.43              |
| 1:B:586:ASP:OD1   | 1:B:586:ASP:C     | 2.62                     | 0.43              |
| 1:B:742:LYS:H     | 1:B:742:LYS:HG2   | 1.49                     | 0.43              |
| 1:B:1027:ILE:H    | 1:B:1027:ILE:HG12 | 1.78                     | 0.43              |
| 1:D:391:MET:HE3   | 1:D:407:CYS:SG    | 2.59                     | 0.43              |
| 1:A:456:TYR:CD1   | 1:A:456:TYR:C     | 2.97                     | 0.42              |
| 1:B:834:TYR:HA    | 1:B:910:VAL:O     | 2.19                     | 0.42              |
| 1:C:697:ASP:HB3   | 1:C:701:MET:HG3   | 2.01                     | 0.42              |
| 1:D:625:ILE:HG12  | 1:D:648:ILE:HB    | 2.01                     | 0.42              |
| 1:B:625:ILE:HG12  | 1:B:648:ILE:HB    | 2.00                     | 0.42              |
| 1:B:897:PRO:O     | 1:B:898:LYS:C     | 2.62                     | 0.42              |
| 1:C:399:GLN:HA    | 1:C:399:GLN:OE1   | 2.18                     | 0.42              |
| 1:C:723:ARG:HH21  | 1:C:830:ASP:HA    | 1.84                     | 0.42              |
| 1:D:714:LYS:HB2   | 1:D:714:LYS:HE2   | 1.95                     | 0.42              |
| 1:A:533:TYR:OH    | 1:A:616:ASP:OD1   | 2.30                     | 0.42              |
| 1:A:860:ASN:HA    | 1:B:1024:ASP:OD2  | 2.19                     | 0.42              |
| 1:A:873:GLU:N     | 1:A:874:PRO:HD2   | 2.34                     | 0.42              |
| 1:B:401:VAL:O     | 1:B:402:GLN:C     | 2.62                     | 0.42              |
| 1:B:424:ASN:O     | 1:B:427:SER:HB2   | 2.19                     | 0.42              |
| 1:B:918:ASN:ND2   | 1:B:943:SER:HA    | 2.34                     | 0.42              |
| 1:C:330:GLN:H     | 1:C:330:GLN:HG3   | 1.57                     | 0.42              |
| 1:B:707:LYS:HE2   | 1:B:762:LEU:CD2   | 2.49                     | 0.42              |
| 1:B:772:ILE:O     | 1:B:773:ALA:C     | 2.62                     | 0.42              |
| 1:C:977:LEU:N     | 1:C:977:LEU:HD23  | 2.35                     | 0.42              |
| 1:D:353:ALA:O     | 1:D:354:HIS:C     | 2.63                     | 0.42              |
| 2:K:5:PRO:HG2     | 2:K:5:PRO:O       | 2.18                     | 0.42              |
| 1:A:483:VAL:O     | 1:A:484:ALA:C     | 2.63                     | 0.42              |
| 1:A:491:ARG:HD2   | 1:A:491:ARG:HA    | 1.78                     | 0.42              |
| 1:A:660:GLY:HA2   | 1:A:683:SER:CB    | 2.50                     | 0.42              |
| 1:C:361:LEU:HA    | 1:C:361:LEU:HD23  | 1.86                     | 0.42              |
| 1:C:403:GLY:O     | 1:C:404:ALA:C     | 2.61                     | 0.42              |
| 1:D:738:LEU:HD23  | 1:D:738:LEU:HA    | 1.92                     | 0.42              |
| 1:A:881:GLN:NE2   | 1:A:887:GLN:HA    | 2.33                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:522:LEU:HD23 | 1:B:525:ILE:HD11 | 2.02                     | 0.42              |
| 1:B:538:ASP:C    | 1:B:539:LEU:HD23 | 2.45                     | 0.42              |
| 1:B:850:MET:HE2  | 1:B:963:ARG:NE   | 2.34                     | 0.42              |
| 1:C:400:ASP:C    | 1:C:400:ASP:OD1  | 2.61                     | 0.42              |
| 1:C:525:ILE:O    | 1:C:528:LEU:HB2  | 2.20                     | 0.42              |
| 1:D:451:ASP:C    | 1:D:451:ASP:OD1  | 2.63                     | 0.42              |
| 1:D:740:ASP:CB   | 1:D:768:PRO:HG3  | 2.45                     | 0.42              |
| 1:D:742:LYS:CE   | 1:D:768:PRO:HB3  | 2.50                     | 0.42              |
| 1:D:764:MET:HE3  | 1:D:764:MET:HB3  | 1.88                     | 0.42              |
| 1:A:344:LEU:HD23 | 1:A:344:LEU:HA   | 1.85                     | 0.42              |
| 1:A:513:ILE:O    | 1:A:514:ALA:C    | 2.61                     | 0.42              |
| 1:A:926:VAL:CG1  | 1:A:927:LEU:N    | 2.82                     | 0.42              |
| 1:B:979:TYR:O    | 1:B:980:LEU:C    | 2.63                     | 0.42              |
| 1:D:405:LEU:HD12 | 1:D:405:LEU:HA   | 1.85                     | 0.42              |
| 1:A:697:ASP:O    | 1:A:698:HIS:C    | 2.61                     | 0.42              |
| 1:A:704:HIS:ND1  | 1:A:704:HIS:N    | 2.67                     | 0.42              |
| 1:C:559:PRO:O    | 1:C:560:THR:C    | 2.61                     | 0.42              |
| 1:C:986:LYS:O    | 1:C:990:GLN:CG   | 2.68                     | 0.42              |
| 1:D:561:SER:O    | 1:D:565:GLN:HG2  | 2.19                     | 0.42              |
| 1:A:873:GLU:O    | 1:A:874:PRO:C    | 2.63                     | 0.42              |
| 1:B:651:MET:HB3  | 1:B:651:MET:HE3  | 1.62                     | 0.42              |
| 1:B:863:LEU:HD12 | 1:B:864:TRP:H    | 1.85                     | 0.42              |
| 1:B:885:LEU:HA   | 1:B:886:PRO:HD2  | 1.77                     | 0.42              |
| 1:B:1014:TRP:O   | 1:B:1015:GLU:C   | 2.61                     | 0.42              |
| 1:C:638:ASN:C    | 1:C:640:LEU:N    | 2.77                     | 0.42              |
| 1:C:774:GLU:O    | 1:C:778:GLU:HB2  | 2.19                     | 0.42              |
| 1:D:651:MET:HE3  | 1:D:651:MET:HB3  | 1.73                     | 0.42              |
| 1:A:617:ARG:O    | 1:A:620:GLN:HB3  | 2.20                     | 0.42              |
| 1:B:405:LEU:HD12 | 1:B:405:LEU:HA   | 1.70                     | 0.42              |
| 1:B:545:ARG:NH1  | 1:B:576:PHE:O    | 2.53                     | 0.42              |
| 1:C:626:LEU:HA   | 1:C:626:LEU:HD12 | 1.80                     | 0.42              |
| 1:D:330:GLN:H    | 1:D:330:GLN:HG3  | 1.68                     | 0.42              |
| 1:D:742:LYS:C    | 1:D:743:ILE:HG12 | 2.44                     | 0.42              |
| 1:A:525:ILE:O    | 1:A:528:LEU:HB2  | 2.20                     | 0.41              |
| 1:B:936:MET:HB2  | 1:B:966:TYR:HD2  | 1.85                     | 0.41              |
| 1:C:491:ARG:HD2  | 1:C:491:ARG:HA   | 1.68                     | 0.41              |
| 1:C:539:LEU:HD21 | 1:C:1014:TRP:CE2 | 2.55                     | 0.41              |
| 1:A:986:LYS:O    | 1:A:990:GLN:HG2  | 2.20                     | 0.41              |
| 1:B:348:PRO:C    | 1:B:350:PHE:H    | 2.28                     | 0.41              |
| 1:C:960:ALA:HB1  | 1:C:965:GLU:HB3  | 2.02                     | 0.41              |
| 1:D:930:GLY:HA2  | 1:D:987:VAL:HG12 | 2.03                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:471:ASP:O    | 1:C:472:TYR:C    | 2.62                     | 0.41              |
| 1:C:979:TYR:O    | 1:C:980:LEU:C    | 2.63                     | 0.41              |
| 1:D:329:GLU:C    | 1:D:331:GLY:H    | 2.27                     | 0.41              |
| 1:B:572:ASN:HA   | 1:B:573:PRO:HD2  | 1.81                     | 0.41              |
| 1:D:405:LEU:HD13 | 1:D:428:ILE:HG21 | 2.01                     | 0.41              |
| 1:D:815:ARG:HH11 | 1:D:815:ARG:CG   | 2.33                     | 0.41              |
| 1:A:564:MET:SD   | 1:A:564:MET:C    | 3.03                     | 0.41              |
| 1:A:625:ILE:HD13 | 1:A:625:ILE:HG21 | 1.90                     | 0.41              |
| 1:A:792:PHE:CE1  | 1:D:1004:MET:HE1 | 2.55                     | 0.41              |
| 1:B:539:LEU:HD23 | 1:B:539:LEU:N    | 2.34                     | 0.41              |
| 1:B:625:ILE:HG21 | 1:B:625:ILE:HD13 | 1.89                     | 0.41              |
| 1:C:480:VAL:HG13 | 1:C:505:LEU:HD23 | 2.00                     | 0.41              |
| 1:C:522:LEU:HD23 | 1:C:525:ILE:HD11 | 2.02                     | 0.41              |
| 1:D:538:ASP:C    | 1:D:539:LEU:HD23 | 2.45                     | 0.41              |
| 1:D:780:ILE:HD13 | 1:D:780:ILE:HA   | 1.94                     | 0.41              |
| 1:B:813:VAL:HG13 | 1:B:814:PRO:HD2  | 2.03                     | 0.41              |
