



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 12:05 PM EDT

PDB ID : 4YFL / pdb\_00004yfl  
Title : Crystal structure of VH1-46 germline-derived CD4-binding site-directed anti-body 1B2530 in complex with HIV-1 clade A/E 93TH057 gp120  
Authors : Acharya, P.; Zhou, T.; Moquin, S.; Kwong, P.D.  
Deposited on : 2015-02-25  
Resolution : 3.39 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  
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

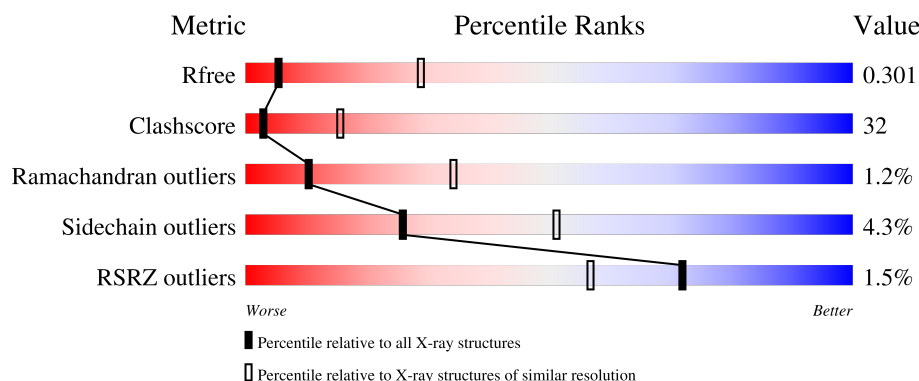
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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                      | 1047 (3.42-3.34)                                      |
| Clashscore            | 190562                      | 1067 (3.42-3.34)                                      |
| Ramachandran outliers | 187476                      | 1056 (3.42-3.34)                                      |
| Sidechain outliers    | 187428                      | 1056 (3.42-3.34)                                      |
| RSRZ outliers         | 180081                      | 1047 (3.42-3.34)                                      |

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   | E     | 353    | <div> <div>46%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>               |
| 1   | G     | 353    | <div> <div>43%</div> <div>46%</div> <div>8%</div> <div>••</div> </div>              |
| 2   | F     | 227    | <div> <div>38%</div> <div>55%</div> <div>•</div> <div>•</div> </div>                |
| 2   | H     | 227    | <div> <div>3%</div> <div>34%</div> <div>56%</div> <div>8%</div> <div>•</div> </div> |
| 3   | I     | 215    | <div> <div>2%</div> <div>40%</div> <div>48%</div> <div>•</div> <div>7%</div> </div> |

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| Mol | Chain | Length | Quality of chain                                                                                   |
|-----|-------|--------|----------------------------------------------------------------------------------------------------|
| 3   | L     | 215    | <div><div></div><div>2%</div><div>32%</div><div>57%</div><div>7%</div><div></div><div></div></div> |

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23777 atoms, of which 11731 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 Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160.

| Mol | Chain | Residues | Atoms |      |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|----|---------|---------|-------|
| 1   | G     | 347      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5360  | 1700 | 2647 | 472 | 518 | 23 |         |         |       |
| 1   | E     | 347      | Total | C    | H    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 5356  | 1700 | 2643 | 472 | 518 | 23 |         |         |       |

There are 16 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| G     | 124     | GLY      | -      | linker  | UNP Q0ED31 |
| G     | 198     | GLY      | -      | linker  | UNP Q0ED31 |
| G     | 318     | GLY      | -      | linker  | UNP Q0ED31 |
| G     | 319     | GLY      | -      | linker  | UNP Q0ED31 |
| G     | 320     | SER      | -      | linker  | UNP Q0ED31 |
| G     | 321     | GLY      | -      | linker  | UNP Q0ED31 |
| G     | 322     | SER      | -      | linker  | UNP Q0ED31 |
| G     | 323     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 124     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 198     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 318     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 319     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 320     | SER      | -      | linker  | UNP Q0ED31 |
| E     | 321     | GLY      | -      | linker  | UNP Q0ED31 |
| E     | 322     | SER      | -      | linker  | UNP Q0ED31 |
| E     | 323     | GLY      | -      | linker  | UNP Q0ED31 |

- Molecule 2 is a protein called 1B2530 heavy chain.

| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 2   | H     | 223      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3350  | 1069 | 1661 | 290 | 322 | 8 |         |         |       |

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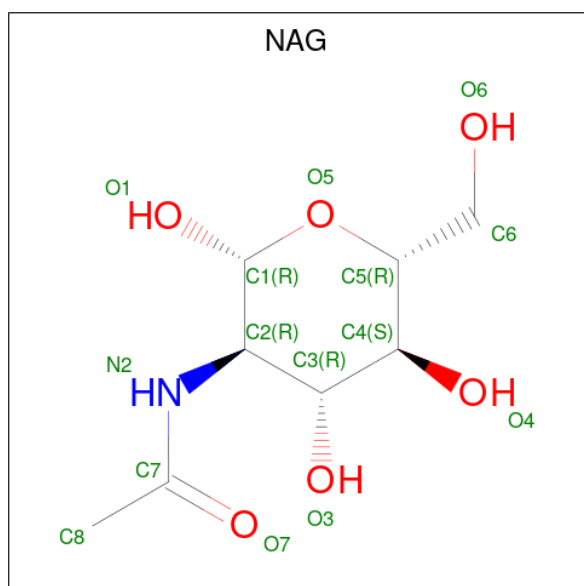
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| Mol | Chain | Residues | Atoms |      |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|------|-----|-----|---|---------|---------|-------|
| 2   | F     | 221      | Total | C    | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3329  | 1063 | 1651 | 288 | 319 | 8 |         |         |       |

- Molecule 3 is a protein called 1B2530 Light chain.

| Mol | Chain | Residues | Atoms |     |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 3   | L     | 209      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 3020  | 964 | 1479 | 261 | 312 | 4 |         |         |       |
| 3   | I     | 200      | Total | C   | H    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 2914  | 932 | 1426 | 251 | 301 | 4 |         |         |       |

- 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   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |
| 4   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |
| 4   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |
| 4   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |
| 4   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |
| 4   | G     | 1        | Total | C | H  | N | O |  | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |  |         |         |

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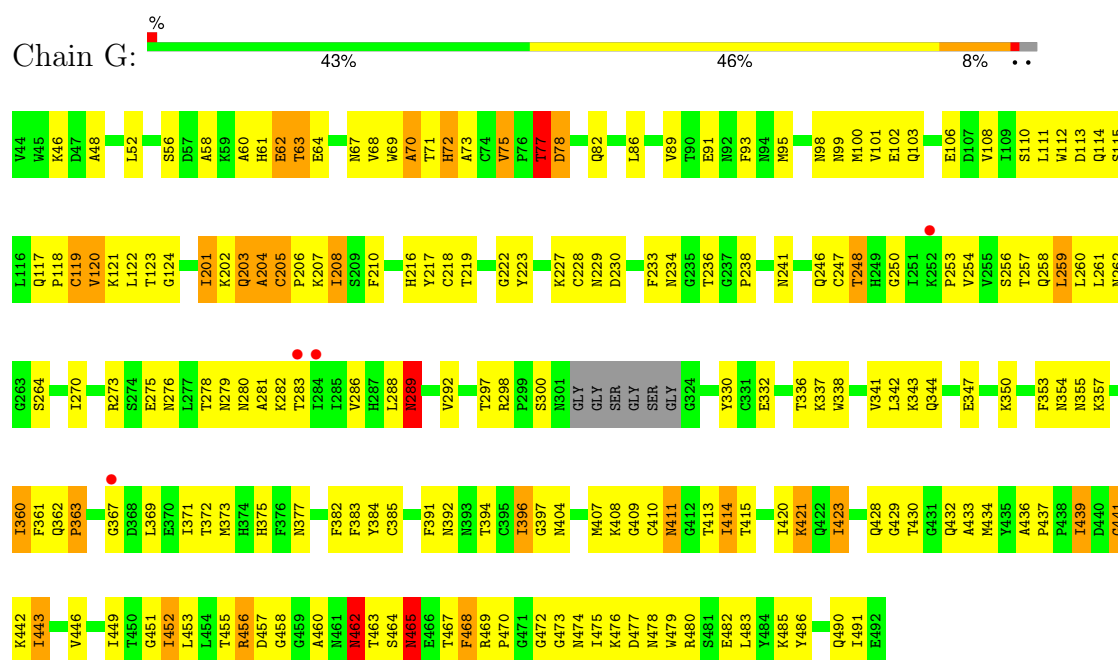
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| Mol | Chain | Residues | Atoms |   |    |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|----|---|---|---------|---------|
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |
| 4   | E     | 1        | Total | C | H  | N | O | 0       | 0       |
|     |       |          | 28    | 8 | 14 | 1 | 5 |         |         |

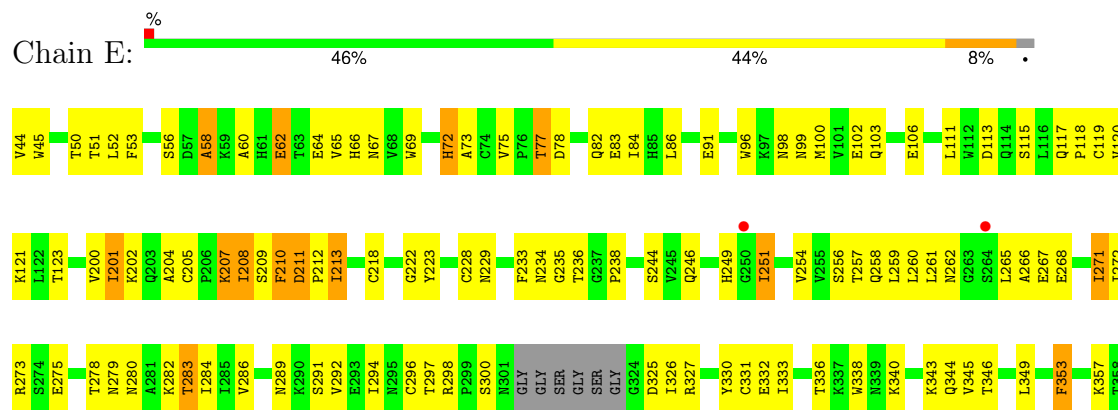
### 3 Residue-property plots [i](#)

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

- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160

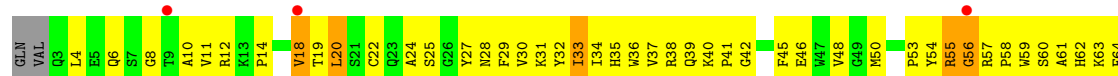


- Molecule 1: Envelope glycoprotein gp160,Envelope glycoprotein gp160,Envelope glycoprotein gp160

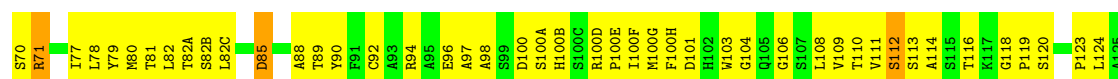




### • Molecule 2: 1B2530 heavy chain



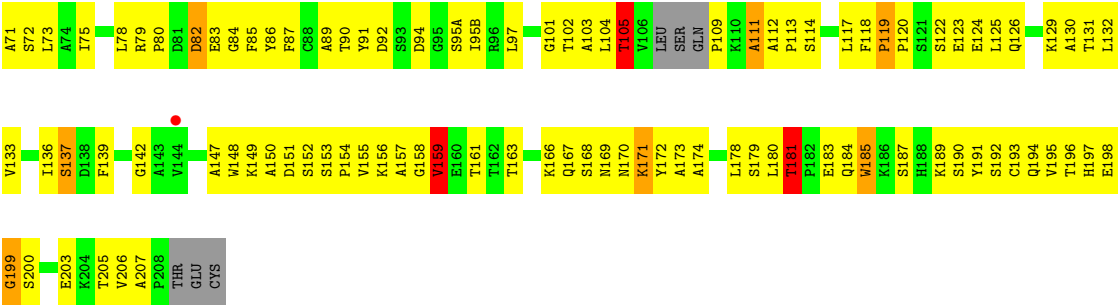
### • Molecule 2: 1B2530 heavy chain



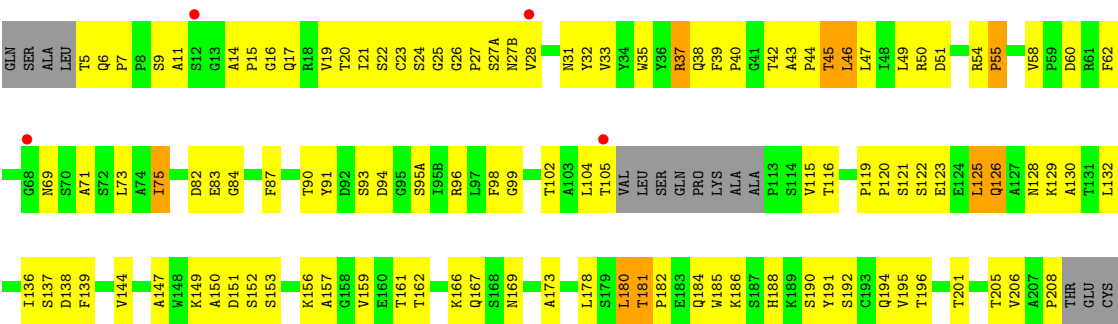
### • Molecule 3: 1B2530 Light chain







● Molecule 3: 1B2530 Light chain



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 66.96Å 57.32Å 254.72Å<br>90.00° 90.11° 90.00°               | Depositor        |
| Resolution (Å)                                                          | 28.77 – 3.39<br>28.77 – 3.39                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 90.0 (28.77-3.39)<br>85.3 (28.77-3.39)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.08 (at 3.39Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX 1.9_1692                                             | Depositor        |
| R, $R_{free}$                                                           | 0.268 , 0.326<br>0.265 , 0.301                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1257 reflections (4.57%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 113.5                                                       | Xtriage          |
| Anisotropy                                                              | 0.271                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 588.5                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$ | Xtriage          |
| Estimated twinning fraction                                             | 0.408 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 23777                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 223.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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: 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   | E     | 0.65         | 0/2770      | 1.49        | 54/3760 (1.4%)   |
| 1   | G     | 0.68         | 0/2770      | 1.54        | 60/3760 (1.6%)   |
| 2   | F     | 0.53         | 0/1722      | 1.08        | 14/2341 (0.6%)   |
| 2   | H     | 0.64         | 0/1733      | 1.18        | 12/2355 (0.5%)   |
| 3   | I     | 0.52         | 0/1527      | 1.10        | 11/2083 (0.5%)   |
| 3   | L     | 0.61         | 0/1580      | 1.24        | 20/2157 (0.9%)   |
| All | All   | 0.62         | 0/12102     | 1.33        | 171/16456 (1.0%) |

There are no bond length outliers.

