



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:07 AM UTC

PDB ID : 2QTS / pdb\_00002qts  
Title : Structure of an acid-sensing ion channel 1 at 1.9 Å resolution and low pH  
Authors : Jasti, J.; Furukawa, H.; Gonzales, E.B.; Gouaux, E.  
Deposited on : 2007-08-02  
Resolution : 1.90 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:

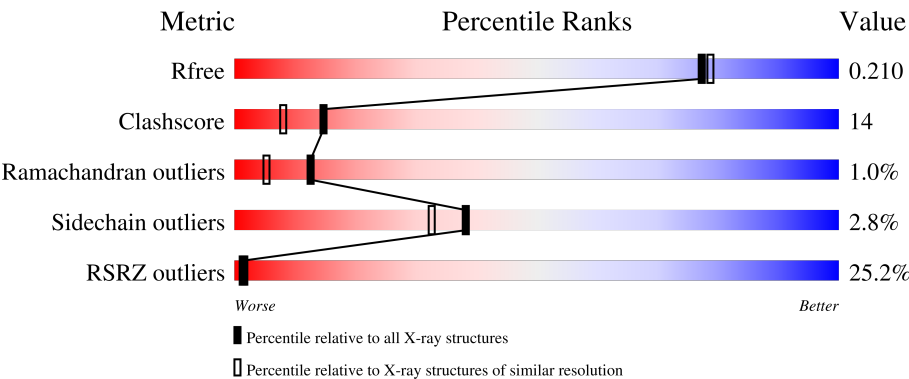
MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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                      | 7789 (1.90-1.90)                                      |
| Clashscore            | 190562                      | 8410 (1.90-1.90)                                      |
| Ramachandran outliers | 187476                      | 8333 (1.90-1.90)                                      |
| Sidechain outliers    | 187428                      | 8333 (1.90-1.90)                                      |
| RSRZ outliers         | 180081                      | 7790 (1.90-1.90)                                      |

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

| Mol | Chain | Length | Quality of chain                                                   |
|-----|-------|--------|--------------------------------------------------------------------|
| 1   | A     | 438    | <div><div>23%</div><div>67%</div><div>25%</div><div>5%</div></div> |
| 1   | B     | 438    | <div><div>21%</div><div>70%</div><div>23%</div><div>5%</div></div> |
| 1   | C     | 438    | <div><div>21%</div><div>68%</div><div>23%</div><div>5%</div></div> |
| 1   | D     | 438    | <div><div>26%</div><div>67%</div><div>26%</div><div>5%</div></div> |
| 1   | E     | 438    | <div><div>30%</div><div>66%</div><div>28%</div><div>5%</div></div> |

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| Mol | Chain | Length | Quality of chain                                                              |
|-----|-------|--------|-------------------------------------------------------------------------------|
| 1   | F     | 438    | <div><div></div><div>22%</div><div>68%</div><div>24%</div><div>6%</div></div> |
| 2   | G     | 2      | <div><div></div><div>100%</div></div>                                         |
| 2   | H     | 2      | <div><div></div><div>50%</div><div>50%</div></div>                            |
| 2   | I     | 2      | <div><div></div><div>50%</div><div>50%</div></div>                            |

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 22034 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acid-sensing ion channel.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 417      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3345  | 2144 | 541 | 633 | 27 |         |         |       |
| 1   | B     | 420      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3369  | 2161 | 545 | 636 | 27 |         |         |       |
| 1   | C     | 418      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3350  | 2148 | 542 | 633 | 27 |         |         |       |
| 1   | D     | 415      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3324  | 2130 | 539 | 628 | 27 |         |         |       |
| 1   | E     | 421      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3375  | 2164 | 546 | 638 | 27 |         |         |       |
| 1   | F     | 412      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 3299  | 2114 | 536 | 622 | 27 |         |         |       |

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|---------|-------|
| 2   | G     | 2        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 23    | 12 | 11 |         |         |       |
| 2   | H     | 2        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 23    | 12 | 11 |         |         |       |
| 2   | I     | 2        | Total | C  | O  | 0       | 0       | 0     |
|     |       |          | 23    | 12 | 11 |         |         |       |