| 1:C:566:SER:HB2  | 1:C:697:ASP:OD1  | 2.21                     | 0.41              |
| 1:A:330:GLN:H    | 1:A:330:GLN:HG3  | 1.54                     | 0.41              |
| 1:A:834:TYR:HA   | 1:A:910:VAL:O    | 2.20                     | 0.41              |
| 1:B:501:MET:HE3  | 1:B:501:MET:HB3  | 1.87                     | 0.41              |
| 1:B:700:ASN:O    | 1:B:703:PRO:HD3  | 2.20                     | 0.41              |
| 1:B:846:SER:HB2  | 1:B:963:ARG:NH2  | 2.36                     | 0.41              |
| 1:C:367:LEU:O    | 1:C:368:GLN:C    | 2.64                     | 0.41              |
| 1:C:426:ALA:HB2  | 1:C:441:SER:CB   | 2.48                     | 0.41              |
| 1:C:476:MET:O    | 1:C:477:LYS:C    | 2.62                     | 0.41              |
| 1:C:719:ILE:O    | 1:C:719:ILE:HG22 | 2.20                     | 0.41              |
| 1:C:928:TRP:O    | 1:C:991:ARG:NH1  | 2.48                     | 0.41              |
| 1:D:886:PRO:HG2  | 1:D:889:ARG:HG2  | 2.02                     | 0.41              |
| 1:A:530:LYS:HE2  | 1:A:533:TYR:OH   | 2.21                     | 0.41              |
| 1:A:626:LEU:HA   | 1:A:626:LEU:HD12 | 1.76                     | 0.41              |
| 1:C:428:ILE:HG23 | 1:C:428:ILE:HD12 | 1.71                     | 0.41              |
| 1:C:841:TYR:CD1  | 1:C:841:TYR:C    | 2.99                     | 0.41              |
| 1:C:930:GLY:HA2  | 1:C:987:VAL:HG12 | 2.03                     | 0.41              |
| 1:D:557:ASN:HB2  | 1:D:589:THR:HG21 | 2.03                     | 0.41              |
| 1:D:626:LEU:HA   | 1:D:626:LEU:HD12 | 1.87                     | 0.41              |
| 1:D:920:HIS:HB2  | 3:D:1201:UDP:O2B | 2.21                     | 0.41              |
| 1:D:950:LEU:HD23 | 1:D:950:LEU:HA   | 1.90                     | 0.41              |
| 1:A:452:PHE:C    | 1:A:452:PHE:CD1  | 2.98                     | 0.41              |
| 1:A:769:MET:HE3  | 1:A:774:GLU:HG3  | 2.02                     | 0.41              |
| 1:A:804:ASN:OD1  | 1:A:804:ASN:C    | 2.64                     | 0.41              |
| 1:A:889:ARG:HG3  | 1:A:889:ARG:HH11 | 1.85                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:326:ILE:O    | 1:B:329:GLU:HB2  | 2.21                     | 0.41              |
| 1:B:428:ILE:HG23 | 1:B:428:ILE:HD12 | 1.54                     | 0.41              |
| 1:B:555:PHE:O    | 1:B:592:ARG:HD3  | 2.21                     | 0.41              |
| 1:B:695:ILE:HB   | 1:B:1002:TYR:CD2 | 2.56                     | 0.41              |
| 1:B:858:VAL:HG22 | 1:B:975:THR:HG23 | 2.03                     | 0.41              |
| 1:B:924:MET:H    | 1:B:924:MET:HG2  | 1.68                     | 0.41              |
| 1:B:935:THR:HG23 | 1:B:937:PRO:HD3  | 2.02                     | 0.41              |
| 1:C:617:ARG:HA   | 1:C:617:ARG:HD2  | 1.74                     | 0.41              |
| 1:C:655:TYR:HA   | 1:C:656:PRO:HD3  | 1.71                     | 0.41              |
| 1:D:465:ILE:HA   | 1:D:841:TYR:HB3  | 2.03                     | 0.41              |
| 1:D:517:HIS:O    | 1:D:520:LEU:HB2  | 2.20                     | 0.41              |
| 1:D:670:ASP:OD2  | 1:D:692:THR:HA   | 2.20                     | 0.41              |
| 1:D:689:MET:HE3  | 1:D:689:MET:HB3  | 1.95                     | 0.41              |
| 1:D:804:ASN:C    | 1:D:804:ASN:OD1  | 2.62                     | 0.41              |
| 1:D:815:ARG:HG3  | 1:D:815:ARG:HH11 | 1.86                     | 0.41              |
| 1:D:1022:LYS:O   | 1:D:1023:PRO:C   | 2.64                     | 0.41              |
| 1:B:335:GLU:O    | 1:B:336:ALA:C    | 2.63                     | 0.41              |
| 1:C:483:VAL:O    | 1:C:484:ALA:C    | 2.63                     | 0.41              |
| 1:D:881:GLN:NE2  | 1:D:887:GLN:HA   | 2.35                     | 0.41              |
| 1:A:522:LEU:O    | 1:A:523:ASP:C    | 2.63                     | 0.40              |
| 1:A:695:ILE:HG13 | 1:A:696:GLY:H    | 1.85                     | 0.40              |
| 1:C:328:ARG:NH2  | 1:C:360:VAL:HG13 | 2.36                     | 0.40              |
| 1:C:435:ILE:O    | 1:C:436:PRO:C    | 2.61                     | 0.40              |
| 1:C:488:GLU:C    | 1:C:490:ASN:H    | 2.28                     | 0.40              |
| 1:A:662:LEU:H    | 1:A:662:LEU:CD1  | 2.22                     | 0.40              |
| 1:A:941:LEU:C    | 1:A:941:LEU:CD2  | 2.94                     | 0.40              |
| 1:B:430:LYS:HE2  | 1:B:462:CYS:SG   | 2.61                     | 0.40              |
| 1:B:603:ILE:HG12 | 1:B:617:ARG:NH2  | 2.37                     | 0.40              |
| 1:C:405:LEU:HA   | 1:C:405:LEU:HD12 | 1.72                     | 0.40              |
| 1:C:415:ASN:OD1  | 1:C:415:ASN:C    | 2.64                     | 0.40              |
| 1:C:738:LEU:HA   | 1:C:738:LEU:HD23 | 1.81                     | 0.40              |
| 1:C:850:MET:HE2  | 1:C:963:ARG:NE   | 2.35                     | 0.40              |
| 1:D:937:PRO:HB2  | 1:D:944:ARG:NH1  | 2.35                     | 0.40              |
| 1:A:697:ASP:OD2  | 1:A:700:ASN:HB3  | 2.21                     | 0.40              |
| 1:A:866:LEU:HA   | 1:A:866:LEU:HD23 | 1.69                     | 0.40              |
| 1:B:559:PRO:HA   | 1:B:562:HIS:ND1  | 2.36                     | 0.40              |
| 1:C:950:LEU:HD23 | 1:C:950:LEU:HA   | 1.94                     | 0.40              |
| 1:D:449:LYS:HA   | 1:D:450:PRO:HD3  | 1.85                     | 0.40              |
| 1:D:828:PRO:HG2  | 1:D:831:ALA:HB3  | 2.03                     | 0.40              |
| 2:L:8:SER:O      | 2:L:9:ALA:O      | 2.40                     | 0.40              |
| 1:A:323:LEU:O    | 1:A:326:ILE:HB   | 2.21                     | 0.40              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:742:LYS:HE3  | 1:A:768:PRO:HB3  | 2.02                     | 0.40              |
| 1:A:764:MET:HA   | 1:A:765:PRO:HD2  | 1.77                     | 0.40              |
| 1:B:652:TRP:O    | 1:B:654:GLY:N    | 2.47                     | 0.40              |
| 1:B:701:MET:HE2  | 1:B:701:MET:HB3  | 1.95                     | 0.40              |
| 1:C:312:SER:O    | 1:C:314:PRO:HD3  | 2.20                     | 0.40              |
| 1:C:510:ARG:HG3  | 1:C:510:ARG:HH11 | 1.86                     | 0.40              |
| 1:C:785:ILE:CG2  | 1:C:786:GLN:HG2  | 2.51                     | 0.40              |
| 1:D:435:ILE:N    | 1:D:436:PRO:CD   | 2.83                     | 0.40              |
| 1:D:607:GLN:OE1  | 1:D:607:GLN:CA   | 2.68                     | 0.40              |
| 1:B:491:ARG:HD2  | 1:B:491:ARG:HA   | 1.69                     | 0.40              |
| 1:B:644:ARG:HA   | 1:B:649:GLN:OE1  | 2.22                     | 0.40              |
| 1:B:846:SER:O    | 1:B:849:GLN:HB3  | 2.22                     | 0.40              |
| 1:C:463:LEU:HD23 | 1:C:463:LEU:HA   | 1.83                     | 0.40              |
| 1:C:772:ILE:HD12 | 1:C:772:ILE:H    | 1.87                     | 0.40              |
| 1:C:796:ASN:O    | 1:C:798:LEU:N    | 2.54                     | 0.40              |
| 1:D:983:VAL:O    | 1:D:986:LYS:HB3  | 2.21                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|---------|----------|-------------|----|
| 1   | A     | 692/723 (96%) | 622 (90%) | 63 (9%) | 7 (1%)   | 12          | 41 |
| 1   | B     | 692/723 (96%) | 623 (90%) | 59 (8%) | 10 (1%)  | 9           | 34 |
| 1   | C     | 692/723 (96%) | 618 (89%) | 65 (9%) | 9 (1%)   | 9           | 36 |
| 1   | D     | 692/723 (96%) | 624 (90%) | 58 (8%) | 10 (1%)  | 9           | 34 |
| 2   | I     | 9/11 (82%)    | 6 (67%)   | 0       | 3 (33%)  | 0           | 0  |
| 2   | J     | 9/11 (82%)    | 6 (67%)   | 0       | 3 (33%)  | 0           | 0  |
| 2   | K     | 9/11 (82%)    | 6 (67%)   | 0       | 3 (33%)  | 0           | 0  |