All (171) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 443 | ILE  | N-CA-C | 11.67 | 125.03      | 107.99   |
| 1   | G     | 420 | ILE  | N-CA-C | 11.50 | 125.14      | 108.58   |
| 1   | E     | 437 | PRO  | CA-C-N | 10.63 | 130.59      | 119.85   |
| 1   | E     | 437 | PRO  | C-N-CA | 10.63 | 130.59      | 119.85   |
| 1   | G     | 411 | ASN  | N-CA-C | 10.35 | 125.80      | 110.17   |
| 1   | G     | 382 | PHE  | N-CA-C | 10.31 | 125.00      | 108.41   |
| 1   | G     | 437 | PRO  | CA-C-N | 10.22 | 130.17      | 119.85   |
| 1   | G     | 437 | PRO  | C-N-CA | 10.22 | 130.17      | 119.85   |
| 1   | G     | 219 | THR  | CA-C-N | 9.82  | 130.24      | 120.52   |
| 1   | G     | 219 | THR  | C-N-CA | 9.82  | 130.24      | 120.52   |
| 1   | E     | 462 | ASN  | N-CA-C | -9.66 | 99.81       | 111.69   |
| 1   | E     | 201 | ILE  | N-CA-C | 9.57  | 121.51      | 108.11   |
| 1   | E     | 86  | LEU  | N-CA-C | 9.54  | 124.79      | 107.99   |
| 1   | G     | 62  | GLU  | N-CA-C | -9.30 | 95.50       | 110.20   |
| 1   | G     | 201 | ILE  | N-CA-C | 9.30  | 121.33      | 107.75   |
| 1   | E     | 360 | ILE  | N-CA-C | 9.18  | 120.95      | 108.11   |
| 1   | E     | 449 | ILE  | N-CA-C | 9.04  | 121.93      | 108.54   |
| 1   | G     | 219 | THR  | N-CA-C | 9.01  | 121.42      | 110.07   |

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| Mol | Chain | Res   | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-------|------|---------|-------|-------------|----------|
| 1   | E     | 420   | ILE  | N-CA-C  | 8.84  | 121.31      | 108.58   |
| 3   | L     | 69    | ASN  | N-CA-C  | -8.44 | 103.00      | 113.38   |
| 3   | L     | 105   | THR  | N-CA-C  | -8.39 | 100.87      | 112.12   |
| 1   | G     | 423   | ILE  | N-CA-C  | 8.34  | 119.89      | 107.80   |
| 2   | H     | 45    | PHE  | N-CA-C  | 8.33  | 120.66      | 110.41   |
| 1   | E     | 211   | ASP  | CA-C-N  | 8.19  | 128.20      | 119.76   |
| 1   | E     | 211   | ASP  | C-N-CA  | 8.19  | 128.20      | 119.76   |
| 1   | G     | 441   | GLY  | N-CA-C  | 8.05  | 127.34      | 112.77   |
| 1   | E     | 213   | ILE  | N-CA-C  | 7.95  | 116.66      | 107.84   |
| 1   | G     | 437   | PRO  | N-CA-C  | 7.74  | 120.14      | 110.70   |
| 3   | L     | 109   | PRO  | N-CA-CB | 7.71  | 111.48      | 103.00   |
| 2   | H     | 11    | VAL  | N-CA-C  | 7.64  | 119.60      | 108.53   |
| 1   | G     | 205   | CYS  | CA-C-N  | 7.61  | 127.54      | 119.85   |
| 1   | G     | 205   | CYS  | C-N-CA  | 7.61  | 127.54      | 119.85   |
| 1   | G     | 360   | ILE  | N-CA-C  | 7.58  | 118.72      | 108.11   |
| 2   | F     | 13    | LYS  | CA-C-N  | 7.57  | 128.02      | 119.92   |
| 2   | F     | 13    | LYS  | C-N-CA  | 7.57  | 128.02      | 119.92   |
| 3   | I     | 27(A) | SER  | N-CA-C  | -7.55 | 104.12      | 112.72   |
| 1   | E     | 490   | GLN  | N-CA-C  | 7.47  | 121.85      | 109.46   |
| 1   | G     | 119   | CYS  | N-CA-C  | -7.46 | 103.15      | 111.28   |
| 1   | E     | 390   | LEU  | N-CA-C  | 7.37  | 120.37      | 111.82   |
| 2   | H     | 20    | LEU  | N-CA-C  | 7.36  | 121.20      | 108.76   |
| 1   | E     | 452   | ILE  | N-CA-C  | 7.33  | 119.30      | 108.45   |
| 1   | E     | 438   | PRO  | N-CA-C  | 7.28  | 122.96      | 111.38   |
| 1   | G     | 449   | ILE  | N-CA-C  | 7.16  | 119.13      | 108.54   |
| 1   | E     | 45    | TRP  | N-CA-C  | 7.14  | 119.59      | 108.96   |
| 1   | E     | 283   | THR  | N-CA-C  | 7.11  | 120.01      | 110.35   |
| 1   | G     | 429   | GLY  | N-CA-C  | -7.06 | 105.48      | 115.30   |
| 2   | F     | 166   | PHE  | CA-C-N  | 7.03  | 127.06      | 119.89   |
| 2   | F     | 166   | PHE  | C-N-CA  | 7.03  | 127.06      | 119.89   |
| 1   | E     | 210   | PHE  | N-CA-C  | 7.01  | 119.89      | 108.26   |
| 1   | G     | 452   | ILE  | N-CA-C  | 6.95  | 118.73      | 108.45   |
| 1   | G     | 78    | ASP  | CA-C-N  | -6.94 | 112.55      | 119.56   |
| 1   | G     | 78    | ASP  | C-N-CA  | -6.94 | 112.55      | 119.56   |
| 1   | G     | 292   | VAL  | N-CA-C  | 6.89  | 117.81      | 107.75   |
| 1   | G     | 207   | LYS  | N-CA-C  | 6.88  | 120.47      | 110.28   |
| 1   | G     | 462   | ASN  | N-CA-C  | -6.78 | 103.69      | 112.23   |
| 1   | E     | 423   | ILE  | N-CA-C  | 6.78  | 117.63      | 107.80   |
| 1   | G     | 336   | THR  | N-CA-C  | 6.74  | 118.28      | 111.07   |
| 1   | E     | 208   | ILE  | N-CA-C  | 6.74  | 118.54      | 108.96   |
| 3   | L     | 119   | PRO  | CA-C-N  | 6.70  | 126.73      | 119.90   |
| 3   | L     | 119   | PRO  | C-N-CA  | 6.70  | 126.73      | 119.90   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 58  | ALA  | N-CA-C  | 6.70  | 119.68      | 110.24   |
| 2   | F     | 71  | ARG  | N-CA-C  | 6.69  | 117.31      | 107.88   |
| 1   | G     | 413 | THR  | N-CA-C  | -6.68 | 99.94       | 109.96   |
| 1   | E     | 336 | THR  | N-CA-C  | 6.68  | 118.22      | 111.07   |
| 1   | E     | 486 | TYR  | N-CA-C  | 6.67  | 120.40      | 109.72   |
| 1   | E     | 272 | ILE  | N-CA-C  | 6.67  | 117.89      | 108.36   |
| 3   | I     | 26  | GLY  | CA-C-N  | -6.65 | 111.53      | 119.84   |
| 3   | I     | 26  | GLY  | C-N-CA  | -6.65 | 111.53      | 119.84   |
| 1   | G     | 347 | GLU  | N-CA-C  | -6.63 | 103.97      | 111.07   |
| 1   | G     | 414 | ILE  | N-CA-C  | 6.62  | 118.36      | 108.23   |
| 1   | E     | 121 | LYS  | N-CA-C  | 6.62  | 119.68      | 108.90   |
| 2   | F     | 30  | VAL  | N-CA-C  | 6.60  | 118.19      | 111.00   |
| 1   | E     | 62  | GLU  | N-CA-C  | -6.59 | 99.79       | 110.20   |
| 3   | L     | 137 | SER  | N-CA-C  | 6.52  | 119.06      | 108.76   |
| 1   | G     | 377 | ASN  | N-CA-C  | 6.50  | 119.53      | 109.07   |
| 3   | L     | 171 | LYS  | N-CA-C  | -6.47 | 100.94      | 110.52   |
| 1   | E     | 365 | SER  | N-CA-C  | -6.45 | 104.34      | 111.82   |
| 2   | H     | 184 | SER  | N-CA-C  | 6.44  | 118.84      | 111.11   |
| 1   | E     | 441 | GLY  | N-CA-C  | 6.44  | 124.42      | 112.77   |
| 1   | E     | 60  | ALA  | N-CA-C  | 6.43  | 120.38      | 112.54   |
| 1   | G     | 456 | ARG  | N-CA-C  | 6.39  | 120.70      | 109.96   |
| 3   | L     | 21  | ILE  | N-CA-C  | 6.39  | 117.08      | 107.75   |
| 1   | E     | 437 | PRO  | N-CA-C  | 6.34  | 118.43      | 110.70   |
| 1   | E     | 261 | LEU  | N-CA-C  | 6.30  | 119.66      | 109.40   |
| 1   | G     | 289 | ASN  | N-CA-C  | -6.28 | 105.26      | 113.17   |
| 3   | I     | 75  | ILE  | N-CA-C  | 6.28  | 117.16      | 108.12   |
| 2   | F     | 49  | GLY  | N-CA-C  | 6.24  | 119.86      | 110.75   |
| 3   | L     | 163 | THR  | N-CA-C  | -6.24 | 101.92      | 109.72   |
| 1   | G     | 120 | VAL  | N-CA-C  | 6.24  | 117.28      | 108.17   |
| 2   | H     | 207 | ILE  | N-CA-C  | 6.23  | 119.02      | 108.86   |
| 1   | G     | 363 | PRO  | O-C-N   | 6.22  | 124.07      | 121.15   |
| 2   | F     | 113 | SER  | N-CA-C  | -6.19 | 104.59      | 111.71   |
| 1   | G     | 203 | GLN  | N-CA-C  | 6.18  | 116.59      | 107.88   |
| 1   | G     | 439 | ILE  | CB-CA-C | -6.16 | 103.31      | 111.13   |
| 1   | E     | 453 | LEU  | N-CA-C  | 6.14  | 119.25      | 109.24   |
| 1   | G     | 446 | VAL  | N-CA-C  | 6.12  | 116.93      | 107.99   |
| 1   | E     | 271 | ILE  | N-CA-C  | 6.10  | 116.71      | 108.17   |
| 1   | E     | 449 | ILE  | CB-CA-C | -6.10 | 103.94      | 111.08   |
| 2   | F     | 43  | LEU  | N-CA-C  | 6.04  | 117.96      | 108.96   |
| 1   | G     | 367 | GLY  | N-CA-C  | 6.03  | 119.41      | 111.52   |
| 2   | H     | 201 | LEU  | N-CA-C  | 6.02  | 117.66      | 110.19   |
| 2   | H     | 209 | ASN  | N-CA-C  | 6.01  | 118.20      | 108.34   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 388 | THR  | N-CA-C  | 5.99  | 118.29      | 111.11   |
| 3   | I     | 126 | GLN  | N-CA-C  | -5.98 | 105.48      | 112.89   |
| 3   | L     | 159 | VAL  | N-CA-C  | 5.98  | 118.49      | 108.81   |
| 1   | G     | 77  | THR  | N-CA-C  | 5.97  | 118.41      | 110.53   |
| 2   | H     | 206 | TYR  | N-CA-C  | 5.96  | 118.21      | 108.55   |
| 3   | I     | 51  | ASP  | N-CA-C  | -5.95 | 104.62      | 112.24   |
| 1   | G     | 476 | LYS  | N-CA-C  | -5.92 | 104.90      | 111.71   |
| 1   | G     | 420 | ILE  | CB-CA-C | -5.88 | 103.62      | 110.91   |
| 1   | E     | 363 | PRO  | CA-C-N  | 5.87  | 127.18      | 119.84   |
| 1   | E     | 363 | PRO  | C-N-CA  | 5.87  | 127.18      | 119.84   |
| 2   | H     | 56  | GLY  | N-CA-C  | -5.87 | 106.39      | 116.01   |
| 3   | L     | 181 | THR  | N-CA-C  | -5.84 | 102.23      | 110.29   |
| 1   | G     | 297 | THR  | N-CA-C  | 5.82  | 119.00      | 108.69   |
| 1   | G     | 248 | THR  | N-CA-C  | 5.80  | 117.54      | 110.41   |
| 1   | E     | 267 | GLU  | N-CA-C  | -5.80 | 106.21      | 113.28   |
| 1   | E     | 382 | PHE  | N-CA-C  | 5.79  | 117.72      | 108.41   |
| 1   | E     | 251 | ILE  | N-CA-C  | 5.78  | 116.19      | 107.80   |
| 1   | G     | 205 | CYS  | N-CA-C  | 5.75  | 124.07      | 111.53   |
| 1   | E     | 443 | ILE  | N-CA-C  | 5.75  | 116.38      | 107.99   |
| 1   | E     | 410 | CYS  | N-CA-C  | -5.73 | 105.17      | 111.82   |
| 3   | L     | 39  | PHE  | CA-C-N  | 5.66  | 126.55      | 119.98   |
| 3   | L     | 39  | PHE  | C-N-CA  | 5.66  | 126.55      | 119.98   |
| 1   | E     | 484 | TYR  | N-CA-C  | 5.65  | 118.21      | 111.71   |
| 1   | E     | 292 | VAL  | N-CA-C  | 5.63  | 115.97      | 107.75   |
| 2   | F     | 165 | THR  | N-CA-C  | 5.63  | 117.47      | 108.41   |
| 1   | E     | 207 | LYS  | N-CA-C  | 5.62  | 118.59      | 110.28   |
| 3   | L     | 82  | ASP  | N-CA-C  | -5.61 | 106.41      | 113.20   |
| 3   | L     | 7   | PRO  | CA-C-N  | 5.60  | 125.36      | 119.76   |
| 3   | L     | 7   | PRO  | C-N-CA  | 5.60  | 125.36      | 119.76   |
| 1   | G     | 205 | CYS  | N-CA-CB | -5.59 | 105.46      | 111.66   |
| 3   | L     | 157 | ALA  | N-CA-C  | 5.57  | 115.73      | 107.88   |
| 2   | F     | 161 | SER  | N-CA-C  | 5.56  | 118.25      | 109.96   |
| 3   | L     | 26  | GLY  | N-CA-C  | -5.55 | 108.32      | 115.09   |
| 3   | L     | 60  | ASP  | N-CA-C  | 5.51  | 119.72      | 112.89   |
| 1   | G     | 202 | LYS  | N-CA-C  | 5.49  | 118.43      | 109.59   |
| 1   | G     | 337 | LYS  | N-CA-C  | -5.48 | 105.21      | 111.07   |
| 3   | L     | 185 | TRP  | N-CA-C  | -5.46 | 105.33      | 111.28   |
| 1   | G     | 208 | ILE  | N-CA-C  | 5.44  | 116.69      | 108.96   |
| 1   | E     | 376 | PHE  | N-CA-C  | 5.43  | 116.53      | 108.60   |
| 2   | H     | 79  | LEU  | N-CA-C  | 5.41  | 118.39      | 109.85   |
| 2   | F     | 191 | THR  | N-CA-C  | -5.40 | 106.82      | 113.41   |
| 1   | E     | 332 | GLU  | N-CA-C  | 5.40  | 118.04      | 109.24   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | I     | 37  | ARG  | N-CA-C   | -5.40 | 102.89      | 110.50   |
| 1   | E     | 368 | ASP  | N-CA-C   | 5.39  | 118.10      | 110.50   |
| 1   | E     | 204 | ALA  | N-CA-C   | 5.33  | 118.17      | 110.28   |
| 1   | G     | 75  | VAL  | N-CA-C   | 5.30  | 120.33      | 108.88   |
| 3   | I     | 156 | LYS  | N-CA-C   | 5.30  | 121.48      | 114.12   |
| 1   | E     | 51  | THR  | N-CA-C   | 5.29  | 116.77      | 109.15   |
| 1   | G     | 465 | ASN  | N-CA-C   | 5.29  | 118.19      | 109.72   |
| 1   | G     | 259 | LEU  | N-CA-C   | 5.29  | 117.58      | 109.07   |
| 2   | F     | 118 | GLY  | CA-C-N   | 5.27  | 125.25      | 120.03   |
| 2   | F     | 118 | GLY  | C-N-CA   | 5.27  | 125.25      | 120.03   |
| 3   | I     | 22  | SER  | N-CA-C   | 5.27  | 118.65      | 110.17   |
| 1   | G     | 468 | PHE  | N-CA-C   | 5.23  | 118.09      | 109.72   |
| 3   | I     | 180 | LEU  | N-CA-C   | 5.22  | 117.32      | 109.23   |
| 1   | G     | 206 | PRO  | N-CA-C   | 5.20  | 119.65      | 111.38   |
| 1   | E     | 434 | MET  | N-CA-C   | 5.20  | 117.38      | 108.90   |
| 3   | I     | 144 | VAL  | N-CA-C   | 5.18  | 117.51      | 108.90   |
| 1   | E     | 425 | ASN  | N-CA-C   | -5.18 | 100.72      | 108.96   |
| 1   | G     | 275 | GLU  | N-CA-C   | 5.17  | 117.66      | 111.71   |
| 1   | G     | 70  | ALA  | N-CA-C   | -5.15 | 105.85      | 111.82   |
| 1   | E     | 353 | PHE  | N-CA-C   | 5.13  | 118.63      | 111.30   |
| 1   | E     | 84  | ILE  | N-CA-C   | 5.11  | 115.21      | 107.80   |
| 1   | G     | 63  | THR  | N-CA-C   | -5.09 | 107.07      | 113.28   |
| 1   | G     | 204 | ALA  | N-CA-C   | 5.06  | 118.71      | 112.54   |
| 1   | G     | 78  | ASP  | N-CA-C   | -5.04 | 102.24      | 109.24   |
| 2   | H     | 178 | PHE  | CA-C-N   | 5.02  | 124.95      | 119.78   |
| 2   | H     | 178 | PHE  | C-N-CA   | 5.02  | 124.95      | 119.78   |
| 1   | G     | 289 | ASN  | CA-CB-CG | 5.01  | 117.61      | 112.60   |

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   | E     | 2713  | 2643     | 2644     | 131     | 0            |
| 1   | G     | 2713  | 2647     | 2647     | 157     | 1            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2   | F     | 1678  | 1651     | 1651     | 128     | 0            |
| 2   | H     | 1689  | 1661     | 1661     | 148     | 22           |
| 3   | I     | 1488  | 1426     | 1426     | 97      | 0            |
| 3   | L     | 1541  | 1479     | 1473     | 137     | 17           |
| 4   | E     | 140   | 140      | 130      | 10      | 0            |
| 4   | G     | 84    | 84       | 78       | 11      | 0            |
| All | All   | 12046 | 11731    | 11710    | 768     | 24           |

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 32.