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | A     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | B     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | C     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | D     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | E     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 3   | F     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 4   | A     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | B     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | C     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | D     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | E     | 1        | Total Cl<br>1 1 | 0       | 0       |
| 4   | F     | 1        | Total Cl<br>1 1 | 0       | 0       |

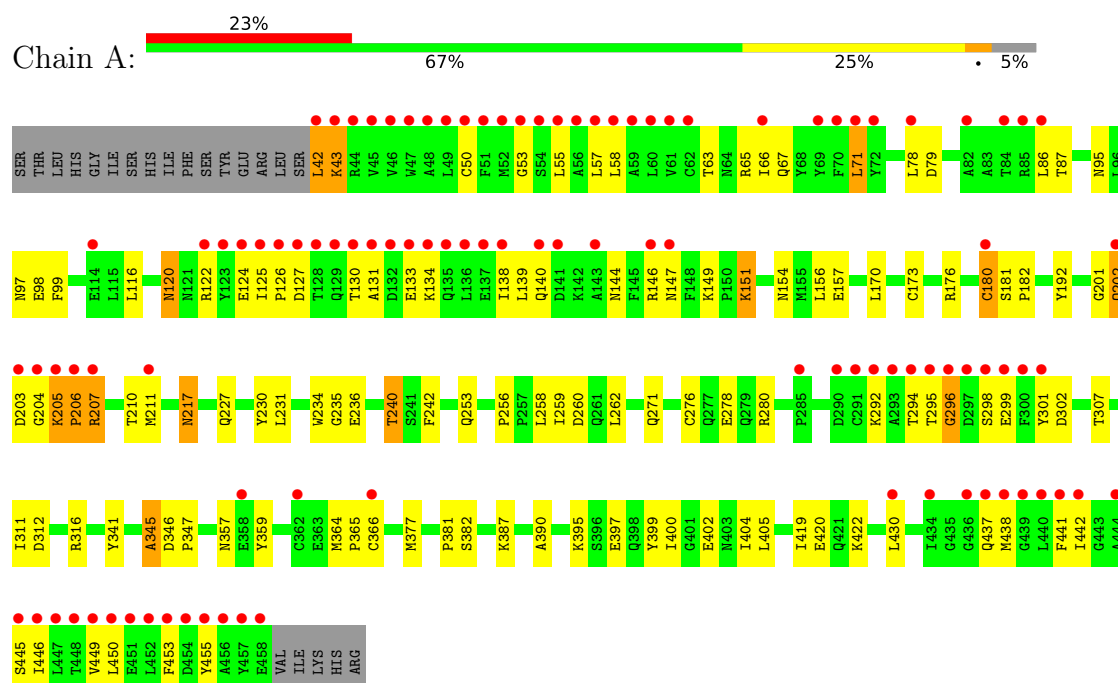
- Molecule 5 is water.

| Mol | Chain | Residues | Atoms              | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 5   | A     | 285      | Total O<br>285 285 | 0       | 0       |
| 5   | B     | 280      | Total O<br>280 280 | 0       | 0       |
| 5   | C     | 302      | Total O<br>302 302 | 0       | 0       |
| 5   | D     | 270      | Total O<br>270 270 | 0       | 0       |
| 5   | E     | 292      | Total O<br>292 292 | 0       | 0       |
| 5   | F     | 300      | Total O<br>300 300 | 0       | 0       |