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| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 2   | L     | 9/11 (82%)      | 6 (67%)    | 0        | 3 (33%)  | 0           | 0  |
| All | All   | 2804/2936 (96%) | 2511 (90%) | 245 (9%) | 48 (2%)  | 7           | 30 |

All (48) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | I     | 2   | VAL  |
| 2   | I     | 9   | ALA  |
| 2   | J     | 2   | VAL  |
| 2   | J     | 9   | ALA  |
| 2   | K     | 2   | VAL  |
| 2   | K     | 9   | ALA  |
| 2   | L     | 2   | VAL  |
| 2   | L     | 9   | ALA  |
| 1   | A     | 331 | GLY  |
| 1   | A     | 334 | GLU  |
| 1   | B     | 331 | GLY  |
| 1   | B     | 334 | GLU  |
| 1   | B     | 763 | ASN  |
| 1   | B     | 797 | GLY  |
| 1   | C     | 331 | GLY  |
| 1   | C     | 334 | GLU  |
| 1   | C     | 620 | GLN  |
| 1   | C     | 770 | ASN  |
| 1   | D     | 331 | GLY  |
| 1   | D     | 334 | GLU  |
| 1   | D     | 402 | GLN  |
| 1   | A     | 620 | GLN  |
| 1   | A     | 763 | ASN  |
| 1   | A     | 888 | ASN  |
| 1   | C     | 763 | ASN  |
| 1   | D     | 620 | GLN  |
| 1   | D     | 733 | ALA  |
| 1   | D     | 763 | ASN  |
| 2   | I     | 10  | GLN  |
| 2   | J     | 10  | GLN  |
| 2   | K     | 10  | GLN  |
| 2   | L     | 10  | GLN  |
| 1   | A     | 733 | ALA  |
| 1   | A     | 770 | ASN  |
| 1   | B     | 330 | GLN  |
| 1   | B     | 620 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 733 | ALA  |
| 1   | D     | 732 | LYS  |
| 1   | D     | 878 | GLN  |
| 1   | B     | 888 | ASN  |
| 1   | C     | 402 | GLN  |
| 1   | B     | 878 | GLN  |
| 1   | C     | 639 | GLU  |
| 1   | B     | 504 | PRO  |
| 1   | C     | 504 | PRO  |
| 1   | C     | 656 | PRO  |
| 1   | D     | 772 | ILE  |
| 1   | D     | 504 | PRO  |

### 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     | 600/618 (97%)   | 530 (88%)  | 70 (12%)  | 5           | 20 |
| 1   | B     | 600/618 (97%)   | 534 (89%)  | 66 (11%)  | 6           | 23 |
| 1   | C     | 600/618 (97%)   | 533 (89%)  | 67 (11%)  | 6           | 22 |
| 1   | D     | 600/618 (97%)   | 535 (89%)  | 65 (11%)  | 6           | 23 |
| 2   | I     | 10/10 (100%)    | 7 (70%)    | 3 (30%)   | 0           | 1  |
| 2   | J     | 10/10 (100%)    | 7 (70%)    | 3 (30%)   | 0           | 1  |
| 2   | K     | 10/10 (100%)    | 6 (60%)    | 4 (40%)   | 0           | 0  |
| 2   | L     | 10/10 (100%)    | 7 (70%)    | 3 (30%)   | 0           | 1  |
| All | All   | 2440/2512 (97%) | 2159 (88%) | 281 (12%) | 5           | 21 |