All (768) 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) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:3:GLN:N      | 2:F:24:ALA:HA   | 1.37                     | 1.36              |
| 2:F:3:GLN:N      | 2:F:24:ALA:CA   | 2.17                     | 1.08              |
| 1:E:113:ASP:O    | 1:E:117:GLN:NE2 | 2.01                     | 0.93              |
| 2:F:5:GLU:OE2    | 2:F:23:GLN:OE1  | 1.88                     | 0.92              |
| 2:F:5:GLU:CG     | 2:F:23:GLN:HB3  | 2.01                     | 0.91              |
| 3:L:151:ASP:OD2  | 3:L:190:SER:HB2 | 1.71                     | 0.90              |
| 2:H:182:LEU:HA   | 2:H:188:TYR:HA  | 1.52                     | 0.90              |
| 3:L:150:ALA:N    | 3:L:153:SER:O   | 2.04                     | 0.89              |
| 2:F:28:ASN:OD1   | 2:F:94:ARG:NH1  | 2.08                     | 0.86              |
| 3:L:153:SER:OG   | 3:L:154:PRO:HD2 | 1.78                     | 0.84              |
| 1:G:98:ASN:ND2   | 1:G:100:MET:SD  | 2.51                     | 0.84              |
| 1:G:229:ASN:CG   | 4:G:501:NAG:H82 | 2.03                     | 0.83              |
| 2:H:226:LYS:NZ   | 3:L:120:PRO:O   | 2.14                     | 0.81              |
| 3:I:166:LYS:NZ   | 3:I:167:GLN:O   | 2.12                     | 0.81              |
| 3:I:14:ALA:O     | 3:I:16:GLY:N    | 2.14                     | 0.81              |
| 3:L:111:ALA:HB1  | 3:L:112:ALA:HB2 | 1.63                     | 0.80              |
| 3:L:90:THR:OG1   | 3:L:97:LEU:N    | 2.15                     | 0.80              |
| 3:L:46:LEU:HD23  | 3:L:47:LEU:N    | 1.97                     | 0.79              |
| 2:H:20:LEU:HD12  | 2:H:81:MET:SD   | 2.22                     | 0.79              |
| 2:H:55:ARG:O     | 2:H:72:ARG:NH2  | 2.16                     | 0.78              |
| 3:L:124:GLU:OE2  | 3:L:131:THR:OG1 | 2.02                     | 0.78              |
| 1:G:58:ALA:HB2   | 1:G:70:ALA:HB3  | 1.66                     | 0.78              |
| 4:E:510:NAG:H3   | 4:E:510:NAG:H83 | 1.67                     | 0.77              |
| 1:G:52:LEU:HD11  | 1:G:100:MET:HG2 | 1.67                     | 0.77              |
| 1:E:455:THR:OG1  | 1:E:471:GLY:O   | 2.03                     | 0.76              |
| 1:G:254:VAL:CG1  | 4:G:502:NAG:H81 | 2.16                     | 0.76              |
| 2:F:124:LEU:HD21 | 2:F:141:LEU:CD2 | 2.15                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:6:GLN:OE1    | 2:H:96:CYS:N     | 2.19                     | 0.75              |
| 2:H:54:TYR:O     | 2:H:56:GLY:N     | 2.19                     | 0.75              |
| 3:L:111:ALA:HB1  | 3:L:112:ALA:CB   | 2.17                     | 0.74              |
| 2:H:6:GLN:O      | 2:H:117:GLN:NE2  | 2.22                     | 0.73              |
| 3:I:138:ASP:OD1  | 3:I:169:ASN:ND2  | 2.22                     | 0.72              |
| 1:E:102:GLU:OE2  | 1:E:476:LYS:NZ   | 2.21                     | 0.72              |
| 2:H:101:ALA:N    | 2:H:109:PRO:O    | 2.22                     | 0.72              |
| 1:E:465:ASN:OD1  | 1:E:465:ASN:N    | 2.20                     | 0.71              |
| 2:H:139:SER:O    | 2:H:141:LYS:NZ   | 2.23                     | 0.71              |
| 3:L:46:LEU:HD23  | 3:L:47:LEU:H     | 1.55                     | 0.71              |
| 2:F:209:LYS:NZ   | 2:F:210:LYS:O    | 2.24                     | 0.70              |
| 3:I:167:GLN:HG2  | 3:I:173:ALA:HB2  | 1.72                     | 0.70              |
| 3:L:1:GLN:N      | 3:L:95(A):SER:O  | 2.24                     | 0.70              |
| 2:F:39:GLN:O     | 2:F:88:ALA:HB1   | 1.91                     | 0.70              |
| 3:I:11:ALA:HB3   | 3:I:19:VAL:HG23  | 1.73                     | 0.70              |
| 1:E:340:LYS:NZ   | 1:E:344:GLN:OE1  | 2.24                     | 0.70              |
| 2:H:150:LEU:HD13 | 2:H:223:VAL:HG11 | 1.72                     | 0.69              |
| 2:F:60:ALA:HB3   | 2:F:63:PHE:CD1   | 2.27                     | 0.69              |
| 3:I:123:GLU:N    | 3:I:123:GLU:OE1  | 2.25                     | 0.69              |
| 2:F:124:LEU:HD21 | 2:F:141:LEU:HD22 | 1.73                     | 0.69              |
| 3:L:193:CYS:N    | 3:L:203:GLU:OE2  | 2.26                     | 0.69              |
| 1:G:410:CYS:SG   | 4:G:506:NAG:O6   | 2.49                     | 0.69              |
| 3:I:159:VAL:HG22 | 3:I:178:LEU:CD1  | 2.23                     | 0.69              |
| 3:I:25:GLY:N     | 3:I:69:ASN:OD1   | 2.27                     | 0.68              |
| 2:H:33:ILE:HD12  | 2:H:50:MET:HB2   | 1.75                     | 0.68              |
| 3:L:147:ALA:O    | 3:L:194:GLN:N    | 2.27                     | 0.68              |
| 3:L:111:ALA:CB   | 3:L:112:ALA:HB2  | 2.23                     | 0.67              |
| 3:L:117:LEU:HD12 | 3:L:133:VAL:O    | 1.95                     | 0.67              |
| 3:L:151:ASP:CG   | 3:L:190:SER:HB2  | 2.19                     | 0.67              |
| 1:E:279:ASN:ND2  | 3:I:94:ASP:OD2   | 2.27                     | 0.67              |
| 3:L:184:GLN:HA   | 3:L:187:SER:HB3  | 1.75                     | 0.67              |
| 1:E:119:CYS:N    | 1:E:434:MET:O    | 2.28                     | 0.67              |
| 1:G:396:ILE:O    | 1:G:404:ASN:N    | 2.26                     | 0.67              |
| 1:E:421:LYS:NZ   | 1:E:423:ILE:O    | 2.24                     | 0.67              |
| 1:E:69:TRP:CG    | 1:E:111:LEU:HD12 | 2.30                     | 0.66              |
| 1:E:283:THR:OG1  | 1:E:473:GLY:N    | 2.22                     | 0.66              |
| 1:G:460:ALA:HB1  | 3:L:1:GLN:NE2    | 2.10                     | 0.66              |
| 3:L:166:LYS:NZ   | 3:L:167:GLN:O    | 2.28                     | 0.66              |
| 1:G:262:ASN:ND2  | 4:G:502:NAG:O7   | 2.29                     | 0.66              |
| 2:H:38:ARG:NE    | 2:H:46:GLU:OE1   | 2.22                     | 0.66              |
| 1:G:369:LEU:HD22 | 1:G:373:MET:SD   | 2.36                     | 0.66              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:408:LYS:O    | 4:G:506:NAG:O6   | 2.12                     | 0.66              |
| 1:E:64:GLU:HG3   | 1:E:211:ASP:H    | 1.61                     | 0.66              |
| 3:I:27:PRO:O     | 3:I:69:ASN:ND2   | 2.28                     | 0.66              |
| 2:F:5:GLU:OE2    | 2:F:23:GLN:HB3   | 1.95                     | 0.65              |
| 2:H:150:LEU:HD13 | 2:H:223:VAL:CG1  | 2.26                     | 0.65              |
| 1:G:60:ALA:HB2   | 1:G:71:THR:HG21  | 1.79                     | 0.65              |
| 1:G:61:HIS:HB3   | 2:F:79:TYR:HB2   | 1.78                     | 0.65              |
| 4:E:503:NAG:O7   | 4:E:503:NAG:O3   | 2.14                     | 0.65              |
| 1:G:278:THR:O    | 1:G:456:ARG:NH2  | 2.30                     | 0.64              |
| 3:L:54:ARG:NH2   | 3:L:62:PHE:O     | 2.30                     | 0.64              |
| 3:L:167:GLN:HG2  | 3:L:173:ALA:HB2  | 1.79                     | 0.64              |
| 1:E:119:CYS:SG   | 1:E:436:ALA:N    | 2.70                     | 0.64              |
| 3:L:111:ALA:HB1  | 3:L:112:ALA:CA   | 2.28                     | 0.64              |
| 1:G:58:ALA:HB1   | 1:G:67:ASN:O     | 1.99                     | 0.63              |
| 1:G:362:GLN:N    | 1:G:468:PHE:O    | 2.30                     | 0.63              |
| 2:H:221:LYS:NZ   | 2:H:222:LYS:O    | 2.32                     | 0.63              |
| 2:F:200:HIS:ND1  | 2:F:203:SER:OG   | 2.19                     | 0.63              |
| 3:I:54:ARG:NH2   | 3:I:62:PHE:O     | 2.32                     | 0.63              |
| 1:G:254:VAL:HG13 | 4:G:502:NAG:H81  | 1.79                     | 0.63              |
| 1:G:276:ASN:HB3  | 1:G:282:LYS:HG3  | 1.81                     | 0.62              |
| 2:H:212:HIS:ND1  | 2:H:215:SER:OG   | 2.22                     | 0.62              |
| 3:L:54:ARG:NE    | 3:L:59:PRO:O     | 2.31                     | 0.62              |
| 1:E:363:PRO:O    | 1:E:469:ARG:NH1  | 2.32                     | 0.62              |
| 1:G:371:ILE:HG21 | 2:H:55:ARG:HB3   | 1.81                     | 0.62              |
| 1:E:373:MET:SD   | 4:E:508:NAG:H81  | 2.40                     | 0.62              |
| 1:G:52:LEU:CD1   | 1:G:100:MET:HG2  | 2.29                     | 0.62              |
| 2:F:4:LEU:N      | 2:F:23:GLN:O     | 2.33                     | 0.62              |
| 2:F:5:GLU:HG3    | 2:F:23:GLN:HB3   | 1.82                     | 0.62              |
| 2:H:4:LEU:HD23   | 2:H:24:ALA:HB2   | 1.82                     | 0.61              |
| 1:E:357:LYS:NZ   | 1:E:465:ASN:O    | 2.32                     | 0.61              |
| 1:G:465:ASN:OD1  | 1:G:465:ASN:N    | 2.32                     | 0.61              |
| 2:H:14:PRO:HB3   | 2:H:87:LYS:HA    | 1.82                     | 0.61              |
| 2:F:20:LEU:HD12  | 2:F:80:MET:SD    | 2.41                     | 0.61              |
| 2:F:124:LEU:HD21 | 2:F:141:LEU:HD23 | 1.81                     | 0.61              |
| 1:G:281:ALA:HB2  | 2:H:50:MET:HE1   | 1.82                     | 0.61              |
| 3:L:28:VAL:O     | 3:L:66:LYS:NZ    | 2.20                     | 0.61              |
| 1:E:254:VAL:HG21 | 1:E:262:ASN:HB2  | 1.83                     | 0.61              |
| 1:G:86:LEU:O     | 1:G:89:VAL:HG12  | 2.01                     | 0.61              |
| 1:G:113:ASP:O    | 1:G:117:GLN:NE2  | 2.34                     | 0.61              |
| 1:G:110:SER:O    | 1:G:114:GLN:HG2  | 2.01                     | 0.60              |
| 1:E:257:THR:O    | 1:E:259:LEU:N    | 2.30                     | 0.60              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:F:38:ARG:NH2   | 2:F:46:GLU:OE1     | 2.34                     | 0.60              |
| 3:L:181:THR:O    | 3:L:185:TRP:N      | 2.31                     | 0.60              |
| 3:L:9:SER:O      | 3:L:103:ALA:N      | 2.35                     | 0.60              |
| 3:I:5:THR:OG1    | 3:I:24:SER:O       | 2.18                     | 0.60              |
| 3:I:159:VAL:HG13 | 3:I:178:LEU:HD13   | 1.84                     | 0.60              |
| 2:F:3:GLN:N      | 2:F:24:ALA:CB      | 2.65                     | 0.60              |
| 2:F:5:GLU:HG2    | 2:F:23:GLN:HB3     | 1.82                     | 0.60              |
| 3:I:150:ALA:O    | 3:I:152:SER:N      | 2.34                     | 0.60              |
| 1:E:64:GLU:CG    | 1:E:211:ASP:H      | 2.15                     | 0.59              |
| 2:F:200:HIS:O    | 2:F:204:ASN:N      | 2.35                     | 0.59              |
| 1:G:48:ALA:CB    | 1:G:490:GLN:HB2    | 2.32                     | 0.59              |
| 3:L:153:SER:OG   | 3:L:154:PRO:CD     | 2.50                     | 0.59              |
| 2:F:9:THR:O      | 2:F:12:ARG:NH2     | 2.35                     | 0.59              |
| 2:F:96:GLU:HA    | 2:F:100:ASP:HB3    | 1.84                     | 0.59              |
| 3:L:123:GLU:N    | 3:L:123:GLU:OE1    | 2.32                     | 0.59              |
| 3:I:37:ARG:NE    | 3:I:45:THR:HB      | 2.18                     | 0.59              |
| 3:I:46:LEU:HD12  | 3:I:47:LEU:H       | 1.68                     | 0.59              |
| 2:F:97:ALA:N     | 2:F:100(E):PRO:O   | 2.35                     | 0.58              |
| 1:E:56:SER:N     | 1:E:75:VAL:O       | 2.31                     | 0.58              |
| 2:H:14:PRO:HA    | 2:H:86:LEU:HB2     | 1.84                     | 0.58              |
| 2:H:101:ALA:HA   | 2:H:110:ILE:HG22   | 1.86                     | 0.58              |
| 4:E:504:NAG:O3   | 4:E:504:NAG:O7     | 2.21                     | 0.58              |
| 3:I:122:SER:O    | 3:I:125:LEU:N      | 2.36                     | 0.58              |
| 2:F:5:GLU:CD     | 2:F:23:GLN:HB3     | 2.28                     | 0.58              |
| 2:H:182:LEU:HD12 | 2:H:182:LEU:O      | 2.03                     | 0.57              |
| 1:E:404:ASN:ND2  | 1:E:404:ASN:O      | 2.37                     | 0.57              |
| 3:I:150:ALA:HB3  | 3:I:153:SER:HB3    | 1.86                     | 0.57              |
| 1:G:298:ARG:NH2  | 1:G:441:GLY:O      | 2.29                     | 0.57              |
| 3:L:34:TYR:HB3   | 3:L:46:LEU:HD21    | 1.86                     | 0.57              |
| 2:F:124:LEU:HD22 | 3:I:121:SER:H      | 1.69                     | 0.57              |
| 1:E:62:GLU:HG3   | 1:E:64:GLU:HB3     | 1.86                     | 0.57              |
| 1:E:457:ASP:OD2  | 1:E:469:ARG:NE     | 2.36                     | 0.57              |
| 2:H:180:ALA:HB2  | 2:H:190:LEU:HD12   | 1.86                     | 0.57              |
| 4:E:510:NAG:H3   | 4:E:510:NAG:C8     | 2.34                     | 0.57              |
| 2:F:195:ILE:HG12 | 2:F:210:LYS:HA     | 1.86                     | 0.57              |
| 2:F:116:THR:HA   | 2:F:146:PHE:CD1    | 2.40                     | 0.57              |
| 1:E:52:LEU:CD1   | 1:E:100:MET:HE3    | 2.35                     | 0.57              |
| 3:I:181:THR:OG1  | 3:I:184:GLN:N      | 2.34                     | 0.57              |
| 3:L:189:LYS:HZ3  | 3:L:207:ALA:HB1    | 1.69                     | 0.57              |
| 1:E:275:GLU:OE2  | 2:F:100(D):ARG:NH2 | 2.38                     | 0.57              |
| 3:L:83:GLU:HG2   | 3:L:105:THR:HA     | 1.86                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:298:ARG:HB3  | 1:G:443:ILE:HB   | 1.87                     | 0.56              |
| 3:L:14:ALA:O     | 3:L:16:GLY:N     | 2.38                     | 0.56              |
| 2:F:96:GLU:O     | 2:F:100:ASP:N    | 2.38                     | 0.56              |
| 3:L:117:LEU:HD23 | 3:L:205:THR:HA   | 1.86                     | 0.56              |
| 1:E:64:GLU:OE2   | 1:E:66:HIS:ND1   | 2.35                     | 0.56              |
| 1:G:260:LEU:O    | 1:G:451:GLY:N    | 2.37                     | 0.56              |
| 3:L:181:THR:OG1  | 3:L:184:GLN:N    | 2.32                     | 0.56              |
| 1:E:256:SER:OG   | 1:E:259:LEU:O    | 2.19                     | 0.56              |
| 3:L:148:TRP:CD1  | 3:L:159:VAL:HG11 | 2.41                     | 0.56              |
| 1:G:119:CYS:N    | 1:G:434:MET:O    | 2.38                     | 0.56              |
| 1:E:260:LEU:HB2  | 1:E:451:GLY:CA   | 2.36                     | 0.56              |
| 1:G:258:GLN:NE2  | 1:G:372:THR:O    | 2.39                     | 0.56              |
| 3:I:14:ALA:HB3   | 3:I:17:GLN:HG3   | 1.88                     | 0.56              |
| 3:L:9:SER:HB3    | 3:L:11:ALA:HB2   | 1.88                     | 0.56              |
| 1:G:260:LEU:HB2  | 1:G:451:GLY:HA3  | 1.88                     | 0.56              |
| 2:H:48:VAL:O     | 2:H:60:SER:OG    | 2.19                     | 0.56              |
| 1:E:257:THR:O    | 1:E:374:HIS:ND1  | 2.37                     | 0.56              |
| 3:L:122:SER:O    | 3:L:126:GLN:N    | 2.38                     | 0.55              |
| 3:I:122:SER:O    | 3:I:126:GLN:N    | 2.39                     | 0.55              |
| 2:H:139:SER:OG   | 2:H:141:LYS:NZ   | 2.35                     | 0.55              |
| 3:L:15:PRO:HA    | 3:L:78:LEU:HD22  | 1.88                     | 0.55              |
| 2:F:11:VAL:HG11  | 2:F:147:PRO:CB   | 2.37                     | 0.55              |
| 2:F:60:ALA:HB3   | 2:F:63:PHE:HD1   | 1.71                     | 0.55              |
| 1:G:350:LYS:HB3  | 1:G:355:ASN:HA   | 1.88                     | 0.55              |
| 1:G:300:SER:HB3  | 1:G:442:LYS:HB2  | 1.87                     | 0.55              |
| 1:E:282:LYS:NZ   | 2:F:98:ALA:O     | 2.40                     | 0.55              |
| 1:G:279:ASN:ND2  | 3:L:94:ASP:OD2   | 2.38                     | 0.55              |
| 2:H:182:LEU:CA   | 2:H:188:TYR:HA   | 2.32                     | 0.55              |
| 1:E:62:GLU:HG3   | 1:E:64:GLU:CB    | 2.37                     | 0.55              |
| 2:F:124:LEU:HD22 | 3:I:120:PRO:HA   | 1.89                     | 0.55              |
| 3:L:27:PRO:O     | 3:L:69:ASN:ND2   | 2.40                     | 0.54              |
| 3:L:46:LEU:HD22  | 3:L:49:LEU:HD23  | 1.90                     | 0.54              |
| 1:E:396:ILE:O    | 1:E:404:ASN:N    | 2.34                     | 0.54              |
| 2:F:103:TRP:HB2  | 3:I:43:ALA:HB1   | 1.88                     | 0.54              |
| 2:F:68:SER:HG    | 2:F:81:THR:HG1   | 1.20                     | 0.54              |
| 2:H:73:ASP:N     | 2:H:78:ILE:O     | 2.41                     | 0.54              |
| 3:L:184:GLN:O    | 3:L:191:TYR:OH   | 2.25                     | 0.54              |
| 2:F:60:ALA:HB3   | 2:F:63:PHE:CE1   | 2.42                     | 0.54              |
| 2:F:68:SER:OG    | 2:F:81:THR:OG1   | 2.01                     | 0.54              |
| 1:G:60:ALA:CB    | 1:G:71:THR:HG21  | 2.37                     | 0.54              |
| 1:G:62:GLU:HG3   | 1:G:64:GLU:CB    | 2.37                     | 0.54              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:167:GLN:CG   | 3:I:173:ALA:HB2  | 2.38                     | 0.54              |
| 1:G:205:CYS:SG   | 1:G:436:ALA:HB2  | 2.48                     | 0.54              |
| 2:H:86:LEU:C     | 2:H:87:LYS:HG3   | 2.31                     | 0.54              |
| 2:H:182:LEU:HB3  | 2:H:188:TYR:CZ   | 2.42                     | 0.54              |
| 2:F:161:SER:OG   | 2:F:183:THR:O    | 2.22                     | 0.54              |
| 3:L:189:LYS:NZ   | 3:L:207:ALA:HB1  | 2.23                     | 0.54              |
| 1:E:53:PHE:CE2   | 1:E:218:CYS:HB2  | 2.42                     | 0.54              |
| 1:E:111:LEU:HD23 | 1:E:115:SER:HB2  | 1.89                     | 0.53              |
| 2:F:171:GLN:O    | 2:F:174:GLY:N    | 2.41                     | 0.53              |
| 1:G:407:MET:SD   | 4:G:506:NAG:H62  | 2.49                     | 0.53              |
| 1:G:464:SER:OG   | 1:G:465:ASN:OD1  | 2.24                     | 0.53              |
| 2:H:178:PHE:N    | 2:H:191:SER:O    | 2.41                     | 0.53              |
| 3:L:111:ALA:HB1  | 3:L:112:ALA:HA   | 1.89                     | 0.53              |
| 1:E:98:ASN:OD1   | 1:E:100:MET:HG3  | 2.08                     | 0.53              |
| 2:H:167:ASN:CG   | 2:H:171:LEU:HB2  | 2.33                     | 0.53              |
| 2:H:178:PHE:HB2  | 2:H:191:SER:HB2  | 1.91                     | 0.53              |
| 2:H:215:SER:CB   | 2:H:217:THR:HG1  | 2.19                     | 0.53              |
| 1:E:257:THR:OG1  | 1:E:375:HIS:N    | 2.32                     | 0.53              |
| 1:E:268:GLU:O    | 1:E:289:ASN:ND2  | 2.33                     | 0.53              |
| 1:E:298:ARG:NH2  | 1:E:441:GLY:O    | 2.35                     | 0.53              |
| 2:H:98:ARG:NE    | 2:H:113:ASP:OD2  | 2.41                     | 0.53              |
| 2:H:182:LEU:HA   | 2:H:188:TYR:CA   | 2.32                     | 0.53              |
| 1:G:421:LYS:NZ   | 1:G:423:ILE:O    | 2.32                     | 0.53              |
| 2:H:108:ARG:N    | 2:H:109:PRO:HD3  | 2.24                     | 0.53              |
| 2:H:162:VAL:HB   | 2:H:190:LEU:HD13 | 1.91                     | 0.53              |
| 2:F:33:ILE:HG13  | 2:F:34:ILE:N     | 2.23                     | 0.53              |
| 1:G:62:GLU:HG3   | 1:G:64:GLU:HB3   | 1.90                     | 0.53              |
| 3:I:159:VAL:HG22 | 3:I:178:LEU:HD13 | 1.89                     | 0.53              |
| 1:G:343:LYS:HD3  | 1:G:396:ILE:HG23 | 1.91                     | 0.53              |
| 3:L:4:LEU:HA     | 3:L:25:GLY:HA2   | 1.91                     | 0.53              |
| 1:E:120:VAL:HB   | 1:E:434:MET:HB3  | 1.91                     | 0.53              |
| 1:E:118:PRO:HB3  | 1:E:435:TYR:CE1  | 2.44                     | 0.52              |
| 1:G:428:GLN:OE1  | 1:G:428:GLN:N    | 2.36                     | 0.52              |
| 1:G:91:GLU:O     | 1:G:238:PRO:HA   | 2.10                     | 0.52              |
| 2:H:157:TYR:CZ   | 2:H:188:TYR:HB2  | 2.45                     | 0.52              |
| 2:F:138:LEU:HD12 | 2:F:138:LEU:C    | 2.34                     | 0.52              |
| 2:H:203:THR:HG23 | 2:H:204:GLN:OE1  | 2.09                     | 0.52              |
| 1:G:230:ASP:OD1  | 1:G:241:ASN:N    | 2.41                     | 0.52              |
| 2:H:134:PHE:HB2  | 2:H:153:LEU:HD23 | 1.92                     | 0.52              |
| 2:H:182:LEU:HB3  | 2:H:188:TYR:CE2  | 2.44                     | 0.52              |
| 3:L:36:TYR:O     | 3:L:86:TYR:HA    | 2.10                     | 0.52              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 2:F:55:GLY:HA3    | 2:F:71:ARG:NE    | 2.24                     | 0.52              |
| 2:F:197:ASN:ND2   | 2:F:208:ASP:OD1  | 2.37                     | 0.52              |
| 2:H:139:SER:H     | 3:L:118:PHE:HE1  | 1.57                     | 0.52              |
| 3:L:35:TRP:CD2    | 3:L:73:LEU:HD22  | 2.44                     | 0.52              |
| 1:G:253:PRO:HA    | 1:G:479:TRP:CZ3  | 2.44                     | 0.51              |
| 3:L:189:LYS:NZ    | 3:L:190:SER:OG   | 2.41                     | 0.51              |
| 1:E:325:ASP:OD2   | 1:E:327:ARG:NH1  | 2.44                     | 0.51              |
| 3:L:91:TYR:O      | 3:L:94:ASP:N     | 2.44                     | 0.51              |
| 2:F:142:VAL:HG12  | 2:F:145:TYR:CE1  | 2.45                     | 0.51              |
| 3:I:32:TYR:CD2    | 3:I:50:ARG:HG2   | 2.45                     | 0.51              |
| 1:G:218:CYS:HA    | 1:G:247:CYS:HA   | 1.93                     | 0.51              |
| 2:H:6:GLN:HG2     | 2:H:22:CYS:SG    | 2.50                     | 0.51              |
| 2:H:14:PRO:HD2    | 2:H:125:SER:HA   | 1.92                     | 0.51              |
| 1:E:91:GLU:O      | 1:E:238:PRO:HA   | 2.10                     | 0.51              |
| 1:G:56:SER:N      | 1:G:75:VAL:O     | 2.40                     | 0.51              |
| 3:L:167:GLN:CG    | 3:L:173:ALA:HB2  | 2.41                     | 0.51              |
| 1:G:423:ILE:HA    | 1:G:433:ALA:O    | 2.11                     | 0.51              |
| 1:E:343:LYS:O     | 1:E:346:THR:OG1  | 2.22                     | 0.51              |
| 1:G:276:ASN:ND2   | 1:G:279:ASN:HB2  | 2.26                     | 0.51              |
| 2:H:156:ASP:HA    | 2:H:187:LEU:HD13 | 1.93                     | 0.51              |
| 1:E:283:THR:CG2   | 1:E:472:GLY:HA3  | 2.41                     | 0.51              |
| 2:F:100(G):MET:SD | 3:I:49:LEU:HD22  | 2.51                     | 0.51              |
| 3:L:54:ARG:HB2    | 3:L:58:VAL:HG11  | 1.93                     | 0.51              |
| 1:E:407:MET:HG2   | 1:E:408:LYS:N    | 2.25                     | 0.51              |
| 3:I:20:THR:HA     | 3:I:73:LEU:O     | 2.11                     | 0.51              |
| 3:L:142:GLY:HA3   | 3:L:172:TYR:CG   | 2.46                     | 0.50              |
| 2:H:164:VAL:HG11  | 2:H:192:SER:CB   | 2.41                     | 0.50              |
| 1:E:223:TYR:CE2   | 1:E:490:GLN:HG3  | 2.46                     | 0.50              |
| 2:F:100(A):SER:OG | 2:F:100(B):HIS:N | 2.43                     | 0.50              |
| 1:G:61:HIS:HA     | 2:F:70:SER:CB    | 2.41                     | 0.50              |
| 2:F:96:GLU:CA     | 2:F:100:ASP:HB3  | 2.42                     | 0.50              |
| 2:F:178:LEU:HD23  | 2:F:179:SER:N    | 2.26                     | 0.50              |
| 1:G:82:GLN:O      | 1:G:246:GLN:NE2  | 2.45                     | 0.50              |
| 1:G:330:TYR:CD1   | 1:G:415:THR:HG23 | 2.46                     | 0.50              |
| 2:H:111:MET:SD    | 3:L:49:LEU:HD22  | 2.52                     | 0.50              |
| 3:L:148:TRP:NE1   | 3:L:159:VAL:HG11 | 2.26                     | 0.50              |
| 1:E:297:THR:OG1   | 1:E:444:ASN:OD1  | 2.26                     | 0.50              |
| 2:F:61:HIS:N      | 2:F:61:HIS:CD2   | 2.78                     | 0.50              |
| 3:I:39:PHE:HB3    | 3:I:40:PRO:HD2   | 1.93                     | 0.50              |
| 1:G:375:HIS:ND1   | 1:G:383:PHE:O    | 2.36                     | 0.50              |
| 2:F:145:TYR:CZ    | 2:F:176:TYR:HB3  | 2.47                     | 0.50              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:72:HIS:ND1   | 1:G:72:HIS:C      | 2.69                     | 0.50              |
| 1:G:222:GLY:O    | 1:G:491:ILE:N     | 2.34                     | 0.50              |
| 2:H:124:SER:HB2  | 2:H:158:PHE:CE1   | 2.47                     | 0.50              |
| 2:F:112:SER:OG   | 2:F:114:ALA:O     | 2.29                     | 0.50              |
| 3:L:149:LYS:C    | 3:L:155:VAL:HG23  | 2.37                     | 0.50              |
| 1:E:294:ILE:HD12 | 1:E:333:ILE:HD11  | 1.92                     | 0.50              |
| 2:F:70:SER:OG    | 2:F:79:TYR:O      | 2.29                     | 0.50              |
| 1:E:258:GLN:NE2  | 1:E:373:MET:C     | 2.70                     | 0.50              |
| 3:I:119:PRO:HA   | 3:I:132:LEU:HD23  | 1.94                     | 0.50              |
| 1:G:257:THR:O    | 1:G:259:LEU:N     | 2.42                     | 0.49              |
| 1:G:475:ILE:CG2  | 1:G:479:TRP:CZ2   | 2.95                     | 0.49              |
| 3:L:54:ARG:CZ    | 3:L:60:ASP:HA     | 2.42                     | 0.49              |
| 3:I:46:LEU:HD12  | 3:I:47:LEU:N      | 2.27                     | 0.49              |
| 1:G:392:ASN:OD1  | 4:G:506:NAG:H2    | 2.11                     | 0.49              |
| 2:H:212:HIS:HB3  | 2:H:217:THR:HB    | 1.95                     | 0.49              |
| 1:E:457:ASP:CG   | 1:E:469:ARG:HE    | 2.19                     | 0.49              |
| 3:I:19:VAL:CG1   | 3:I:75:ILE:HB     | 2.42                     | 0.49              |
| 3:L:169:ASN:C    | 3:L:171:LYS:H     | 2.20                     | 0.49              |
| 2:H:36:TRP:O     | 2:H:48:VAL:HG22   | 2.12                     | 0.49              |
| 2:H:182:LEU:HB3  | 2:H:188:TYR:CE1   | 2.47                     | 0.49              |
| 3:L:2:SER:CB     | 3:L:27:PRO:HD3    | 2.42                     | 0.49              |
| 3:L:26:GLY:N     | 3:L:27:PRO:HD2    | 2.27                     | 0.49              |
| 1:E:266:ALA:HB3  | 1:E:289:ASN:HB3   | 1.94                     | 0.49              |
| 2:F:150:VAL:HG13 | 2:F:198:VAL:CG1   | 2.43                     | 0.49              |
| 2:F:169:VAL:HB   | 3:I:162:THR:HG22  | 1.94                     | 0.49              |
| 1:G:453:LEU:HD21 | 1:G:477:ASP:HB3   | 1.94                     | 0.49              |
| 2:H:60:SER:HB3   | 2:H:68:LEU:HD21   | 1.94                     | 0.49              |
| 1:E:423:ILE:HG12 | 1:E:434:MET:HB2   | 1.93                     | 0.49              |
| 1:G:260:LEU:N    | 1:G:451:GLY:O     | 2.40                     | 0.49              |
| 2:H:20:LEU:HB2   | 2:H:81:MET:HG2    | 1.94                     | 0.49              |
| 3:L:33:VAL:HG12  | 3:L:35:TRP:CD1    | 2.47                     | 0.49              |
| 3:L:91:TYR:HD1   | 3:L:91:TYR:H      | 1.60                     | 0.49              |
| 3:L:198:GLU:O    | 3:L:200:SER:N     | 2.43                     | 0.49              |
| 1:E:208:ILE:HD12 | 1:E:210:PHE:HB2   | 1.93                     | 0.49              |
| 1:G:61:HIS:CB    | 2:F:79:TYR:HB2    | 2.42                     | 0.49              |
| 2:H:4:LEU:HD12   | 2:H:114:HIS:ND1   | 2.28                     | 0.49              |
| 2:H:137:ALA:HB1  | 2:H:225:PRO:HA    | 1.94                     | 0.49              |
| 3:L:29:GLY:HA2   | 3:L:31:ASN:N      | 2.27                     | 0.49              |
| 3:L:75:ILE:HG21  | 3:L:78:LEU:HA     | 1.93                     | 0.49              |
| 2:F:15:GLY:H     | 2:F:82(C):LEU:HB2 | 1.77                     | 0.49              |
| 3:I:38:GLN:C     | 3:I:39:PHE:HD1    | 2.20                     | 0.49              |

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| Atom-1           | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|---------------------|--------------------------|-------------------|
| 2:H:180:ALA:HA   | 2:H:190:LEU:HA      | 1.95                     | 0.49              |
| 1:E:62:GLU:OE2   | 1:E:209:SER:OG      | 2.29                     | 0.49              |
| 2:F:119:PRO:HB3  | 2:F:145:TYR:HB3     | 1.94                     | 0.49              |
| 2:F:169:VAL:O    | 2:F:171:GLN:N       | 2.46                     | 0.49              |
| 3:I:196:THR:HA   | 3:I:201:THR:HA      | 1.95                     | 0.49              |
| 2:F:5:GLU:HG2    | 2:F:23:GLN:O        | 2.12                     | 0.49              |
| 2:F:200:HIS:HB3  | 2:F:205:THR:HB      | 1.95                     | 0.49              |
| 2:H:102:ALA:HA   | 2:H:108:ARG:HB3     | 1.95                     | 0.49              |
| 2:H:178:PHE:HE1  | 2:H:193:VAL:HG12    | 1.78                     | 0.49              |
| 1:E:251:ILE:HD13 | 1:E:482:GLU:HB3     | 1.93                     | 0.49              |
| 3:I:21:ILE:HD11  | 3:I:73:LEU:HD23     | 1.94                     | 0.49              |
| 3:I:37:ARG:NH2   | 3:I:46:LEU:O        | 2.46                     | 0.49              |
| 1:G:58:ALA:CB    | 1:G:70:ALA:HB3      | 2.39                     | 0.48              |
| 1:G:228:CYS:SG   | 1:G:233:PHE:CG      | 3.07                     | 0.48              |
| 2:H:137:ALA:HB3  | 2:H:226:LYS:HE3     | 1.96                     | 0.48              |
| 2:H:153:LEU:HD11 | 3:L:131:THR:HG21    | 1.95                     | 0.48              |
| 3:I:32:TYR:CG    | 3:I:50:ARG:HG2      | 2.48                     | 0.48              |
| 1:G:120:VAL:HB   | 1:G:434:MET:HB3     | 1.94                     | 0.48              |
| 1:G:260:LEU:HD22 | 1:G:478:ASN:CG      | 2.38                     | 0.48              |
| 2:F:97:ALA:HA    | 2:F:100(F):ILE:HG22 | 1.95                     | 0.48              |
| 3:I:205:THR:HG22 | 3:I:206:VAL:H       | 1.77                     | 0.48              |
| 1:G:280:ASN:HB3  | 1:G:456:ARG:CZ      | 2.44                     | 0.48              |
| 3:I:23:CYS:HB3   | 3:I:71:ALA:HB3      | 1.95                     | 0.48              |
| 1:G:363:PRO:O    | 1:G:469:ARG:NH1     | 2.41                     | 0.48              |
| 1:G:123:THR:OG1  | 1:G:430:THR:O       | 2.16                     | 0.48              |
| 3:L:27(A):SER:C  | 3:L:69:ASN:HB2      | 2.38                     | 0.48              |
| 3:L:193:CYS:H    | 3:L:203:GLU:CD      | 2.21                     | 0.48              |
| 1:E:249:HIS:ND1  | 1:E:486:TYR:OH      | 2.44                     | 0.48              |
| 2:F:166:PHE:HB2  | 2:F:179:SER:HB2     | 1.95                     | 0.48              |
| 3:I:90:THR:O     | 3:I:96:ARG:NE       | 2.47                     | 0.48              |
| 3:L:67:SER:O     | 3:L:70:SER:OG       | 2.17                     | 0.48              |
| 3:L:69:ASN:O     | 3:L:71:ALA:N        | 2.47                     | 0.48              |
| 3:L:125:LEU:HD23 | 3:L:129:LYS:O       | 2.13                     | 0.48              |
| 1:E:205:CYS:SG   | 1:E:436:ALA:HB2     | 2.54                     | 0.48              |
| 2:F:89:THR:HA    | 2:F:108:LEU:HA      | 1.95                     | 0.48              |
| 1:G:72:HIS:CE1   | 1:G:73:ALA:HB2      | 2.48                     | 0.48              |
| 1:G:475:ILE:HA   | 1:G:478:ASN:OD1     | 2.13                     | 0.48              |
| 3:L:83:GLU:HG2   | 3:L:105:THR:HB      | 1.95                     | 0.48              |
| 2:F:18:VAL:HG22  | 2:F:19:THR:N        | 2.28                     | 0.48              |
| 3:I:39:PHE:CD1   | 3:I:84:GLY:HA3      | 2.49                     | 0.48              |
| 1:E:278:THR:OG1  | 3:I:93:SER:OG       | 2.25                     | 0.48              |