All (281) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 312 | SER  |
| 1   | A     | 315 | THR  |
| 1   | A     | 319 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 330 | GLN  |
| 1   | A     | 346 | VAL  |
| 1   | A     | 360 | VAL  |
| 1   | A     | 367 | LEU  |
| 1   | A     | 371 | LEU  |
| 1   | A     | 372 | MET  |
| 1   | A     | 378 | ILE  |
| 1   | A     | 383 | THR  |
| 1   | A     | 401 | VAL  |
| 1   | A     | 406 | GLN  |
| 1   | A     | 409 | THR  |
| 1   | A     | 410 | ARG  |
| 1   | A     | 412 | ILE  |
| 1   | A     | 434 | ASN  |
| 1   | A     | 437 | GLU  |
| 1   | A     | 439 | ILE  |
| 1   | A     | 441 | SER  |
| 1   | A     | 443 | ARG  |
| 1   | A     | 447 | LYS  |
| 1   | A     | 481 | SER  |
| 1   | A     | 488 | GLU  |
| 1   | A     | 491 | ARG  |
| 1   | A     | 494 | SER  |
| 1   | A     | 501 | MET  |
| 1   | A     | 515 | GLU  |
| 1   | A     | 537 | LYS  |
| 1   | A     | 541 | LEU  |
| 1   | A     | 630 | ASN  |
| 1   | A     | 634 | LYS  |
| 1   | A     | 644 | ARG  |
| 1   | A     | 662 | LEU  |
| 1   | A     | 667 | ILE  |
| 1   | A     | 669 | THR  |
| 1   | A     | 671 | GLN  |
| 1   | A     | 697 | ASP  |
| 1   | A     | 710 | VAL  |
| 1   | A     | 713 | PHE  |
| 1   | A     | 714 | LYS  |
| 1   | A     | 719 | ILE  |
| 1   | A     | 727 | ASN  |
| 1   | A     | 732 | LYS  |
| 1   | A     | 742 | LYS  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 743  | ILE  |
| 1   | A     | 770  | ASN  |
| 1   | A     | 771  | THR  |
| 1   | A     | 778  | GLU  |
| 1   | A     | 793  | SER  |
| 1   | A     | 800  | THR  |
| 1   | A     | 805  | ASN  |
| 1   | A     | 820  | THR  |
| 1   | A     | 829  | GLU  |
| 1   | A     | 832  | ILE  |
| 1   | A     | 846  | SER  |
| 1   | A     | 862  | VAL  |
| 1   | A     | 871  | VAL  |
| 1   | A     | 914  | THR  |
| 1   | A     | 918  | ASN  |
| 1   | A     | 926  | VAL  |
| 1   | A     | 936  | MET  |
| 1   | A     | 978  | GLU  |
| 1   | A     | 981  | LYS  |
| 1   | A     | 990  | GLN  |
| 1   | A     | 991  | ARG  |
| 1   | A     | 1015 | GLU  |
| 1   | A     | 1022 | LYS  |
| 1   | A     | 1027 | ILE  |
| 1   | A     | 1028 | LYS  |
| 1   | B     | 315  | THR  |
| 1   | B     | 319  | SER  |
| 1   | B     | 330  | GLN  |
| 1   | B     | 338  | ARG  |
| 1   | B     | 346  | VAL  |
| 1   | B     | 360  | VAL  |
| 1   | B     | 367  | LEU  |
| 1   | B     | 371  | LEU  |
| 1   | B     | 372  | MET  |
| 1   | B     | 378  | ILE  |
| 1   | B     | 383  | THR  |
| 1   | B     | 401  | VAL  |
| 1   | B     | 406  | GLN  |
| 1   | B     | 410  | ARG  |
| 1   | B     | 412  | ILE  |
| 1   | B     | 434  | ASN  |
| 1   | B     | 437  | GLU  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 439 | ILE  |
| 1   | B     | 441 | SER  |
| 1   | B     | 443 | ARG  |
| 1   | B     | 447 | LYS  |
| 1   | B     | 481 | SER  |
| 1   | B     | 488 | GLU  |
| 1   | B     | 491 | ARG  |
| 1   | B     | 492 | LEU  |
| 1   | B     | 494 | SER  |
| 1   | B     | 501 | MET  |
| 1   | B     | 515 | GLU  |
| 1   | B     | 537 | LYS  |
| 1   | B     | 541 | LEU  |
| 1   | B     | 545 | ARG  |
| 1   | B     | 630 | ASN  |
| 1   | B     | 634 | LYS  |
| 1   | B     | 644 | ARG  |
| 1   | B     | 662 | LEU  |
| 1   | B     | 667 | ILE  |
| 1   | B     | 671 | GLN  |
| 1   | B     | 710 | VAL  |
| 1   | B     | 713 | PHE  |
| 1   | B     | 714 | LYS  |
| 1   | B     | 719 | ILE  |
| 1   | B     | 727 | ASN  |
| 1   | B     | 732 | LYS  |
| 1   | B     | 742 | LYS  |
| 1   | B     | 743 | ILE  |
| 1   | B     | 764 | MET  |
| 1   | B     | 770 | ASN  |
| 1   | B     | 771 | THR  |
| 1   | B     | 774 | GLU  |
| 1   | B     | 778 | GLU  |
| 1   | B     | 793 | SER  |
| 1   | B     | 800 | THR  |
| 1   | B     | 805 | ASN  |
| 1   | B     | 820 | THR  |
| 1   | B     | 832 | ILE  |
| 1   | B     | 846 | SER  |
| 1   | B     | 871 | VAL  |
| 1   | B     | 914 | THR  |
| 1   | B     | 936 | MET  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 978  | GLU  |
| 1   | B     | 981  | LYS  |
| 1   | B     | 991  | ARG  |
| 1   | B     | 1015 | GLU  |
| 1   | B     | 1022 | LYS  |
| 1   | B     | 1027 | ILE  |
| 1   | B     | 1028 | LYS  |
| 1   | C     | 315  | THR  |
| 1   | C     | 319  | SER  |
| 1   | C     | 330  | GLN  |
| 1   | C     | 346  | VAL  |
| 1   | C     | 360  | VAL  |
| 1   | C     | 367  | LEU  |
| 1   | C     | 371  | LEU  |
| 1   | C     | 378  | ILE  |
| 1   | C     | 383  | THR  |
| 1   | C     | 401  | VAL  |
| 1   | C     | 406  | GLN  |
| 1   | C     | 410  | ARG  |
| 1   | C     | 412  | ILE  |
| 1   | C     | 434  | ASN  |
| 1   | C     | 437  | GLU  |
| 1   | C     | 439  | ILE  |
| 1   | C     | 441  | SER  |
| 1   | C     | 443  | ARG  |
| 1   | C     | 447  | LYS  |
| 1   | C     | 481  | SER  |
| 1   | C     | 488  | GLU  |
| 1   | C     | 491  | ARG  |
| 1   | C     | 494  | SER  |
| 1   | C     | 501  | MET  |
| 1   | C     | 515  | GLU  |
| 1   | C     | 527  | VAL  |
| 1   | C     | 537  | LYS  |
| 1   | C     | 541  | LEU  |
| 1   | C     | 545  | ARG  |
| 1   | C     | 617  | ARG  |
| 1   | C     | 630  | ASN  |
| 1   | C     | 634  | LYS  |
| 1   | C     | 644  | ARG  |
| 1   | C     | 662  | LEU  |
| 1   | C     | 667  | ILE  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | C     | 669  | THR  |
| 1   | C     | 671  | GLN  |
| 1   | C     | 694  | PHE  |
| 1   | C     | 697  | ASP  |
| 1   | C     | 713  | PHE  |
| 1   | C     | 714  | LYS  |
| 1   | C     | 719  | ILE  |
| 1   | C     | 732  | LYS  |
| 1   | C     | 742  | LYS  |
| 1   | C     | 743  | ILE  |
| 1   | C     | 764  | MET  |
| 1   | C     | 770  | ASN  |
| 1   | C     | 771  | THR  |
| 1   | C     | 774  | GLU  |
| 1   | C     | 800  | THR  |
| 1   | C     | 805  | ASN  |
| 1   | C     | 820  | THR  |
| 1   | C     | 832  | ILE  |
| 1   | C     | 846  | SER  |
| 1   | C     | 871  | VAL  |
| 1   | C     | 881  | GLN  |
| 1   | C     | 914  | THR  |
| 1   | C     | 926  | VAL  |
| 1   | C     | 936  | MET  |
| 1   | C     | 978  | GLU  |
| 1   | C     | 981  | LYS  |
| 1   | C     | 990  | GLN  |
| 1   | C     | 991  | ARG  |
| 1   | C     | 1015 | GLU  |
| 1   | C     | 1022 | LYS  |
| 1   | C     | 1027 | ILE  |
| 1   | C     | 1028 | LYS  |
| 1   | D     | 315  | THR  |
| 1   | D     | 319  | SER  |
| 1   | D     | 330  | GLN  |
| 1   | D     | 338  | ARG  |
| 1   | D     | 346  | VAL  |
| 1   | D     | 360  | VAL  |
| 1   | D     | 367  | LEU  |
| 1   | D     | 371  | LEU  |
| 1   | D     | 372  | MET  |
| 1   | D     | 378  | ILE  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 383 | THR  |
| 1   | D     | 401 | VAL  |
| 1   | D     | 406 | GLN  |
| 1   | D     | 410 | ARG  |
| 1   | D     | 412 | ILE  |
| 1   | D     | 434 | ASN  |
| 1   | D     | 437 | GLU  |
| 1   | D     | 439 | ILE  |
| 1   | D     | 441 | SER  |
| 1   | D     | 443 | ARG  |
| 1   | D     | 447 | LYS  |
| 1   | D     | 481 | SER  |
| 1   | D     | 488 | GLU  |
| 1   | D     | 491 | ARG  |
| 1   | D     | 494 | SER  |
| 1   | D     | 501 | MET  |
| 1   | D     | 515 | GLU  |
| 1   | D     | 528 | LEU  |
| 1   | D     | 537 | LYS  |
| 1   | D     | 541 | LEU  |
| 1   | D     | 545 | ARG  |
| 1   | D     | 630 | ASN  |
| 1   | D     | 634 | LYS  |
| 1   | D     | 644 | ARG  |
| 1   | D     | 662 | LEU  |
| 1   | D     | 667 | ILE  |
| 1   | D     | 671 | GLN  |
| 1   | D     | 697 | ASP  |
| 1   | D     | 713 | PHE  |
| 1   | D     | 714 | LYS  |
| 1   | D     | 719 | ILE  |
| 1   | D     | 727 | ASN  |
| 1   | D     | 732 | LYS  |
| 1   | D     | 742 | LYS  |
| 1   | D     | 743 | ILE  |
| 1   | D     | 764 | MET  |
| 1   | D     | 770 | ASN  |
| 1   | D     | 771 | THR  |
| 1   | D     | 778 | GLU  |
| 1   | D     | 800 | THR  |
| 1   | D     | 805 | ASN  |
| 1   | D     | 820 | THR  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | D     | 832  | ILE  |
| 1   | D     | 846  | SER  |
| 1   | D     | 871  | VAL  |
| 1   | D     | 914  | THR  |
| 1   | D     | 926  | VAL  |
| 1   | D     | 936  | MET  |
| 1   | D     | 977  | LEU  |
| 1   | D     | 978  | GLU  |
| 1   | D     | 981  | LYS  |
| 1   | D     | 991  | ARG  |
| 1   | D     | 1015 | GLU  |
| 1   | D     | 1022 | LYS  |
| 1   | D     | 1027 | ILE  |
| 2   | I     | 2    | VAL  |
| 2   | I     | 4    | VAL  |
| 2   | I     | 11   | SER  |
| 2   | J     | 2    | VAL  |
| 2   | J     | 4    | VAL  |
| 2   | J     | 11   | SER  |
| 2   | K     | 2    | VAL  |
| 2   | K     | 4    | VAL  |
| 2   | K     | 5    | PRO  |
| 2   | K     | 11   | SER  |
| 2   | L     | 2    | VAL  |
| 2   | L     | 4    | VAL  |
| 2   | L     | 11   | SER  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 322  | ASN  |
| 1   | A     | 325  | ASN  |
| 1   | A     | 332  | ASN  |
| 1   | A     | 406  | GLN  |
| 1   | A     | 691  | HIS  |
| 1   | A     | 805  | ASN  |
| 1   | A     | 878  | GLN  |
| 1   | A     | 901  | HIS  |
| 1   | A     | 990  | GLN  |
| 1   | A     | 1025 | HIS  |
| 1   | B     | 321  | ASN  |
| 1   | B     | 322  | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | B     | 325  | ASN  |
| 1   | B     | 406  | GLN  |
| 1   | B     | 424  | ASN  |
| 1   | B     | 681  | GLN  |
| 1   | B     | 805  | ASN  |
| 1   | B     | 878  | GLN  |
| 1   | B     | 901  | HIS  |
| 1   | B     | 990  | GLN  |
| 1   | C     | 321  | ASN  |
| 1   | C     | 322  | ASN  |
| 1   | C     | 325  | ASN  |
| 1   | C     | 406  | GLN  |
| 1   | C     | 498  | HIS  |
| 1   | C     | 517  | HIS  |
| 1   | C     | 691  | HIS  |
| 1   | C     | 784  | GLN  |
| 1   | C     | 805  | ASN  |
| 1   | C     | 878  | GLN  |
| 1   | C     | 990  | GLN  |
| 1   | C     | 1025 | HIS  |
| 1   | D     | 321  | ASN  |
| 1   | D     | 322  | ASN  |
| 1   | D     | 325  | ASN  |
| 1   | D     | 362  | GLN  |
| 1   | D     | 406  | GLN  |
| 1   | D     | 590  | ASN  |
| 1   | D     | 784  | GLN  |
| 1   | D     | 805  | ASN  |
| 1   | D     | 878  | GLN  |
| 1   | D     | 990  | GLN  |
| 1   | D     | 1025 | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | I     | 1202 | 2    | 14,14,15     | 1.77 | 4 (28%)  | 17,19,21    | 2.56 | 5 (29%)  |
| 4   | NAG  | K     | 1202 | 2    | 14,14,15     | 1.69 | 4 (28%)  | 17,19,21    | 2.32 | 6 (35%)  |
| 4   | NAG  | J     | 1202 | 2    | 14,14,15     | 1.72 | 4 (28%)  | 17,19,21    | 2.55 | 5 (29%)  |
| 3   | UDP  | D     | 1201 | -    | 25,26,26     | 1.32 | 4 (16%)  | 38,40,40    | 1.53 | 7 (18%)  |
| 3   | UDP  | C     | 1201 | -    | 25,26,26     | 1.52 | 5 (20%)  | 38,40,40    | 1.41 | 5 (13%)  |
| 3   | UDP  | A     | 1201 | -    | 25,26,26     | 1.55 | 6 (24%)  | 38,40,40    | 1.74 | 10 (26%) |
| 3   | UDP  | B     | 1201 | -    | 25,26,26     | 1.30 | 4 (16%)  | 38,40,40    | 1.82 | 10 (26%) |
| 4   | NAG  | L     | 1202 | 2    | 14,14,15     | 1.57 | 4 (28%)  | 17,19,21    | 2.21 | 5 (29%)  |

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

| Mol | Type | Chain | Res  | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|------|------|---------|------------|---------|
| 4   | NAG  | I     | 1202 | 2    | -       | 1/6/23/26  | 0/1/1/1 |
| 4   | NAG  | K     | 1202 | 2    | -       | 2/6/23/26  | 0/1/1/1 |
| 4   | NAG  | J     | 1202 | 2    | -       | 1/6/23/26  | 0/1/1/1 |
| 3   | UDP  | D     | 1201 | -    | -       | 3/16/32/32 | 0/2/2/2 |
| 3   | UDP  | C     | 1201 | -    | -       | 4/16/32/32 | 0/2/2/2 |
| 3   | UDP  | A     | 1201 | -    | -       | 2/16/32/32 | 0/2/2/2 |
| 3   | UDP  | B     | 1201 | -    | -       | 3/16/32/32 | 0/2/2/2 |
| 4   | NAG  | L     | 1202 | 2    | -       | 1/6/23/26  | 0/1/1/1 |



All (35) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 4   | I     | 1202 | NAG  | O3-C3  | 4.52  | 1.54        | 1.43     |
| 4   | K     | 1202 | NAG  | O3-C3  | 4.11  | 1.53        | 1.43     |
| 4   | J     | 1202 | NAG  | O5-C1  | -3.73 | 1.37        | 1.43     |
| 3   | C     | 1201 | UDP  | O2-C2  | 3.58  | 1.29        | 1.23     |
| 4   | L     | 1202 | NAG  | O3-C3  | 3.58  | 1.51        | 1.43     |
| 3   | D     | 1201 | UDP  | C2-N1  | 3.43  | 1.43        | 1.38     |
| 3   | A     | 1201 | UDP  | PA-O3A | 3.28  | 1.63        | 1.59     |
| 3   | D     | 1201 | UDP  | O2-C2  | 3.15  | 1.28        | 1.23     |
| 4   | J     | 1202 | NAG  | O3-C3  | 3.14  | 1.50        | 1.43     |
| 3   | C     | 1201 | UDP  | C2-N1  | 3.12  | 1.43        | 1.38     |
| 3   | A     | 1201 | UDP  | C2-N1  | 2.97  | 1.43        | 1.38     |
| 3   | B     | 1201 | UDP  | C2-N1  | 2.86  | 1.42        | 1.38     |
| 3   | C     | 1201 | UDP  | C4-N3  | -2.86 | 1.33        | 1.38     |
| 3   | C     | 1201 | UDP  | C5-C4  | -2.83 | 1.37        | 1.43     |
| 3   | A     | 1201 | UDP  | O2-C2  | 2.60  | 1.27        | 1.23     |
| 3   | A     | 1201 | UDP  | C4-N3  | -2.59 | 1.34        | 1.38     |
| 3   | B     | 1201 | UDP  | C6-C5  | 2.57  | 1.41        | 1.35     |
| 4   | K     | 1202 | NAG  | C3-C2  | 2.55  | 1.57        | 1.52     |
| 3   | A     | 1201 | UDP  | C2-N3  | -2.45 | 1.33        | 1.38     |
| 4   | J     | 1202 | NAG  | C8-C7  | 2.42  | 1.55        | 1.50     |
| 4   | L     | 1202 | NAG  | O5-C1  | -2.34 | 1.39        | 1.43     |
| 3   | B     | 1201 | UDP  | C4-N3  | -2.32 | 1.34        | 1.38     |
| 4   | I     | 1202 | NAG  | C3-C2  | 2.30  | 1.57        | 1.52     |
| 4   | J     | 1202 | NAG  | C1-C2  | 2.29  | 1.55        | 1.52     |
| 4   | K     | 1202 | NAG  | C4-C5  | -2.27 | 1.48        | 1.53     |
| 3   | A     | 1201 | UDP  | C5-C4  | -2.25 | 1.38        | 1.43     |
| 3   | B     | 1201 | UDP  | O2-C2  | 2.23  | 1.27        | 1.23     |
| 3   | D     | 1201 | UDP  | C6-C5  | 2.21  | 1.40        | 1.35     |
| 4   | I     | 1202 | NAG  | O5-C1  | -2.20 | 1.40        | 1.43     |
| 4   | L     | 1202 | NAG  | C3-C2  | 2.16  | 1.57        | 1.52     |
| 4   | K     | 1202 | NAG  | O5-C1  | -2.14 | 1.40        | 1.43     |
| 4   | L     | 1202 | NAG  | C8-C7  | 2.11  | 1.54        | 1.50     |
| 3   | D     | 1201 | UDP  | C4-N3  | -2.10 | 1.35        | 1.38     |
| 4   | I     | 1202 | NAG  | C1-C2  | 2.07  | 1.55        | 1.52     |
| 3   | C     | 1201 | UDP  | C6-C5  | 2.06  | 1.39        | 1.35     |

All (53) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 4   | I     | 1202 | NAG  | C1-O5-C5 | 7.00 | 121.57      | 112.19   |
| 4   | K     | 1202 | NAG  | C1-O5-C5 | 6.92 | 121.46      | 112.19   |
| 4   | J     | 1202 | NAG  | C1-O5-C5 | 6.30 | 120.63      | 112.19   |