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| Atom-1              | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|-------------------|--------------------------|-------------------|
| 1:E:478:ASN:O       | 1:E:481:SER:OG    | 2.31                     | 0.48              |
| 2:F:100(F):ILE:HG13 | 2:F:100(F):ILE:O  | 2.14                     | 0.48              |
| 2:F:145:TYR:OH      | 2:F:178:LEU:HB2   | 2.14                     | 0.48              |
| 3:I:167:GLN:HG2     | 3:I:173:ALA:CB    | 2.40                     | 0.48              |
| 1:G:283:THR:HG23    | 1:G:472:GLY:HA3   | 1.96                     | 0.48              |
| 1:G:477:ASP:HA      | 1:G:480:ARG:HB2   | 1.95                     | 0.48              |
| 1:E:296:CYS:HA      | 1:E:331:CYS:HA    | 1.95                     | 0.48              |
| 2:F:52:ASP:O        | 2:F:55:GLY:HA2    | 2.14                     | 0.48              |
| 1:G:279:ASN:OD1     | 1:G:281:ALA:HB3   | 2.14                     | 0.47              |
| 2:H:166:TRP:HB3     | 2:H:171:LEU:HD23  | 1.96                     | 0.47              |
| 3:L:148:TRP:CZ3     | 3:L:178:LEU:HB2   | 2.48                     | 0.47              |
| 1:E:69:TRP:HA       | 1:E:72:HIS:CD2    | 2.49                     | 0.47              |
| 1:E:469:ARG:HB3     | 2:F:56:ARG:NH2    | 2.28                     | 0.47              |
| 1:G:453:LEU:HB3     | 1:G:472:GLY:HA3   | 1.95                     | 0.47              |
| 3:I:32:TYR:CE2      | 3:I:91:TYR:HB3    | 2.49                     | 0.47              |
| 1:G:99:ASN:O        | 1:G:103:GLN:N     | 2.46                     | 0.47              |
| 1:E:210:PHE:CD1     | 1:E:210:PHE:C     | 2.92                     | 0.47              |
| 2:F:153:SER:HB2     | 2:F:157:GLY:HA2   | 1.96                     | 0.47              |
| 3:I:195:VAL:O       | 3:I:201:THR:HA    | 2.15                     | 0.47              |
| 1:E:120:VAL:HG22    | 1:E:202:LYS:HG2   | 1.97                     | 0.47              |
| 2:F:161:SER:O       | 2:F:183:THR:N     | 2.44                     | 0.47              |
| 2:H:156:ASP:HA      | 2:H:187:LEU:HB3   | 1.97                     | 0.47              |
| 3:L:87:PHE:CE2      | 3:L:101:GLY:HA3   | 2.50                     | 0.47              |
| 2:F:66:ARG:HE       | 2:F:82(B):SER:HB3 | 1.79                     | 0.47              |
| 1:G:122:LEU:HB2     | 1:G:432:GLN:HB2   | 1.96                     | 0.47              |
| 1:G:408:LYS:CG      | 1:G:409:GLY:N     | 2.77                     | 0.47              |
| 2:H:67:ARG:NH2      | 2:H:85:SER:HB3    | 2.29                     | 0.47              |
| 3:L:11:ALA:O        | 3:L:13:GLY:N      | 2.45                     | 0.47              |
| 3:L:33:VAL:CG1      | 3:L:34:TYR:N      | 2.78                     | 0.47              |
| 1:E:362:GLN:N       | 1:E:468:PHE:O     | 2.41                     | 0.47              |
| 2:F:21:SER:HB2      | 2:F:77:ILE:HD11   | 1.96                     | 0.47              |
| 1:G:279:ASN:OD1     | 1:G:281:ALA:N     | 2.42                     | 0.47              |
| 2:H:124:SER:HB2     | 2:H:158:PHE:CZ    | 2.50                     | 0.47              |
| 2:F:138:LEU:HD12    | 2:F:139:GLY:N     | 2.29                     | 0.47              |
| 1:G:63:THR:HG21     | 2:F:68:SER:HB3    | 1.97                     | 0.47              |
| 2:H:121:VAL:CG1     | 2:H:123:VAL:HG23  | 2.44                     | 0.47              |
| 2:H:172:THR:HA      | 2:H:175:VAL:HB    | 1.97                     | 0.47              |
| 2:H:182:LEU:HB3     | 2:H:188:TYR:CD2   | 2.50                     | 0.47              |
| 1:E:474:ASN:N       | 1:E:474:ASN:OD1   | 2.47                     | 0.47              |
| 2:F:198:VAL:HG12    | 2:F:199:ASN:N     | 2.29                     | 0.47              |
| 2:H:29:PHE:O        | 2:H:53:PRO:HB2    | 2.15                     | 0.47              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 2:H:154:VAL:HG12 | 2:H:157:TYR:CE1   | 2.50                     | 0.47              |
| 3:L:149:LYS:CA   | 3:L:155:VAL:HG23  | 2.45                     | 0.47              |
| 1:G:396:ILE:HD12 | 1:G:396:ILE:N     | 2.30                     | 0.46              |
| 2:H:89:ASP:OD1   | 2:H:89:ASP:N      | 2.47                     | 0.46              |
| 2:H:135:PRO:HA   | 2:H:223:VAL:HG22  | 1.97                     | 0.46              |
| 2:H:212:HIS:CE1  | 2:H:214:PRO:HG2   | 2.50                     | 0.46              |
| 3:I:147:ALA:HB3  | 3:I:194:GLN:HB2   | 1.96                     | 0.46              |
| 1:G:391:PHE:HE2  | 1:G:470:PRO:HG3   | 1.81                     | 0.46              |
| 2:H:178:PHE:HE1  | 2:H:193:VAL:CG1   | 2.28                     | 0.46              |
| 1:G:63:THR:HG21  | 2:F:68:SER:CB     | 2.46                     | 0.46              |
| 1:G:234:ASN:C    | 1:G:273:ARG:NH1   | 2.73                     | 0.46              |
| 1:G:408:LYS:HG2  | 1:G:409:GLY:N     | 2.29                     | 0.46              |
| 2:F:164:HIS:NE2  | 3:I:167:GLN:HG2   | 2.29                     | 0.46              |
| 1:G:101:VAL:HG22 | 1:G:483:LEU:CD1   | 2.45                     | 0.46              |
| 2:H:10:ALA:O     | 2:H:12:ARG:NH2    | 2.46                     | 0.46              |
| 2:F:94:ARG:O     | 2:F:100(H):PHE:HA | 2.16                     | 0.46              |
| 1:G:204:ALA:C    | 1:G:205:CYS:SG    | 2.98                     | 0.46              |
| 2:H:128:THR:HA   | 2:H:158:PHE:HD2   | 1.80                     | 0.46              |
| 1:E:207:LYS:NZ   | 1:E:439:ILE:HG23  | 2.31                     | 0.46              |
| 2:F:67:LEU:HG    | 2:F:68:SER:N      | 2.30                     | 0.46              |
| 1:G:120:VAL:HA   | 1:G:201:ILE:O     | 2.16                     | 0.46              |
| 3:L:119:PRO:HA   | 3:L:132:LEU:HD23  | 1.97                     | 0.46              |
| 2:F:82:LEU:HD12  | 2:F:82(A):THR:H   | 1.80                     | 0.46              |
| 3:I:184:GLN:O    | 3:I:191:TYR:CZ    | 2.69                     | 0.46              |
| 3:L:159:VAL:HG22 | 3:L:178:LEU:HD13  | 1.98                     | 0.46              |
| 1:E:58:ALA:HB1   | 1:E:67:ASN:O      | 2.15                     | 0.46              |
| 1:E:120:VAL:CG2  | 1:E:434:MET:HE2   | 2.46                     | 0.46              |
| 4:E:504:NAG:O6   | 3:I:32:TYR:OH     | 2.17                     | 0.46              |
| 2:H:210:VAL:HG12 | 2:H:211:ASN:N     | 2.30                     | 0.46              |
| 4:E:504:NAG:H5   | 3:I:93:SER:HA     | 1.98                     | 0.46              |
| 2:F:31:LYS:HE3   | 2:F:100:ASP:HA    | 1.97                     | 0.46              |
| 3:I:82:ASP:O     | 3:I:84:GLY:N      | 2.48                     | 0.46              |
| 1:G:95:MET:HG2   | 1:G:236:THR:HG22  | 1.98                     | 0.46              |
| 1:G:208:ILE:HD12 | 1:G:210:PHE:HB2   | 1.98                     | 0.46              |
| 3:L:78:LEU:HD23  | 3:L:79:ARG:N      | 2.31                     | 0.46              |
| 1:E:361:PHE:HE1  | 1:E:454:LEU:HD11  | 1.81                     | 0.46              |
| 2:F:101:ASP:HA   | 3:I:46:LEU:HD23   | 1.98                     | 0.46              |
| 2:F:166:PHE:HZ   | 3:I:137:SER:HB3   | 1.81                     | 0.46              |
| 3:I:139:PHE:CE2  | 3:I:173:ALA:HA    | 2.51                     | 0.46              |
| 1:G:407:MET:O    | 1:G:411:ASN:ND2   | 2.49                     | 0.45              |
| 3:L:66:LYS:HG2   | 3:L:67:SER:N      | 2.31                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:F:61:HIS:CD2   | 2:F:61:HIS:H       | 2.33                     | 0.45              |
| 1:G:439:ILE:HD11 | 1:G:443:ILE:HG12   | 1.99                     | 0.45              |
| 3:L:122:SER:O    | 3:L:125:LEU:N      | 2.49                     | 0.45              |
| 1:E:210:PHE:CE1  | 1:E:212:PRO:HD3    | 2.50                     | 0.45              |
| 2:F:36:TRP:HE1   | 2:F:78:LEU:CD2     | 2.28                     | 0.45              |
| 2:F:193:THR:HB   | 2:F:210:LYS:HE2    | 1.99                     | 0.45              |
| 1:G:457:ASP:HB2  | 1:G:467:THR:HB     | 1.98                     | 0.45              |
| 2:H:164:VAL:HG11 | 2:H:192:SER:OG     | 2.17                     | 0.45              |
| 3:L:111:ALA:HA   | 3:L:197:HIS:HD1    | 1.81                     | 0.45              |
| 1:E:284:ILE:HB   | 1:E:454:LEU:HB2    | 1.97                     | 0.45              |
| 2:F:195:ILE:HG21 | 2:F:208:ASP:HB3    | 1.97                     | 0.45              |
| 3:I:39:PHE:CE2   | 3:I:82:ASP:HA      | 2.52                     | 0.45              |
| 3:I:136:ILE:HG22 | 3:I:139:PHE:CE2    | 2.50                     | 0.45              |
| 1:G:280:ASN:HD22 | 1:G:458:GLY:CA     | 2.29                     | 0.45              |
| 1:G:286:VAL:HB   | 1:G:452:ILE:HB     | 1.98                     | 0.45              |
| 1:G:411:ASN:OD1  | 1:G:411:ASN:N      | 2.47                     | 0.45              |
| 2:H:224:GLU:HG2  | 2:H:225:PRO:O      | 2.17                     | 0.45              |
| 3:L:205:THR:HG22 | 3:L:206:VAL:H      | 1.81                     | 0.45              |
| 1:E:120:VAL:HA   | 1:E:201:ILE:O      | 2.16                     | 0.45              |
| 1:E:210:PHE:CD1  | 1:E:379:ARG:HA     | 2.50                     | 0.45              |
| 1:E:283:THR:HG23 | 1:E:472:GLY:HA3    | 1.99                     | 0.45              |
| 1:G:48:ALA:HB3   | 1:G:490:GLN:HB2    | 1.98                     | 0.45              |
| 3:L:151:ASP:OD1  | 3:L:190:SER:HB2    | 2.16                     | 0.45              |
| 2:F:116:THR:HG22 | 2:F:147:PRO:HD3    | 1.98                     | 0.45              |
| 1:G:77:THR:CG2   | 1:G:78:ASP:N       | 2.78                     | 0.45              |
| 3:L:30:GLY:O     | 3:L:66:LYS:NZ      | 2.47                     | 0.45              |
| 1:E:423:ILE:HA   | 1:E:433:ALA:O      | 2.17                     | 0.45              |
| 2:F:127:SER:O    | 2:F:129:LYS:NZ     | 2.48                     | 0.45              |
| 3:I:19:VAL:HG13  | 3:I:75:ILE:HB      | 1.98                     | 0.45              |
| 2:H:30:VAL:HG13  | 2:H:31:LYS:CG      | 2.47                     | 0.45              |
| 1:G:230:ASP:HB2  | 1:G:233:PHE:HB2    | 1.97                     | 0.45              |
| 1:E:228:CYS:O    | 1:E:485:LYS:HB2    | 2.17                     | 0.45              |
| 1:E:235:GLY:N    | 1:E:273:ARG:NH1    | 2.65                     | 0.45              |
| 1:E:374:HIS:CD2  | 1:E:376:PHE:CD1    | 3.05                     | 0.45              |
| 2:F:67:LEU:HD13  | 2:F:82:LEU:HD13    | 1.99                     | 0.45              |
| 2:F:100(F):ILE:O | 2:F:100(G):MET:HB3 | 2.16                     | 0.45              |
| 1:G:354:ASN:HB2  | 1:G:357:LYS:HG3    | 1.98                     | 0.45              |
| 3:L:65:SER:O     | 3:L:72:SER:OG      | 2.30                     | 0.45              |
| 3:L:117:LEU:CD2  | 3:L:205:THR:HA     | 2.46                     | 0.45              |
| 1:E:118:PRO:HB3  | 1:E:435:TYR:CZ     | 2.52                     | 0.45              |
| 1:G:408:LYS:CG   | 1:G:409:GLY:H      | 2.30                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:133:VAL:HG21 | 2:H:219:VAL:HG11 | 1.99                     | 0.45              |
| 2:H:181:VAL:O    | 2:H:183:GLN:N    | 2.50                     | 0.45              |
| 3:L:38:GLN:C     | 3:L:39:PHE:HD1   | 2.25                     | 0.45              |
| 1:E:65:VAL:O     | 1:E:69:TRP:CB    | 2.65                     | 0.45              |
| 1:E:123:THR:OG1  | 1:E:430:THR:O    | 2.16                     | 0.45              |
| 1:G:373:MET:HE2  | 1:G:385:CYS:C    | 2.42                     | 0.44              |
| 2:H:33:ILE:HD11  | 2:H:35:HIS:NE2   | 2.32                     | 0.44              |
| 2:H:109:PRO:HB2  | 2:H:111:MET:HE3  | 1.99                     | 0.44              |
| 3:L:136:ILE:CG2  | 3:L:195:VAL:HG11 | 2.47                     | 0.44              |
| 3:I:54:ARG:HB2   | 3:I:58:VAL:HG11  | 1.99                     | 0.44              |
| 1:G:396:ILE:N    | 1:G:396:ILE:CD1  | 2.80                     | 0.44              |
| 1:G:455:THR:OG1  | 2:H:57:ARG:NH1   | 2.50                     | 0.44              |
| 1:G:475:ILE:O    | 1:G:478:ASN:HB2  | 2.17                     | 0.44              |
| 2:H:73:ASP:HB3   | 2:H:78:ILE:HG22  | 1.98                     | 0.44              |
| 3:L:9:SER:O      | 3:L:102:THR:HB   | 2.17                     | 0.44              |
| 3:L:113:PRO:HB3  | 3:L:139:PHE:HB3  | 1.99                     | 0.44              |
| 1:E:96:TRP:HE1   | 1:E:236:THR:HG22 | 1.82                     | 0.44              |
| 1:E:330:TYR:HB2  | 1:E:416:LEU:O    | 2.18                     | 0.44              |
| 1:G:216:HIS:CE1  | 1:G:250:GLY:N    | 2.86                     | 0.44              |
| 1:G:227:LYS:HG3  | 1:G:486:TYR:CE1  | 2.53                     | 0.44              |
| 2:H:25:SER:HG    | 2:H:28:ASN:HB2   | 1.82                     | 0.44              |
| 2:H:55:ARG:H     | 2:H:55:ARG:HH11  | 1.64                     | 0.44              |
| 2:H:173:SER:C    | 2:H:175:VAL:H    | 2.25                     | 0.44              |
| 1:E:229:ASN:ND2  | 4:E:503:NAG:H62  | 2.32                     | 0.44              |
| 2:F:100(H):PHE:O | 2:F:103:TRP:NE1  | 2.44                     | 0.44              |
| 3:I:6:GLN:HE21   | 3:I:102:THR:HG23 | 1.83                     | 0.44              |
| 3:I:9:SER:CB     | 3:I:21:ILE:HG22  | 2.47                     | 0.44              |
| 2:H:20:LEU:O     | 2:H:81:MET:N     | 2.51                     | 0.44              |
| 2:H:90:ASP:HB2   | 2:H:123:VAL:HG21 | 2.00                     | 0.44              |
| 3:L:46:LEU:HD22  | 3:L:49:LEU:CD2   | 2.47                     | 0.44              |
| 1:E:286:VAL:O    | 1:E:451:GLY:HA2  | 2.17                     | 0.44              |
| 2:F:90:TYR:HE1   | 2:F:109:VAL:HG21 | 1.83                     | 0.44              |
| 1:G:121:LYS:HB3  | 1:G:201:ILE:HB   | 2.00                     | 0.44              |
| 1:G:462:ASN:C    | 1:G:464:SER:H    | 2.25                     | 0.44              |
| 2:H:166:TRP:O    | 2:H:169:GLY:N    | 2.50                     | 0.44              |
| 3:I:188:HIS:HB2  | 3:I:191:TYR:CZ   | 2.53                     | 0.44              |
| 2:H:37:VAL:HG23  | 2:H:95:PHE:HB2   | 2.00                     | 0.44              |
| 2:H:137:ALA:CB   | 2:H:226:LYS:HG3  | 2.47                     | 0.44              |
| 1:E:77:THR:CG2   | 1:E:78:ASP:N     | 2.80                     | 0.44              |
| 1:E:222:GLY:HA2  | 1:E:491:ILE:HD12 | 2.00                     | 0.44              |
| 3:I:39:PHE:HB2   | 3:I:42:THR:HG21  | 2.00                     | 0.44              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:258:GLN:NE2  | 1:G:373:MET:HA     | 2.33                     | 0.44              |
| 1:G:456:ARG:HD3  | 1:G:468:PHE:HE2    | 1.83                     | 0.44              |
| 2:H:137:ALA:CB   | 2:H:225:PRO:HA     | 2.48                     | 0.44              |
| 3:L:4:LEU:HD23   | 3:L:25:GLY:HA2     | 2.00                     | 0.44              |
| 3:L:15:PRO:HA    | 3:L:78:LEU:CD2     | 2.48                     | 0.44              |
| 3:L:117:LEU:HD23 | 3:L:205:THR:CA     | 2.47                     | 0.44              |
| 4:E:509:NAG:H82  | 4:E:509:NAG:C1     | 2.48                     | 0.44              |
| 2:H:108:ARG:N    | 2:H:109:PRO:CD     | 2.81                     | 0.44              |
| 1:E:67:ASN:HA    | 1:E:213:ILE:HD13   | 2.00                     | 0.44              |
| 2:F:18:VAL:O     | 2:F:81:THR:HG22    | 2.18                     | 0.44              |
| 2:F:166:PHE:HB3  | 2:F:167:PRO:HD2    | 2.00                     | 0.44              |
| 1:G:453:LEU:HD21 | 1:G:477:ASP:CB     | 2.47                     | 0.44              |
| 2:H:121:VAL:HG12 | 2:H:123:VAL:HG23   | 2.00                     | 0.44              |
| 2:H:178:PHE:HB2  | 2:H:191:SER:C      | 2.42                     | 0.44              |
| 1:E:349:LEU:HD22 | 1:E:353:PHE:HE2    | 1.82                     | 0.44              |
| 1:E:462:ASN:C    | 1:E:464:SER:H      | 2.26                     | 0.44              |
| 2:H:38:ARG:NH2   | 2:H:40:LYS:HE2     | 2.33                     | 0.43              |
| 1:E:64:GLU:CD    | 1:E:66:HIS:H       | 2.26                     | 0.43              |
| 2:F:94:ARG:HE    | 2:F:101:ASP:HB2    | 1.82                     | 0.43              |
| 3:I:6:GLN:HG3    | 3:I:99:GLY:HA3     | 1.99                     | 0.43              |
| 3:I:9:SER:HB2    | 3:I:21:ILE:HG22    | 2.00                     | 0.43              |
| 3:I:60:ASP:C     | 3:I:62:PHE:H       | 2.26                     | 0.43              |
| 1:G:460:ALA:H    | 3:L:95(B):ILE:HG23 | 1.83                     | 0.43              |
| 2:H:10:ALA:HA    | 2:H:120:LEU:HD13   | 2.00                     | 0.43              |
| 3:L:136:ILE:HB   | 3:L:174:ALA:HB3    | 2.01                     | 0.43              |
| 2:F:90:TYR:O     | 2:F:106:GLY:HA2    | 2.18                     | 0.43              |
| 1:G:453:LEU:HB3  | 1:G:472:GLY:CA     | 2.48                     | 0.43              |
| 3:L:120:PRO:HB3  | 3:L:130:ALA:HA     | 2.00                     | 0.43              |
| 1:G:223:TYR:CD2  | 1:G:490:GLN:HA     | 2.53                     | 0.43              |
| 3:L:183:GLU:CD   | 3:L:183:GLU:H      | 2.26                     | 0.43              |
| 1:E:69:TRP:O     | 1:E:73:ALA:N       | 2.49                     | 0.43              |
| 1:E:82:GLN:HB3   | 1:E:246:GLN:HE22   | 1.84                     | 0.43              |
| 1:E:111:LEU:HD23 | 1:E:111:LEU:C      | 2.43                     | 0.43              |
| 1:E:265:LEU:HD13 | 1:E:291:SER:N      | 2.33                     | 0.43              |
| 2:H:92:ALA:H     | 2:H:121:VAL:HB     | 1.83                     | 0.43              |
| 2:H:166:TRP:CB   | 2:H:171:LEU:HB3    | 2.48                     | 0.43              |
| 3:L:80:PRO:O     | 3:L:83:GLU:HG3     | 2.18                     | 0.43              |
| 3:L:84:GLY:O     | 3:L:103:ALA:HA     | 2.18                     | 0.43              |
| 1:E:280:ASN:HB3  | 1:E:456:ARG:CZ     | 2.49                     | 0.43              |
| 1:E:300:SER:HA   | 1:E:441:GLY:O      | 2.18                     | 0.43              |
| 1:E:359:ILE:HG23 | 1:E:468:PHE:HE2    | 1.84                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:52:LEU:HD11  | 1:E:100:MET:HE3  | 2.00                     | 0.43              |
| 2:H:4:LEU:CD1    | 2:H:114:HIS:HB3  | 2.49                     | 0.43              |
| 2:H:8:GLY:O      | 2:H:120:LEU:HD11 | 2.19                     | 0.43              |
| 2:H:64:PHE:O     | 2:H:67:ARG:N     | 2.47                     | 0.43              |
| 2:H:134:PHE:HB2  | 2:H:153:LEU:HB3  | 1.99                     | 0.43              |
| 3:L:35:TRP:CE3   | 3:L:73:LEU:HD22  | 2.54                     | 0.43              |
| 3:L:85:PHE:C     | 3:L:86:TYR:CD1   | 2.96                     | 0.43              |
| 2:F:194:TYR:HB2  | 2:F:211:VAL:HB   | 2.01                     | 0.43              |
| 2:H:27:TYR:O     | 2:H:30:VAL:HG12  | 2.19                     | 0.43              |
| 2:H:205:THR:C    | 2:H:206:TYR:CD1  | 2.97                     | 0.43              |
| 3:L:166:LYS:HD2  | 3:L:170:ASN:HA   | 1.99                     | 0.43              |
| 1:E:280:ASN:HB2  | 1:E:456:ARG:HB3  | 2.01                     | 0.43              |
| 4:E:509:NAG:H2   | 4:E:509:NAG:C6   | 2.49                     | 0.43              |
| 3:I:178:LEU:CD2  | 3:I:180:LEU:HD21 | 2.48                     | 0.43              |
| 1:G:373:MET:SD   | 1:G:384:TYR:HB3  | 2.59                     | 0.43              |
| 2:H:99:ALA:HB1   | 2:H:111:MET:H    | 1.83                     | 0.43              |
| 2:H:111:MET:HB3  | 3:L:34:TYR:CZ    | 2.54                     | 0.43              |
| 3:L:114:SER:O    | 3:L:137:SER:OG   | 2.35                     | 0.43              |
| 3:L:117:LEU:HD12 | 3:L:118:PHE:H    | 1.83                     | 0.43              |
| 1:G:62:GLU:O     | 1:G:68:VAL:HG23  | 2.19                     | 0.43              |
| 1:G:408:LYS:C    | 1:G:410:CYS:H    | 2.26                     | 0.43              |
| 2:H:92:ALA:O     | 2:H:121:VAL:HB   | 2.18                     | 0.43              |
| 2:F:20:LEU:O     | 2:F:79:TYR:HA    | 2.18                     | 0.43              |
| 1:G:52:LEU:CD1   | 1:G:100:MET:HE3  | 2.49                     | 0.42              |
| 1:G:254:VAL:O    | 1:G:478:ASN:ND2  | 2.46                     | 0.42              |
| 1:G:474:ASN:O    | 1:G:477:ASP:HB2  | 2.18                     | 0.42              |
| 2:H:138:PRO:HD2  | 2:H:225:PRO:N    | 2.33                     | 0.42              |
| 2:F:68:SER:OG    | 2:F:81:THR:O     | 2.37                     | 0.42              |
| 3:I:190:SER:HB2  | 3:I:205:THR:HG22 | 2.01                     | 0.42              |
| 1:G:254:VAL:HG11 | 1:G:261:LEU:HB2  | 2.01                     | 0.42              |
| 1:G:341:VAL:O    | 1:G:344:GLN:HB2  | 2.19                     | 0.42              |
| 3:L:4:LEU:HD23   | 3:L:25:GLY:CA    | 2.50                     | 0.42              |
| 3:L:16:GLY:N     | 3:L:78:LEU:HD22  | 2.34                     | 0.42              |
| 1:E:50:THR:HG21  | 1:E:223:TYR:CD2  | 2.54                     | 0.42              |
| 1:E:472:GLY:O    | 1:E:473:GLY:C    | 2.62                     | 0.42              |
| 2:F:200:HIS:CE1  | 2:F:202:PRO:HG2  | 2.54                     | 0.42              |
| 3:I:157:ALA:C    | 3:I:159:VAL:HG23 | 2.43                     | 0.42              |
| 3:I:205:THR:HG22 | 3:I:206:VAL:N    | 2.34                     | 0.42              |
| 2:H:154:VAL:HB   | 2:H:190:LEU:O    | 2.19                     | 0.42              |
| 1:G:270:ILE:HG12 | 1:G:288:LEU:HA   | 2.02                     | 0.42              |
| 1:G:270:ILE:HG13 | 1:G:289:ASN:ND2  | 2.34                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:H:34:ILE:CG2   | 2:H:96:CYS:HB2   | 2.49                     | 0.42              |
| 3:L:33:VAL:HG13  | 3:L:89:ALA:H     | 1.84                     | 0.42              |
| 1:E:102:GLU:O    | 1:E:106:GLU:HG3  | 2.19                     | 0.42              |
| 1:E:233:PHE:O    | 1:E:271:ILE:HG21 | 2.19                     | 0.42              |
| 1:E:258:GLN:NE2  | 1:E:371:ILE:O    | 2.52                     | 0.42              |
| 3:I:49:LEU:HD21  | 3:I:55:PRO:CG    | 2.49                     | 0.42              |
| 2:H:58:PRO:HB2   | 2:H:70:LEU:HD12  | 2.02                     | 0.42              |
| 2:H:166:TRP:C    | 2:H:171:LEU:HB3  | 2.44                     | 0.42              |
| 2:H:182:LEU:HB3  | 2:H:188:TYR:CD1  | 2.53                     | 0.42              |
| 3:L:38:GLN:HA    | 3:L:44:PRO:HA    | 2.00                     | 0.42              |
| 3:L:54:ARG:HB2   | 3:L:58:VAL:CG1   | 2.48                     | 0.42              |
| 1:E:83:GLU:HA    | 1:E:244:SER:O    | 2.20                     | 0.42              |
| 2:F:45:PHE:HB2   | 3:I:98:PHE:CD2   | 2.55                     | 0.42              |
| 2:F:189:LEU:C    | 2:F:191:THR:H    | 2.27                     | 0.42              |
| 1:G:69:TRP:HA    | 1:G:72:HIS:CD2   | 2.54                     | 0.42              |
| 2:H:39:GLN:N     | 2:H:93:THR:O     | 2.41                     | 0.42              |
| 3:L:117:LEU:HD23 | 3:L:205:THR:C    | 2.44                     | 0.42              |
| 3:L:158:GLY:O    | 3:L:179:SER:N    | 2.51                     | 0.42              |
| 2:F:33:ILE:HD11  | 2:F:50:MET:HE2   | 2.02                     | 0.42              |
| 1:G:354:ASN:OD1  | 1:G:354:ASN:N    | 2.52                     | 0.42              |
| 2:H:102:ALA:HA   | 2:H:108:ARG:CA   | 2.49                     | 0.42              |
| 3:L:27(A):SER:HA | 3:L:69:ASN:HB2   | 2.02                     | 0.42              |
| 3:L:37:ARG:HB2   | 3:L:45:THR:OG1   | 2.19                     | 0.42              |
| 3:L:196:THR:HG23 | 3:L:199:GLY:HA2  | 2.01                     | 0.42              |
| 1:E:82:GLN:O     | 1:E:246:GLN:NE2  | 2.52                     | 0.42              |
| 1:E:99:ASN:OD1   | 1:E:103:GLN:NE2  | 2.49                     | 0.42              |
| 1:E:273:ARG:NH2  | 1:E:484:TYR:CD2  | 2.88                     | 0.42              |
| 2:F:40:LYS:CG    | 2:F:88:ALA:HB2   | 2.49                     | 0.42              |
| 1:G:332:GLU:HA   | 1:G:414:ILE:O    | 2.19                     | 0.42              |
| 2:H:164:VAL:CG2  | 2:H:177:THR:HG23 | 2.50                     | 0.42              |
| 3:L:22:SER:OG    | 3:L:71:ALA:HB3   | 2.20                     | 0.42              |
| 3:L:149:LYS:HB2  | 3:L:194:GLN:HE22 | 1.84                     | 0.42              |
| 3:L:150:ALA:HB3  | 3:L:153:SER:HB3  | 2.01                     | 0.42              |
| 1:E:52:LEU:HD13  | 1:E:100:MET:HE3  | 2.00                     | 0.42              |
| 1:E:260:LEU:HB2  | 1:E:451:GLY:HA3  | 1.98                     | 0.42              |
| 1:E:298:ARG:HD2  | 1:E:298:ARG:C    | 2.45                     | 0.42              |
| 1:E:374:HIS:CD2  | 1:E:376:PHE:CE1  | 3.07                     | 0.42              |
| 1:E:376:PHE:CZ   | 1:E:383:PHE:HB3  | 2.54                     | 0.42              |
| 2:F:150:VAL:HG13 | 2:F:198:VAL:HG13 | 2.01                     | 0.42              |
| 3:I:115:VAL:CG1  | 3:I:116:THR:N    | 2.82                     | 0.42              |
| 3:I:188:HIS:N    | 3:I:191:TYR:OH   | 2.44                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:69:TRP:O     | 1:G:73:ALA:N     | 2.51                     | 0.42              |
| 1:G:227:LYS:HD3  | 1:G:229:ASN:HD21 | 1.84                     | 0.42              |
| 2:H:115:TRP:HB3  | 3:L:44:PRO:HD2   | 2.02                     | 0.42              |
| 2:H:152:CYS:SG   | 2:H:223:VAL:CG2  | 3.08                     | 0.42              |
| 2:H:182:LEU:CB   | 2:H:188:TYR:CE1  | 3.03                     | 0.42              |
| 2:F:33:ILE:CG1   | 2:F:34:ILE:N     | 2.82                     | 0.42              |
| 2:F:55:GLY:HA3   | 2:F:71:ARG:CZ    | 2.50                     | 0.42              |
| 1:G:217:TYR:H    | 1:G:248:THR:HG1  | 1.64                     | 0.42              |
| 1:E:111:LEU:O    | 1:E:115:SER:N    | 2.53                     | 0.42              |
| 1:E:280:ASN:ND2  | 1:E:458:GLY:CA   | 2.83                     | 0.42              |
| 1:E:345:VAL:HG12 | 1:E:349:LEU:CD1  | 2.50                     | 0.42              |
| 3:I:21:ILE:HG13  | 3:I:35:TRP:CZ3   | 2.54                     | 0.42              |
| 1:G:280:ASN:HB2  | 1:G:456:ARG:O    | 2.20                     | 0.41              |
| 1:G:360:ILE:HD12 | 1:G:465:ASN:HB2  | 2.02                     | 0.41              |
| 1:G:361:PHE:CD1  | 1:G:391:PHE:CD1  | 3.08                     | 0.41              |
| 2:H:33:ILE:CD1   | 2:H:50:MET:HE2   | 2.50                     | 0.41              |
| 3:L:87:PHE:CD1   | 3:L:87:PHE:N     | 2.87                     | 0.41              |
| 3:L:124:GLU:CD   | 3:L:131:THR:HG1  | 2.16                     | 0.41              |
| 3:L:132:LEU:CD1  | 3:L:180:LEU:HD11 | 2.50                     | 0.41              |
| 2:F:67:LEU:HD12  | 2:F:68:SER:H     | 1.84                     | 0.41              |
| 1:G:63:THR:CG2   | 2:F:68:SER:HB2   | 2.50                     | 0.41              |
| 2:H:178:PHE:CB   | 2:H:191:SER:HB2  | 2.50                     | 0.41              |
| 3:L:83:GLU:CG    | 3:L:105:THR:HA   | 2.50                     | 0.41              |
| 1:E:234:ASN:OD1  | 1:E:234:ASN:C    | 2.64                     | 0.41              |
| 2:F:120:SER:O    | 2:F:143:LYS:HB2  | 2.20                     | 0.41              |
| 2:F:203:SER:CB   | 2:F:205:THR:HG1  | 2.33                     | 0.41              |
| 1:G:108:VAL:O    | 1:G:112:TRP:CD1  | 2.73                     | 0.41              |
| 1:G:338:TRP:CE2  | 1:G:342:LEU:HD22 | 2.55                     | 0.41              |
| 2:H:61:ALA:C     | 2:H:63:LYS:H     | 2.27                     | 0.41              |
| 2:H:152:CYS:N    | 2:H:208:CYS:SG   | 2.93                     | 0.41              |
| 1:E:65:VAL:O     | 1:E:69:TRP:HB3   | 2.20                     | 0.41              |
| 1:E:280:ASN:HD22 | 1:E:458:GLY:N    | 2.18                     | 0.41              |
| 1:E:338:TRP:CH2  | 1:E:452:ILE:HD11 | 2.55                     | 0.41              |
| 2:F:92:CYS:O     | 2:F:104:GLY:N    | 2.52                     | 0.41              |
| 1:G:93:PHE:HB2   | 1:G:233:PHE:HZ   | 1.84                     | 0.41              |
| 1:G:423:ILE:HG12 | 1:G:434:MET:HB2  | 2.02                     | 0.41              |
| 1:E:460:ALA:HB2  | 3:I:95(A):SER:OG | 2.20                     | 0.41              |
| 3:I:125:LEU:N    | 3:I:125:LEU:HD23 | 2.36                     | 0.41              |
| 2:H:182:LEU:HB3  | 2:H:188:TYR:CG   | 2.56                     | 0.41              |
| 3:L:80:PRO:C     | 3:L:82:ASP:N     | 2.78                     | 0.41              |
| 3:I:7:PRO:O      | 3:I:102:THR:HG22 | 2.20                     | 0.41              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 3:I:23:CYS:HB2   | 3:I:35:TRP:CZ2    | 2.56                     | 0.41              |
| 1:G:264:SER:N    | 1:G:482:GLU:OE2   | 2.45                     | 0.41              |
| 2:H:171:LEU:HD21 | 2:H:194:VAL:HG21  | 2.03                     | 0.41              |
| 3:L:83:GLU:HG2   | 3:L:105:THR:CB    | 2.51                     | 0.41              |
| 3:L:149:LYS:HB2  | 3:L:192:SER:HB2   | 2.02                     | 0.41              |
| 3:L:184:GLN:HA   | 3:L:187:SER:CB    | 2.46                     | 0.41              |
| 1:E:294:ILE:HD11 | 1:E:331:CYS:HB3   | 2.03                     | 0.41              |
| 2:F:38:ARG:HA    | 2:F:89:THR:O      | 2.20                     | 0.41              |
| 2:F:100(D):ARG:N | 2:F:100(E):PRO:CD | 2.84                     | 0.41              |
| 2:F:103:TRP:CZ3  | 3:I:44:PRO:HG2    | 2.56                     | 0.41              |
| 2:H:137:ALA:HB3  | 2:H:226:LYS:CE    | 2.50                     | 0.41              |
| 3:L:166:LYS:HG2  | 3:L:167:GLN:N     | 2.36                     | 0.41              |
| 1:E:298:ARG:NH1  | 1:E:326:ILE:HB    | 2.36                     | 0.41              |
| 1:E:462:ASN:O    | 1:E:464:SER:N     | 2.53                     | 0.41              |
| 2:F:14:PRO:HG3   | 2:F:111:VAL:CG1   | 2.50                     | 0.41              |
| 2:F:52:ASP:HB3   | 2:F:52(A):PRO:HD2 | 2.02                     | 0.41              |
| 3:I:186:LYS:HG2  | 3:I:208:PRO:HG2   | 2.03                     | 0.41              |
| 1:G:118:PRO:HB2  | 1:G:434:MET:O     | 2.20                     | 0.41              |
| 1:G:353:PHE:O    | 1:G:357:LYS:HB2   | 2.20                     | 0.41              |
| 1:G:357:LYS:HE3  | 1:G:463:THR:C     | 2.46                     | 0.41              |
| 2:F:11:VAL:HG23  | 2:F:110:THR:CG2   | 2.50                     | 0.41              |
| 2:F:21:SER:HA    | 2:F:78:LEU:O      | 2.20                     | 0.41              |
| 3:I:128:ASN:HA   | 3:I:182:PRO:HG2   | 2.02                     | 0.41              |
| 3:I:130:ALA:N    | 3:I:180:LEU:O     | 2.54                     | 0.41              |
| 1:G:52:LEU:HD11  | 1:G:100:MET:HE3   | 2.03                     | 0.41              |
| 1:G:102:GLU:O    | 1:G:106:GLU:HG3   | 2.20                     | 0.41              |
| 1:G:108:VAL:HG12 | 1:G:112:TRP:CD1   | 2.56                     | 0.41              |
| 1:G:119:CYS:O    | 1:G:203:GLN:N     | 2.54                     | 0.41              |
| 1:G:254:VAL:HG13 | 4:G:502:NAG:C8    | 2.48                     | 0.41              |
| 2:H:18:VAL:HG22  | 2:H:19:THR:N      | 2.35                     | 0.41              |
| 2:H:34:ILE:HG21  | 2:H:96:CYS:HB2    | 2.03                     | 0.41              |
| 2:H:102:ALA:C    | 2:H:108:ARG:HE    | 2.29                     | 0.41              |
| 2:H:150:LEU:HD12 | 2:H:151:GLY:N     | 2.35                     | 0.41              |
| 3:L:16:GLY:CA    | 3:L:78:LEU:HB3    | 2.51                     | 0.41              |
| 3:L:95(A):SER:HA | 3:L:95(B):ILE:HA  | 1.80                     | 0.41              |
| 1:E:72:HIS:ND1   | 1:E:72:HIS:C      | 2.78                     | 0.41              |
| 2:F:45:PHE:HE1   | 3:I:87:PHE:CG     | 2.39                     | 0.41              |
| 2:F:126:PRO:HG2  | 2:F:213:PRO:HB3   | 2.03                     | 0.41              |
| 2:F:145:TYR:CE2  | 2:F:176:TYR:HB3   | 2.55                     | 0.41              |
| 2:F:171:GLN:O    | 2:F:172:SER:C     | 2.63                     | 0.41              |
| 3:I:27:PRO:C     | 3:I:27(B):ASN:H   | 2.29                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 3:I:49:LEU:HG    | 3:I:55:PRO:HG3   | 2.03                     | 0.41              |
| 1:G:111:LEU:O    | 1:G:115:SER:N    | 2.54                     | 0.41              |
| 1:G:362:GLN:HG3  | 1:G:467:THR:HG21 | 2.01                     | 0.41              |
| 4:G:504:NAG:O7   | 4:G:504:NAG:O3   | 2.33                     | 0.41              |
| 2:H:64:PHE:HB2   | 2:H:68:LEU:HB2   | 2.03                     | 0.41              |
| 2:H:97:ALA:HB1   | 2:H:112:PHE:HB3  | 2.02                     | 0.41              |
| 3:I:28:VAL:HG22  | 3:I:31:ASN:ND2   | 2.36                     | 0.41              |
| 2:H:4:LEU:HD12   | 2:H:114:HIS:HB3  | 2.02                     | 0.40              |
| 2:H:27:TYR:OH    | 2:H:32:TYR:OH    | 2.17                     | 0.40              |
| 2:H:40:LYS:O     | 2:H:42:GLY:N     | 2.54                     | 0.40              |
| 2:H:136:LEU:HD21 | 2:H:153:LEU:HB2  | 2.02                     | 0.40              |
| 2:H:182:LEU:CB   | 2:H:188:TYR:CD1  | 3.04                     | 0.40              |
| 3:L:80:PRO:O     | 3:L:83:GLU:N     | 2.50                     | 0.40              |
| 3:L:91:TYR:CG    | 3:L:92:ASP:N     | 2.89                     | 0.40              |
| 1:E:368:ASP:O    | 1:E:371:ILE:HG12 | 2.21                     | 0.40              |
| 3:I:188:HIS:ND1  | 3:I:191:TYR:OH   | 2.45                     | 0.40              |
| 1:G:256:SER:H    | 1:G:475:ILE:CD1  | 2.34                     | 0.40              |
| 2:H:4:LEU:CD2    | 2:H:24:ALA:HB2   | 2.51                     | 0.40              |
| 1:E:72:HIS:CE1   | 1:E:73:ALA:HB2   | 2.56                     | 0.40              |
| 1:E:120:VAL:O    | 1:E:434:MET:N    | 2.53                     | 0.40              |
| 1:E:392:ASN:HB3  | 1:E:395:CYS:HB2  | 2.01                     | 0.40              |
| 3:I:31:ASN:HB2   | 3:I:91:TYR:CZ    | 2.56                     | 0.40              |
| 3:I:129:LYS:HA   | 3:I:182:PRO:HD3  | 2.03                     | 0.40              |
| 3:I:149:LYS:HB2  | 3:I:192:SER:HB2  | 2.02                     | 0.40              |
| 1:G:210:PHE:CD1  | 1:G:210:PHE:C    | 2.99                     | 0.40              |
| 1:G:229:ASN:ND2  | 4:G:501:NAG:H82  | 2.35                     | 0.40              |
| 2:H:102:ALA:HA   | 2:H:108:ARG:HA   | 2.02                     | 0.40              |
| 3:I:49:LEU:HD21  | 3:I:55:PRO:HG2   | 2.02                     | 0.40              |
| 3:I:185:TRP:CZ3  | 3:I:206:VAL:HB   | 2.56                     | 0.40              |
| 1:G:407:MET:HG2  | 1:G:408:LYS:N    | 2.36                     | 0.40              |
| 1:G:457:ASP:CG   | 2:H:59:TRP:CH2   | 2.99                     | 0.40              |
| 2:H:94:TYR:CE1   | 2:H:121:VAL:HG21 | 2.57                     | 0.40              |
| 2:H:138:PRO:HD2  | 2:H:225:PRO:CD   | 2.51                     | 0.40              |
| 2:H:156:ASP:CB   | 2:H:187:LEU:HD13 | 2.52                     | 0.40              |
| 2:H:173:SER:C    | 2:H:175:VAL:N    | 2.77                     | 0.40              |
| 3:L:117:LEU:HD12 | 3:L:118:PHE:N    | 2.36                     | 0.40              |
| 3:L:178:LEU:HD12 | 3:L:179:SER:H    | 1.85                     | 0.40              |
| 1:E:67:ASN:HA    | 1:E:213:ILE:CD1  | 2.52                     | 0.40              |
| 2:F:85:ASP:OD1   | 2:F:85:ASP:N     | 2.54                     | 0.40              |
| 2:F:124:LEU:HD13 | 3:I:120:PRO:HA   | 2.03                     | 0.40              |
| 3:I:37:ARG:CD    | 3:I:47:LEU:HD21  | 2.51                     | 0.40              |