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| Mol | Chain | Res  | Type | Atoms      | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|------------|-------|-------------|----------|
| 4   | L     | 1202 | NAG  | C1-O5-C5   | 6.23  | 120.53      | 112.19   |
| 4   | J     | 1202 | NAG  | O5-C5-C6   | -5.49 | 96.98       | 107.66   |
| 3   | A     | 1201 | UDP  | C5-C4-N3   | 4.71  | 121.40      | 114.80   |
| 4   | I     | 1202 | NAG  | O5-C5-C6   | -4.64 | 98.63       | 107.66   |
| 3   | A     | 1201 | UDP  | C4-N3-C2   | -3.95 | 121.71      | 126.61   |
| 4   | L     | 1202 | NAG  | O5-C5-C6   | -3.92 | 100.04      | 107.66   |
| 3   | B     | 1201 | UDP  | O2A-PA-O1A | 3.77  | 129.98      | 112.44   |
| 4   | J     | 1202 | NAG  | C2-N2-C7   | -3.72 | 117.92      | 122.90   |
| 3   | B     | 1201 | UDP  | O2B-PB-O3A | -3.68 | 92.29       | 104.64   |
| 3   | B     | 1201 | UDP  | C4-N3-C2   | -3.57 | 122.18      | 126.61   |
| 3   | D     | 1201 | UDP  | C4-N3-C2   | -3.55 | 122.20      | 126.61   |
| 3   | D     | 1201 | UDP  | C5-C4-N3   | 3.55  | 119.77      | 114.80   |
| 3   | B     | 1201 | UDP  | C5-C4-N3   | 3.40  | 119.56      | 114.80   |
| 4   | I     | 1202 | NAG  | O3-C3-C2   | 3.36  | 116.37      | 109.40   |
| 3   | B     | 1201 | UDP  | N3-C2-N1   | 3.32  | 119.22      | 114.89   |
| 3   | B     | 1201 | UDP  | O4-C4-C5   | -3.26 | 119.54      | 125.16   |
| 3   | A     | 1201 | UDP  | O4-C4-C5   | -3.22 | 119.61      | 125.16   |
| 3   | D     | 1201 | UDP  | O2B-PB-O3A | -3.18 | 93.97       | 104.64   |
| 3   | A     | 1201 | UDP  | O2B-PB-O3A | -3.16 | 94.03       | 104.64   |
| 3   | C     | 1201 | UDP  | C5-C4-N3   | 3.13  | 119.18      | 114.80   |
| 3   | A     | 1201 | UDP  | C2'-C1'-N1 | 3.07  | 121.80      | 113.25   |
| 3   | C     | 1201 | UDP  | O2A-PA-O1A | 2.88  | 125.84      | 112.44   |
| 3   | D     | 1201 | UDP  | O2A-PA-O1A | 2.88  | 125.83      | 112.44   |
| 4   | I     | 1202 | NAG  | C2-N2-C7   | -2.75 | 119.22      | 122.90   |
| 3   | C     | 1201 | UDP  | O4-C4-C5   | -2.71 | 120.49      | 125.16   |
| 4   | K     | 1202 | NAG  | O5-C5-C6   | -2.69 | 102.42      | 107.66   |
| 3   | A     | 1201 | UDP  | O3B-PB-O2B | 2.68  | 117.87      | 107.80   |
| 4   | K     | 1202 | NAG  | C2-N2-C7   | -2.64 | 119.36      | 122.90   |
| 3   | B     | 1201 | UDP  | O3B-PB-O1B | 2.63  | 121.10      | 110.83   |
| 3   | D     | 1201 | UDP  | N3-C2-N1   | 2.55  | 118.21      | 114.89   |
| 4   | L     | 1202 | NAG  | O3-C3-C2   | 2.53  | 114.67      | 109.40   |
| 3   | C     | 1201 | UDP  | C2'-C1'-N1 | 2.49  | 120.19      | 113.25   |
| 4   | L     | 1202 | NAG  | C2-N2-C7   | -2.47 | 119.59      | 122.90   |
| 4   | I     | 1202 | NAG  | C6-C5-C4   | -2.44 | 107.03      | 113.02   |
| 4   | J     | 1202 | NAG  | O3-C3-C2   | 2.42  | 114.42      | 109.40   |
| 3   | B     | 1201 | UDP  | O2B-PB-O1B | 2.39  | 120.14      | 110.83   |
| 3   | A     | 1201 | UDP  | N3-C2-N1   | 2.34  | 117.94      | 114.89   |
| 4   | K     | 1202 | NAG  | O3-C3-C2   | 2.33  | 114.25      | 109.40   |
| 3   | C     | 1201 | UDP  | C4-N3-C2   | -2.32 | 123.73      | 126.61   |
| 4   | K     | 1202 | NAG  | O5-C1-C2   | -2.27 | 107.78      | 111.29   |
| 4   | L     | 1202 | NAG  | C1-C2-N2   | -2.27 | 106.86      | 110.43   |
| 3   | A     | 1201 | UDP  | O2A-PA-O1A | 2.26  | 122.95      | 112.44   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res  | Type | Atoms       | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-------------|-------|-------------|----------|
| 4   | K     | 1202 | NAG  | O5-C5-C4    | -2.23 | 105.40      | 110.83   |
| 3   | D     | 1201 | UDP  | O2B-PB-O1B  | 2.15  | 119.22      | 110.83   |
| 3   | B     | 1201 | UDP  | C2'-C1'-N1  | 2.11  | 119.13      | 113.25   |
| 3   | A     | 1201 | UDP  | C3'-C2'-C1' | -2.07 | 97.55       | 101.46   |
| 3   | A     | 1201 | UDP  | O3B-PB-O1B  | 2.06  | 118.86      | 110.83   |
| 3   | B     | 1201 | UDP  | O4'-C1'-C2' | -2.06 | 102.22      | 106.62   |
| 3   | D     | 1201 | UDP  | C5-C6-N1    | -2.04 | 118.53      | 121.84   |
| 4   | J     | 1202 | NAG  | O3-C3-C4    | -2.01 | 105.63      | 110.38   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms           |
|-----|-------|------|------|-----------------|
| 3   | A     | 1201 | UDP  | O4'-C4'-C5'-O5' |
| 3   | B     | 1201 | UDP  | O4'-C4'-C5'-O5' |
| 3   | C     | 1201 | UDP  | O4'-C4'-C5'-O5' |
| 3   | C     | 1201 | UDP  | PA-O3A-PB-O2B   |
| 3   | C     | 1201 | UDP  | PA-O3A-PB-O3B   |
| 3   | D     | 1201 | UDP  | O4'-C4'-C5'-O5' |
| 3   | D     | 1201 | UDP  | PA-O3A-PB-O2B   |
| 3   | A     | 1201 | UDP  | C3'-C4'-C5'-O5' |
| 3   | B     | 1201 | UDP  | C3'-C4'-C5'-O5' |
| 3   | C     | 1201 | UDP  | C3'-C4'-C5'-O5' |
| 3   | D     | 1201 | UDP  | C3'-C4'-C5'-O5' |
| 4   | K     | 1202 | NAG  | O5-C5-C6-O6     |
| 3   | B     | 1201 | UDP  | PA-O3A-PB-O2B   |
| 4   | J     | 1202 | NAG  | O5-C5-C6-O6     |
| 4   | L     | 1202 | NAG  | O5-C5-C6-O6     |
| 4   | I     | 1202 | NAG  | O5-C5-C6-O6     |
| 4   | K     | 1202 | NAG  | C4-C5-C6-O6     |

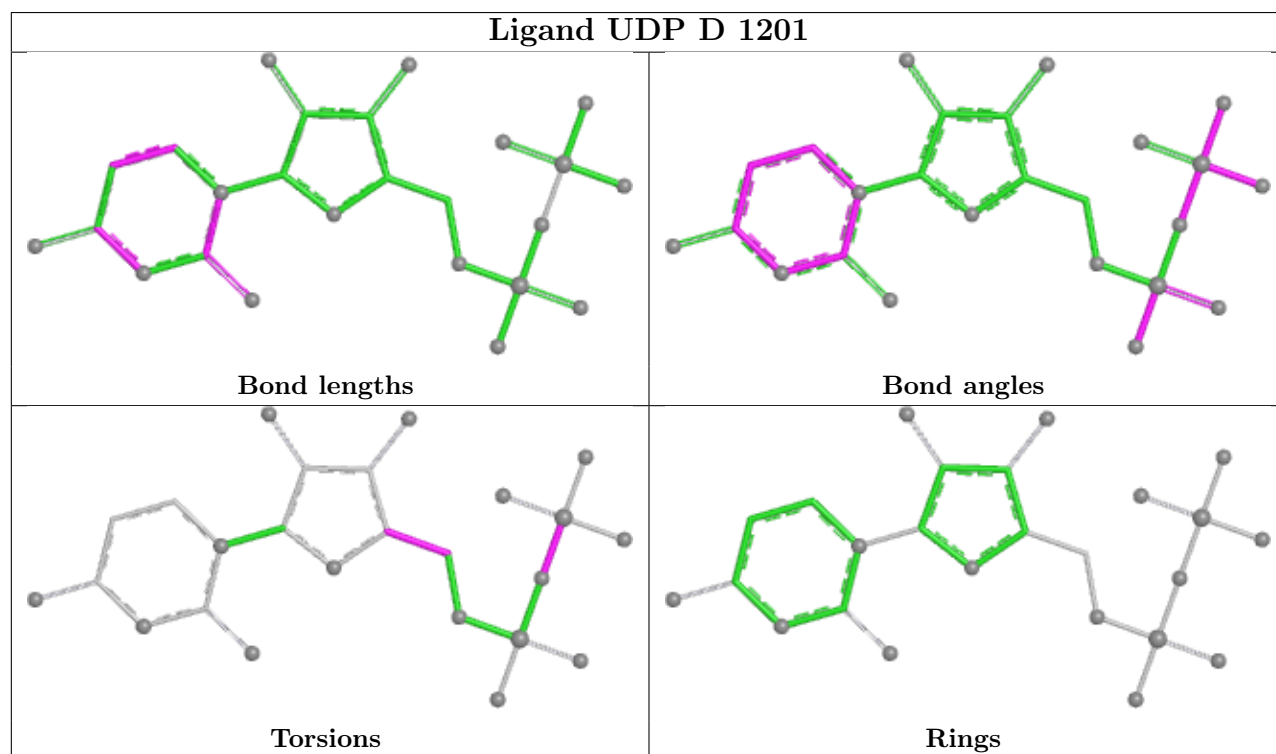
There are no ring outliers.

4 monomers are involved in 9 short contacts:

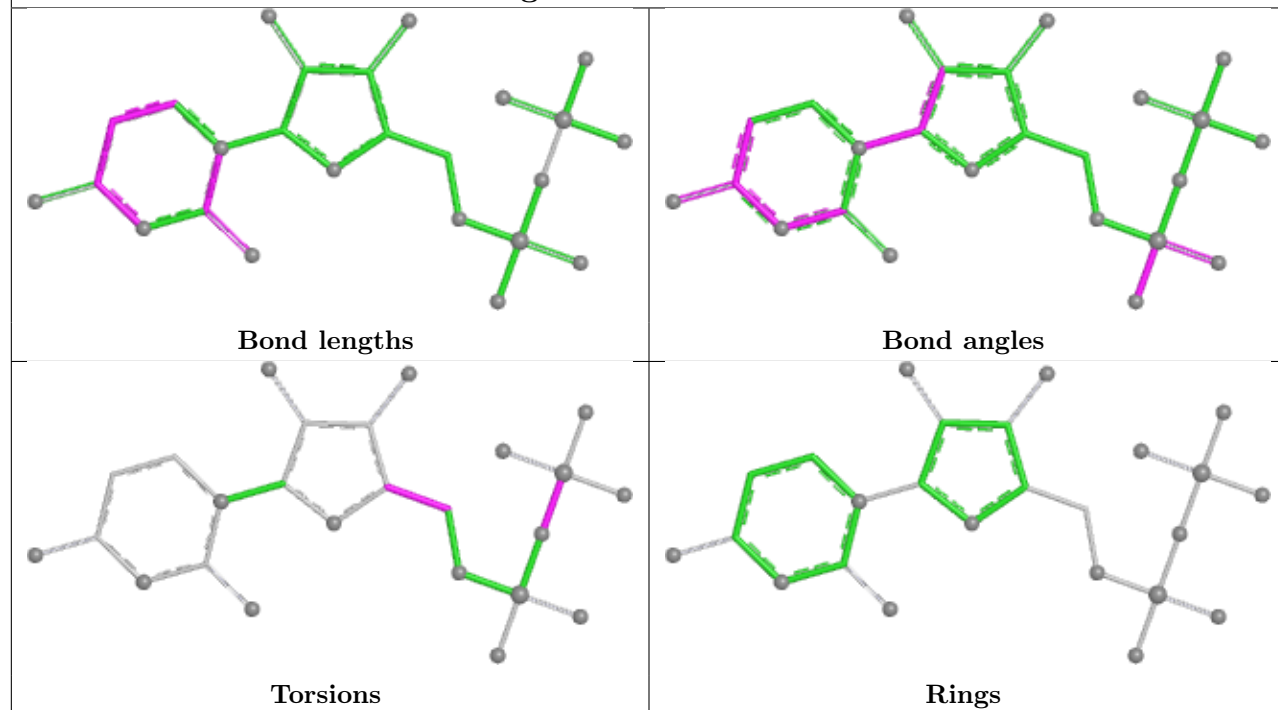
| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | D     | 1201 | UDP  | 3       | 0            |
| 3   | C     | 1201 | UDP  | 2       | 0            |
| 3   | A     | 1201 | UDP  | 2       | 0            |
| 3   | B     | 1201 | UDP  | 2       | 0            |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

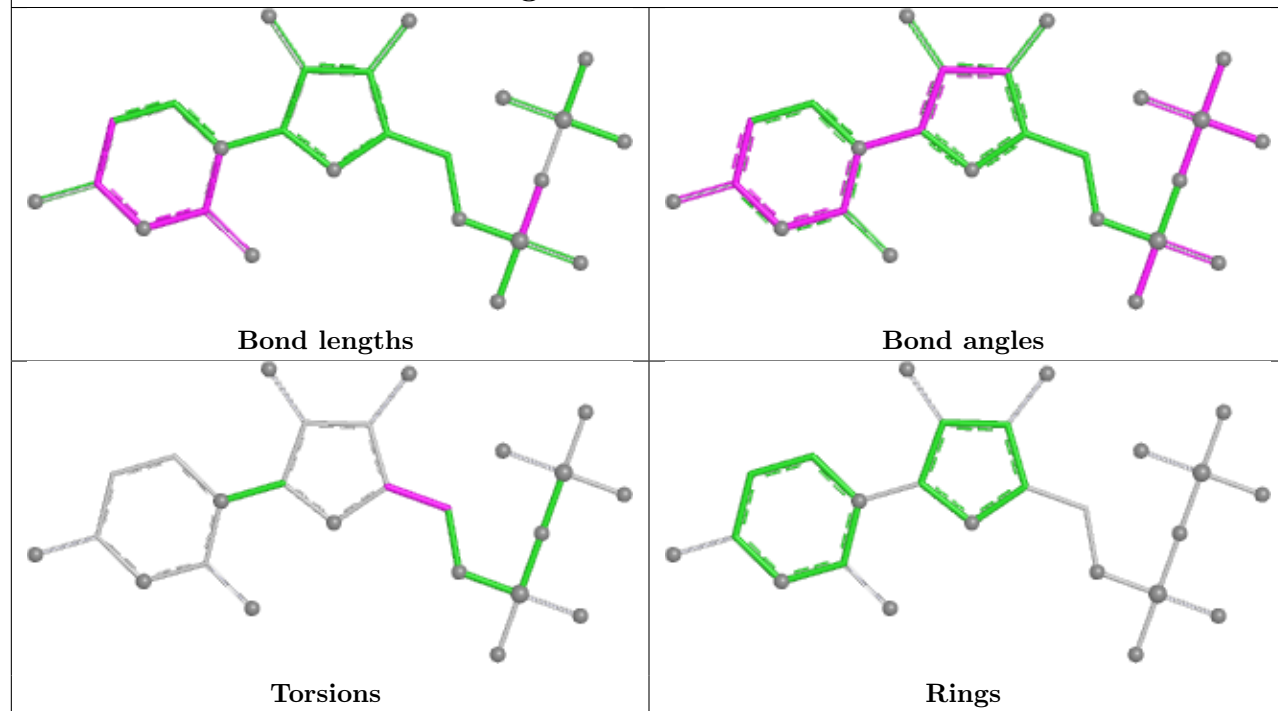
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

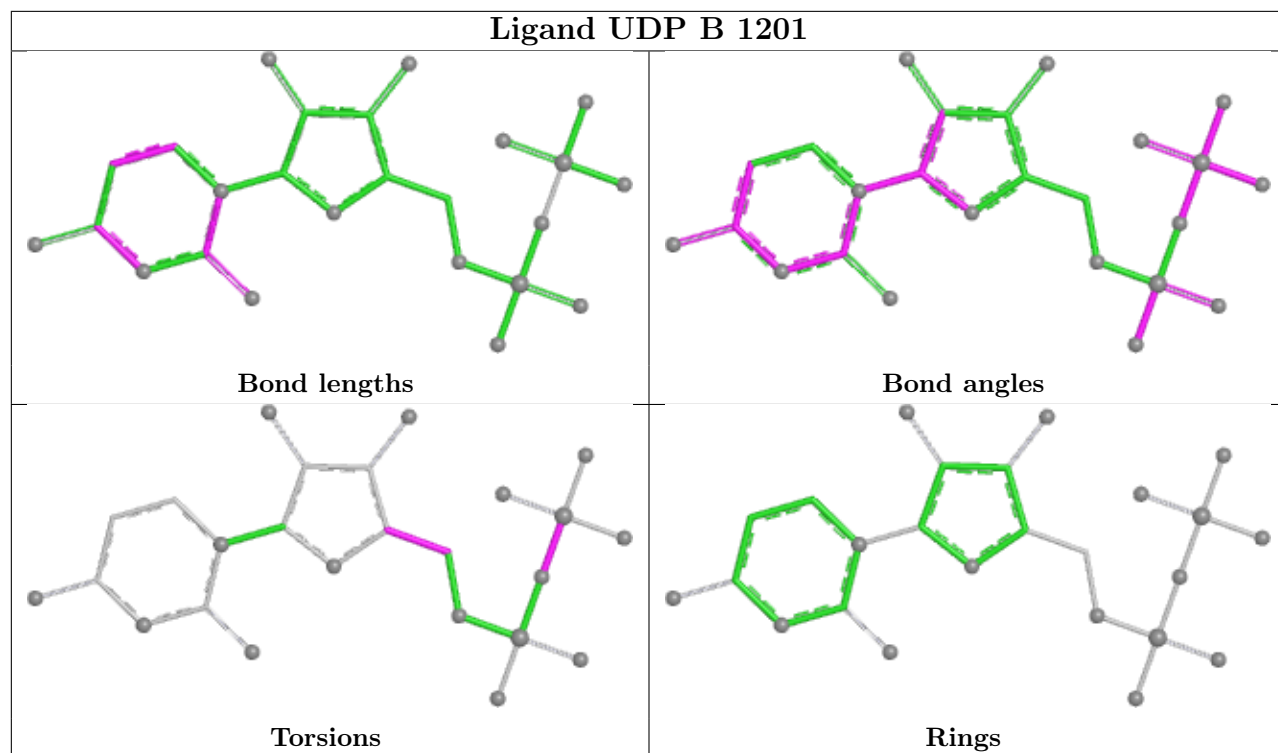


## Ligand UDP C 1201



## Ligand UDP A 1201





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2     | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1   | A     | 698/723 (96%)   | -0.58  | 2 (0%) 90 81  | 30, 53, 95, 148       | 0       |
| 1   | B     | 698/723 (96%)   | -0.66  | 3 (0%) 88 78  | 27, 54, 91, 137       | 0       |
| 1   | C     | 698/723 (96%)   | -0.75  | 1 (0%) 92 88  | 30, 51, 88, 122       | 0       |
| 1   | D     | 698/723 (96%)   | -0.63  | 4 (0%) 85 72  | 36, 66, 97, 134       | 0       |
| 2   | I     | 11/11 (100%)    | 0.53   | 1 (9%) 15 8   | 67, 82, 106, 108      | 0       |
| 2   | J     | 11/11 (100%)    | 0.96   | 2 (18%) 3 2   | 74, 85, 121, 140      | 0       |
| 2   | K     | 11/11 (100%)    | 1.05   | 2 (18%) 3 2   | 66, 86, 111, 142      | 0       |
| 2   | L     | 11/11 (100%)    | 0.81   | 1 (9%) 15 8   | 82, 101, 121, 129     | 0       |
| All | All   | 2836/2936 (96%) | -0.63  | 16 (0%) 85 72 | 27, 56, 97, 148       | 0       |

All (16) RSRZ outliers are listed below:

| Mol | Chain | Res  | Type | RSRZ |
|-----|-------|------|------|------|
| 2   | K     | 11   | SER  | 6.6  |
| 2   | L     | 11   | SER  | 5.2  |
| 2   | J     | 11   | SER  | 5.1  |
| 2   | I     | 11   | SER  | 4.1  |
| 1   | A     | 762  | LEU  | 2.9  |
| 1   | B     | 713  | PHE  | 2.8  |
| 1   | C     | 714  | LYS  | 2.7  |
| 1   | B     | 762  | LEU  | 2.4  |
| 1   | D     | 680  | GLU  | 2.4  |
| 1   | D     | 762  | LEU  | 2.2  |
| 1   | D     | 1028 | LYS  | 2.2  |
| 1   | B     | 714  | LYS  | 2.1  |
| 1   | D     | 714  | LYS  | 2.1  |
| 1   | A     | 860  | ASN  | 2.1  |
| 2   | K     | 9    | ALA  | 2.1  |
| 2   | J     | 2    | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