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| Atom-1         | Atom-2        | Interatomic distance (Å) | Clash overlap (Å) |
|----------------|---------------|--------------------------|-------------------|
| 1:G:227:LYS:HA | 1:G:485:LYS:O | 2.21                     | 0.40              |
| 2:H:37:VAL:HA  | 2:H:46:GLU:O  | 2.22                     | 0.40              |
| 3:I:6:GLN:HE22 | 3:I:87:PHE:HA | 1.86                     | 0.40              |

All (24) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1           | Atom-2                  | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------------|--------------------------|-------------------|
| 2:H:63:LYS:C     | 3:L:152:SER:OG[2_656]   | 1.03                     | 1.17              |
| 2:H:63:LYS:HA    | 3:L:152:SER:HG[2_656]   | 0.62                     | 0.98              |
| 2:H:140:SER:HB2  | 2:H:182:LEU:HD12[2_646] | 0.90                     | 0.70              |
| 2:H:63:LYS:O     | 3:L:152:SER:OG[2_656]   | 1.62                     | 0.58              |
| 2:H:63:LYS:CA    | 3:L:152:SER:HG[2_656]   | 1.06                     | 0.54              |
| 2:H:63:LYS:HA    | 3:L:152:SER:OG[2_656]   | 1.21                     | 0.39              |
| 2:H:140:SER:HB2  | 2:H:182:LEU:CD1[2_646]  | 1.21                     | 0.39              |
| 2:H:63:LYS:O     | 3:L:152:SER:CB[2_656]   | 1.84                     | 0.36              |
| 2:H:140:SER:CB   | 2:H:182:LEU:HD12[2_646] | 1.28                     | 0.32              |
| 2:H:140:SER:HG   | 2:H:182:LEU:O[2_646]    | 1.32                     | 0.28              |
| 2:H:63:LYS:C     | 3:L:152:SER:CB[2_656]   | 1.95                     | 0.25              |
| 2:H:155:LYS:NZ   | 2:H:201:LEU:O[2_656]    | 1.96                     | 0.24              |
| 2:H:38:ARG:NH2   | 3:L:189:LYS:O[2_656]    | 1.98                     | 0.22              |
| 2:H:205:THR:O    | 3:L:179:SER:HG[2_646]   | 1.41                     | 0.19              |
| 2:H:140:SER:CB   | 2:H:182:LEU:CD1[2_646]  | 2.03                     | 0.17              |
| 2:H:205:THR:O    | 3:L:179:SER:OG[2_646]   | 2.07                     | 0.13              |
| 2:H:64:PHE:N     | 3:L:152:SER:OG[2_656]   | 2.08                     | 0.12              |
| 3:L:53:GLN:OE1   | 3:L:168:SER:OG[2_556]   | 2.09                     | 0.11              |
| 2:H:63:LYS:O     | 3:L:152:SER:HB3[2_656]  | 1.53                     | 0.07              |
| 2:H:205:THR:OG1  | 3:L:158:GLY:O[2_646]    | 2.14                     | 0.06              |
| 2:H:140:SER:OG   | 2:H:182:LEU:O[2_646]    | 2.15                     | 0.05              |
| 1:G:46:LYS:HZ2   | 3:L:196:THR:OG1[2_556]  | 1.56                     | 0.04              |
| 2:H:90:ASP:OD1   | 3:L:207:ALA:H[2_656]    | 1.58                     | 0.02              |
| 2:H:209:ASN:HD21 | 3:L:156:LYS:O[2_646]    | 1.58                     | 0.02              |

## 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   | E     | 343/353 (97%)   | 323 (94%)  | 18 (5%)   | 2 (1%)   | 21          | 49 |
| 1   | G     | 343/353 (97%)   | 325 (95%)  | 15 (4%)   | 3 (1%)   | 14          | 41 |
| 2   | F     | 217/227 (96%)   | 184 (85%)  | 31 (14%)  | 2 (1%)   | 14          | 41 |
| 2   | H     | 219/227 (96%)   | 180 (82%)  | 35 (16%)  | 4 (2%)   | 6           | 26 |
| 3   | I     | 196/215 (91%)   | 171 (87%)  | 21 (11%)  | 4 (2%)   | 6           | 24 |
| 3   | L     | 205/215 (95%)   | 172 (84%)  | 29 (14%)  | 4 (2%)   | 6           | 24 |
| All | All   | 1523/1590 (96%) | 1355 (89%) | 149 (10%) | 19 (1%)  | 10          | 34 |

All (19) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 473 | GLY  |
| 2   | H     | 55  | ARG  |
| 3   | L     | 199 | GLY  |
| 1   | E     | 473 | GLY  |
| 1   | G     | 397 | GLY  |
| 3   | L     | 15  | PRO  |
| 1   | E     | 397 | GLY  |
| 2   | F     | 170 | LEU  |
| 3   | I     | 15  | PRO  |
| 3   | L     | 111 | ALA  |
| 3   | I     | 83  | GLU  |
| 3   | I     | 55  | PRO  |
| 2   | H     | 113 | ASP  |
| 3   | L     | 55  | PRO  |
| 3   | I     | 151 | ASP  |
| 1   | G     | 124 | GLY  |
| 2   | F     | 123 | PRO  |
| 2   | H     | 41  | PRO  |
| 2   | H     | 161 | 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   | E     | 309/311 (99%)   | 300 (97%)  | 9 (3%)   | 37          | 60 |
| 1   | G     | 309/311 (99%)   | 301 (97%)  | 8 (3%)   | 40          | 61 |
| 2   | F     | 188/194 (97%)   | 177 (94%)  | 11 (6%)  | 18          | 44 |
| 2   | H     | 190/194 (98%)   | 178 (94%)  | 12 (6%)  | 16          | 42 |
| 3   | I     | 165/177 (93%)   | 157 (95%)  | 8 (5%)   | 23          | 49 |
| 3   | L     | 168/177 (95%)   | 159 (95%)  | 9 (5%)   | 20          | 47 |
| All | All   | 1329/1364 (97%) | 1272 (96%) | 57 (4%)  | 26          | 51 |

All (57) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 72  | HIS  |
| 1   | G     | 77  | THR  |
| 1   | G     | 289 | ASN  |
| 1   | G     | 394 | THR  |
| 1   | G     | 396 | ILE  |
| 1   | G     | 421 | LYS  |
| 1   | G     | 462 | ASN  |
| 1   | G     | 465 | ASN  |
| 2   | H     | 18  | VAL  |
| 2   | H     | 33  | ILE  |
| 2   | H     | 62  | HIS  |
| 2   | H     | 79  | LEU  |
| 2   | H     | 81  | MET  |
| 2   | H     | 89  | ASP  |
| 2   | H     | 110 | ILE  |
| 2   | H     | 120 | LEU  |
| 2   | H     | 128 | THR  |
| 2   | H     | 150 | LEU  |
| 2   | H     | 181 | VAL  |
| 2   | H     | 204 | GLN  |
| 3   | L     | 33  | VAL  |
| 3   | L     | 45  | THR  |
| 3   | L     | 49  | LEU  |
| 3   | L     | 58  | VAL  |
| 3   | L     | 104 | LEU  |
| 3   | L     | 105 | THR  |
| 3   | L     | 159 | VAL  |
| 3   | L     | 161 | THR  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | L     | 181 | THR  |
| 1   | E     | 44  | VAL  |
| 1   | E     | 72  | HIS  |
| 1   | E     | 77  | THR  |
| 1   | E     | 200 | VAL  |
| 1   | E     | 394 | THR  |
| 1   | E     | 396 | ILE  |
| 1   | E     | 404 | ASN  |
| 1   | E     | 421 | LYS  |
| 1   | E     | 465 | ASN  |
| 2   | F     | 33  | ILE  |
| 2   | F     | 48  | VAL  |
| 2   | F     | 61  | HIS  |
| 2   | F     | 85  | ASP  |
| 2   | F     | 112 | SER  |
| 2   | F     | 128 | SER  |
| 2   | F     | 146 | PHE  |
| 2   | F     | 169 | VAL  |
| 2   | F     | 191 | THR  |
| 2   | F     | 192 | GLN  |
| 2   | F     | 196 | CYS  |
| 3   | I     | 33  | VAL  |
| 3   | I     | 45  | THR  |
| 3   | I     | 46  | LEU  |
| 3   | I     | 104 | LEU  |
| 3   | I     | 105 | THR  |
| 3   | I     | 125 | LEU  |
| 3   | I     | 161 | THR  |
| 3   | I     | 181 | THR  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 276 | ASN  |
| 2   | H     | 23  | GLN  |
| 1   | E     | 72  | HIS  |
| 1   | E     | 339 | ASN  |
| 1   | E     | 393 | ASN  |
| 2   | F     | 23  | GLN  |
| 3   | I     | 6   | GLN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

16 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  | E     | 502 | 1    | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.63 | 1 (5%)      |
| 4   | NAG  | G     | 503 | 1    | 14,14,15     | 0.69 | 1 (7%)      | 17,19,21    | 0.90 | 1 (5%)      |
| 4   | NAG  | E     | 503 | 1    | 14,14,15     | 0.74 | 1 (7%)      | 17,19,21    | 0.55 | 0           |
| 4   | NAG  | E     | 507 | 1    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.66 | 0           |
| 4   | NAG  | G     | 501 | 1    | 14,14,15     | 0.55 | 0           | 17,19,21    | 0.96 | 1 (5%)      |
| 4   | NAG  | E     | 501 | -    | 14,14,15     | 0.24 | 0           | 17,19,21    | 0.78 | 1 (5%)      |
| 4   | NAG  | G     | 506 | 1    | 14,14,15     | 0.48 | 0           | 17,19,21    | 0.73 | 0           |
| 4   | NAG  | E     | 504 | 1    | 14,14,15     | 0.83 | 1 (7%)      | 17,19,21    | 0.80 | 1 (5%)      |
| 4   | NAG  | E     | 510 | 1    | 14,14,15     | 0.39 | 0           | 17,19,21    | 1.18 | 1 (5%)      |
| 4   | NAG  | G     | 504 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.45 | 0           |
| 4   | NAG  | E     | 509 | 1    | 14,14,15     | 0.39 | 0           | 17,19,21    | 1.76 | 3 (17%)     |
| 4   | NAG  | E     | 505 | 1    | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.93 | 1 (5%)      |
| 4   | NAG  | E     | 506 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.87 | 0           |
| 4   | NAG  | G     | 502 | 1    | 14,14,15     | 0.21 | 0           | 17,19,21    | 1.06 | 1 (5%)      |
| 4   | NAG  | E     | 508 | 1    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.73 | 1 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | G     | 505 | 1    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.56 | 0        |

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  | E     | 502 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 503 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 503 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 507 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 501 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 501 | -    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 506 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 504 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 510 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 504 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 509 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 505 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 506 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 502 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | E     | 508 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 505 | 1    | -       | 4/6/23/26 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | E     | 504 | NAG  | C1-C2 | 3.01 | 1.56        | 1.52     |
| 4   | E     | 503 | NAG  | C1-C2 | 2.41 | 1.55        | 1.52     |
| 4   | G     | 503 | NAG  | O5-C1 | 2.13 | 1.47        | 1.43     |

All (12) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | E     | 509 | NAG  | C1-O5-C5 | 4.62 | 118.38      | 112.19   |
| 4   | E     | 509 | NAG  | C2-N2-C7 | 4.27 | 128.63      | 122.90   |
| 4   | E     | 510 | NAG  | C2-N2-C7 | 3.91 | 128.15      | 122.90   |
| 4   | G     | 502 | NAG  | C1-O5-C5 | 3.59 | 116.99      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 4   | G     | 501 | NAG  | C1-O5-C5 | 3.51 | 116.90      | 112.19   |
| 4   | G     | 503 | NAG  | C1-O5-C5 | 3.38 | 116.72      | 112.19   |
| 4   | E     | 505 | NAG  | C1-O5-C5 | 3.29 | 116.59      | 112.19   |
| 4   | E     | 501 | NAG  | C1-O5-C5 | 2.83 | 115.98      | 112.19   |
| 4   | E     | 509 | NAG  | C1-C2-N2 | 2.68 | 114.66      | 110.43   |
| 4   | E     | 508 | NAG  | C1-O5-C5 | 2.25 | 115.21      | 112.19   |
| 4   | E     | 502 | NAG  | C1-O5-C5 | 2.07 | 114.96      | 112.19   |
| 4   | E     | 504 | NAG  | C1-O5-C5 | 2.04 | 114.92      | 112.19   |

There are no chirality outliers.

All (42) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | E     | 501 | NAG  | C1-C2-N2-C7 |
| 4   | E     | 509 | NAG  | C1-C2-N2-C7 |
| 4   | E     | 505 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 503 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 507 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 506 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 509 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 501 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 502 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 505 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 505 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 503 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 506 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 504 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 502 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 507 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 505 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 501 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 509 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 504 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 505 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 505 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 506 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 506 | NAG  | O7-C7-N2-C2 |
| 4   | E     | 507 | NAG  | C8-C7-N2-C2 |
| 4   | E     | 507 | NAG  | O7-C7-N2-C2 |
| 4   | E     | 509 | NAG  | C8-C7-N2-C2 |
| 4   | E     | 509 | NAG  | O7-C7-N2-C2 |
| 4   | E     | 510 | NAG  | C8-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | E     | 510 | NAG  | O7-C7-N2-C2 |
| 4   | E     | 508 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 510 | NAG  | O5-C5-C6-O6 |
| 4   | E     | 510 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 502 | NAG  | C3-C2-N2-C7 |
| 4   | E     | 503 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 502 | NAG  | C1-C2-N2-C7 |
| 4   | E     | 508 | NAG  | C4-C5-C6-O6 |
| 4   | E     | 504 | NAG  | C3-C2-N2-C7 |
| 4   | E     | 510 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 504 | NAG  | C3-C2-N2-C7 |
| 4   | E     | 502 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 504 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

9 monomers are involved in 21 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | E     | 503 | NAG  | 2       | 0            |
| 4   | G     | 501 | NAG  | 2       | 0            |
| 4   | G     | 506 | NAG  | 4       | 0            |
| 4   | E     | 504 | NAG  | 3       | 0            |
| 4   | E     | 510 | NAG  | 2       | 0            |
| 4   | G     | 504 | NAG  | 1       | 0            |
| 4   | E     | 509 | NAG  | 2       | 0            |
| 4   | G     | 502 | NAG  | 4       | 0            |
| 4   | E     | 508 | NAG  | 1       | 0            |

## 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   | E     | 347/353 (98%)   | -0.32  | 3 (0%) 81 68  | 77, 180, 442, 606     | 0     |
| 1   | G     | 347/353 (98%)   | -0.36  | 4 (1%) 76 62  | 71, 167, 384, 622     | 0     |
| 2   | F     | 221/227 (97%)   | -0.25  | 1 (0%) 87 77  | 97, 207, 535, 636     | 0     |
| 2   | H     | 223/227 (98%)   | -0.33  | 6 (2%) 56 41  | 84, 184, 504, 597     | 0     |
| 3   | I     | 200/215 (93%)   | -0.25  | 4 (2%) 65 49  | 99, 192, 509, 629     | 0     |
| 3   | L     | 209/215 (97%)   | -0.18  | 5 (2%) 59 44  | 97, 198, 570, 627     | 0     |
| All | All   | 1547/1590 (97%) | -0.29  | 23 (1%) 72 57 | 71, 185, 507, 636     | 0     |

All (23) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 264 | SER  | 3.6  |
| 2   | H     | 18  | VAL  | 3.3  |
| 1   | E     | 463 | THR  | 3.0  |
| 3   | L     | 12  | SER  | 2.4  |
| 3   | I     | 12  | SER  | 2.4  |
| 3   | I     | 28  | VAL  | 2.4  |
| 3   | I     | 68  | GLY  | 2.4  |
| 2   | H     | 213 | LYS  | 2.3  |
| 3   | I     | 105 | THR  | 2.3  |
| 1   | E     | 250 | GLY  | 2.3  |
| 1   | G     | 283 | THR  | 2.3  |
| 2   | H     | 56  | GLY  | 2.2  |
| 1   | G     | 284 | ILE  | 2.2  |
| 3   | L     | 46  | LEU  | 2.2  |
| 1   | G     | 367 | GLY  | 2.2  |
| 2   | F     | 181 | VAL  | 2.2  |
| 3   | L     | 144 | VAL  | 2.1  |
| 3   | L     | 47  | LEU  | 2.1  |
| 3   | L     | 56  | SER  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2   | H     | 66  | GLY  | 2.1  |
| 2   | H     | 200 | SER  | 2.1  |
| 1   | G     | 252 | LYS  | 2.1  |
| 2   | H     | 9   | THR  | 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  | G     | 501 | 14/15 | 0.95 | 0.09 | 98,157,226,334              | 0     |
| 4   | NAG  | E     | 503 | 14/15 | 0.95 | 0.06 | 73,114,157,193              | 0     |
| 4   | NAG  | E     | 509 | 14/15 | 0.95 | 0.08 | 57,73,118,127               | 0     |
| 4   | NAG  | G     | 504 | 14/15 | 0.96 | 0.11 | 98,144,250,250              | 0     |
| 4   | NAG  | E     | 506 | 14/15 | 0.96 | 0.09 | 117,150,180,183             | 0     |
| 4   | NAG  | G     | 505 | 14/15 | 0.96 | 0.08 | 84,139,189,227              | 0     |
| 4   | NAG  | E     | 510 | 14/15 | 0.96 | 0.07 | 74,153,204,223              | 0     |
| 4   | NAG  | E     | 504 | 14/15 | 0.97 | 0.06 | 98,148,184,193              | 0     |
| 4   | NAG  | G     | 506 | 14/15 | 0.97 | 0.09 | 96,186,232,279              | 0     |
| 4   | NAG  | E     | 508 | 14/15 | 0.97 | 0.09 | 97,126,157,181              | 0     |
| 4   | NAG  | E     | 501 | 14/15 | 0.97 | 0.06 | 71,103,199,199              | 0     |
| 4   | NAG  | G     | 503 | 14/15 | 0.97 | 0.08 | 100,140,214,237             | 0     |
| 4   | NAG  | E     | 507 | 14/15 | 0.98 | 0.06 | 88,116,149,179              | 0     |
| 4   | NAG  | E     | 502 | 14/15 | 0.98 | 0.08 | 94,127,225,267              | 0     |
| 4   | NAG  | E     | 505 | 14/15 | 0.98 | 0.07 | 117,155,206,210             | 0     |
| 4   | NAG  | G     | 502 | 14/15 | 0.98 | 0.09 | 81,133,246,246              | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.