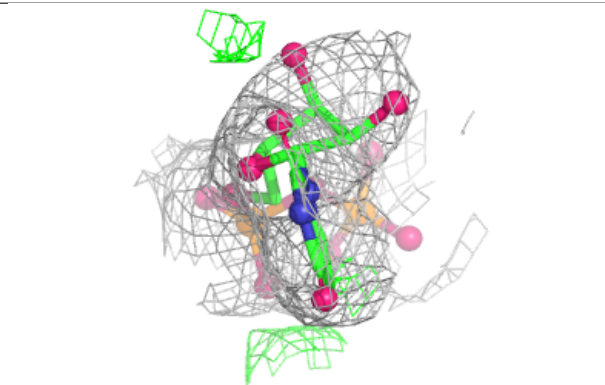
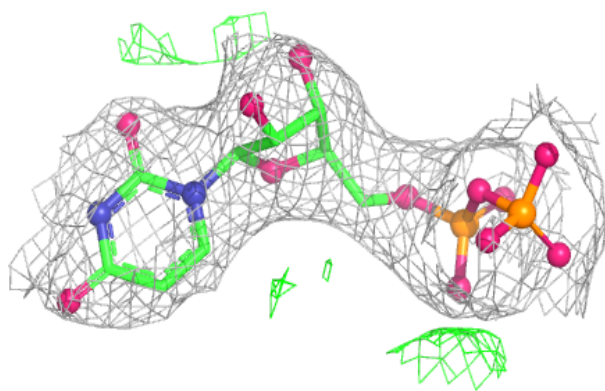
| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | NAG  | J     | 1202 | 14/15 | 0.95 | 0.10 | 56,69,83,85                 | 0     |
| 4   | NAG  | I     | 1202 | 14/15 | 0.96 | 0.08 | 57,67,77,81                 | 0     |
| 4   | NAG  | L     | 1202 | 14/15 | 0.96 | 0.10 | 63,79,93,94                 | 0     |
| 3   | UDP  | D     | 1201 | 25/25 | 0.97 | 0.06 | 60,76,83,85                 | 0     |
| 4   | NAG  | K     | 1202 | 14/15 | 0.97 | 0.08 | 54,59,76,81                 | 0     |
| 3   | UDP  | B     | 1201 | 25/25 | 0.97 | 0.07 | 35,62,72,76                 | 0     |
| 3   | UDP  | C     | 1201 | 25/25 | 0.98 | 0.06 | 44,57,63,64                 | 0     |
| 3   | UDP  | A     | 1201 | 25/25 | 0.98 | 0.06 | 32,55,61,64                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

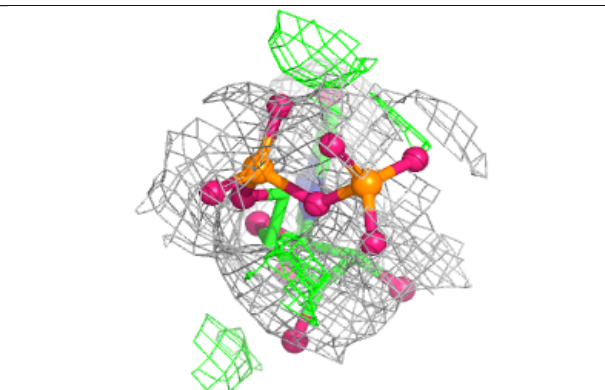
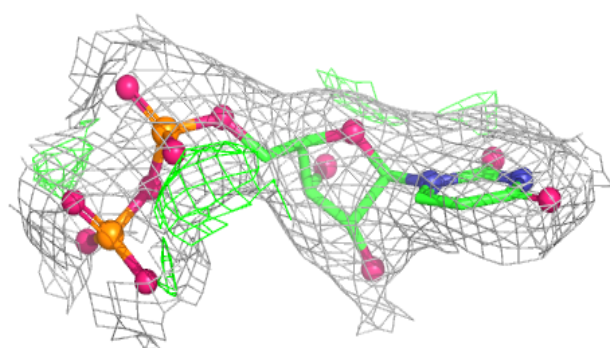
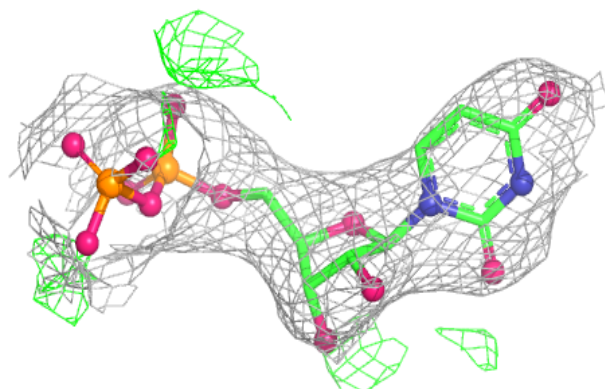


**Electron density around UDP D 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

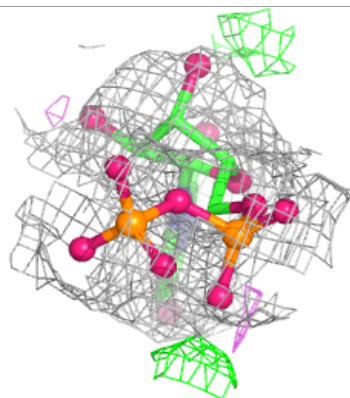
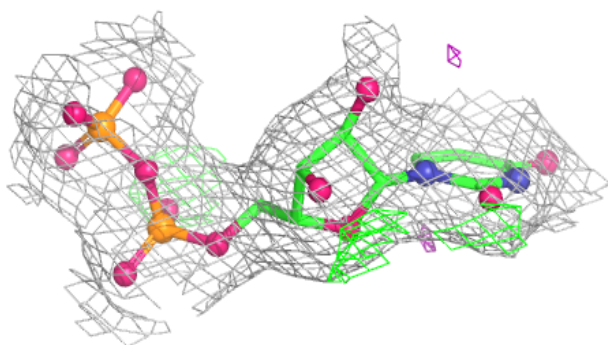
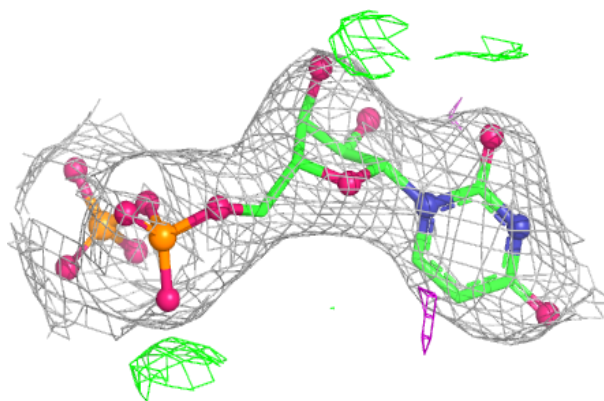
**Electron density around UDP B 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

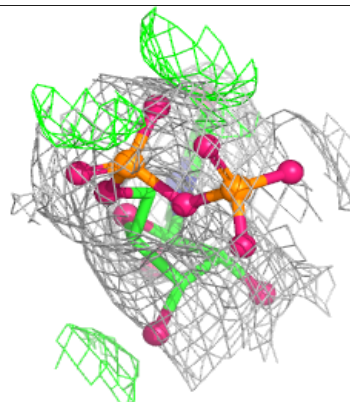
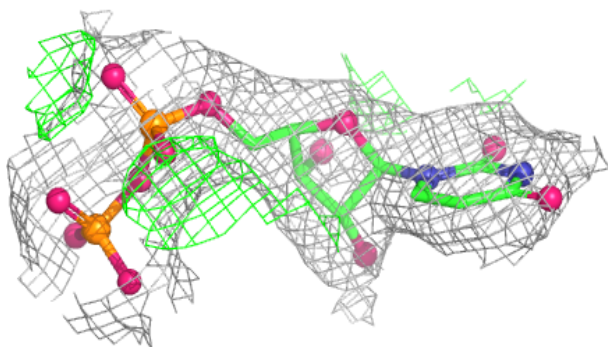
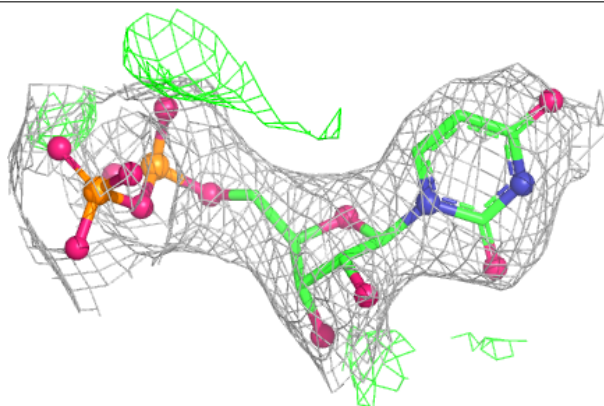


**Electron density around UDP C 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around UDP A 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.