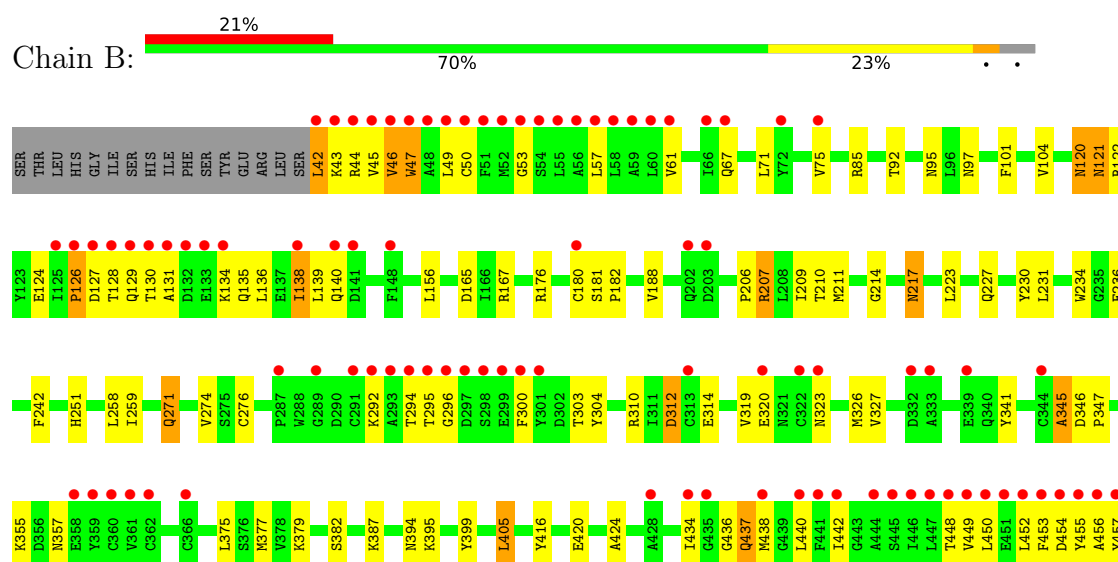
### 3 Residue-property plots [i](#)

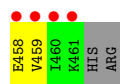
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: Acid-sensing ion channel

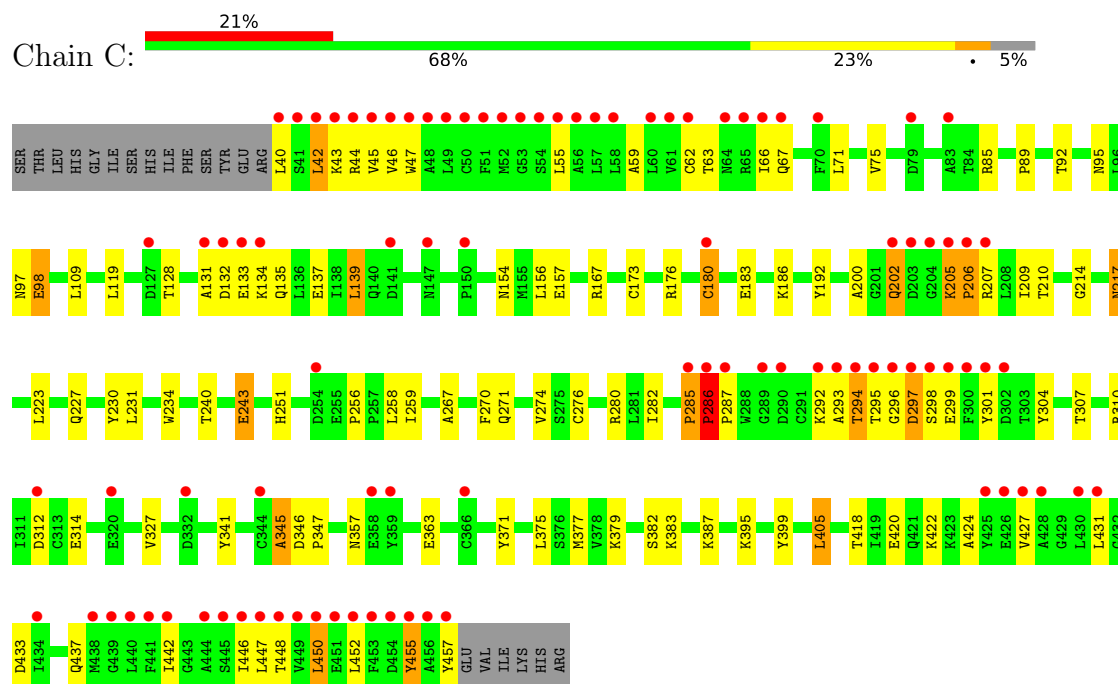


#### • Molecule 1: Acid-sensing ion channel

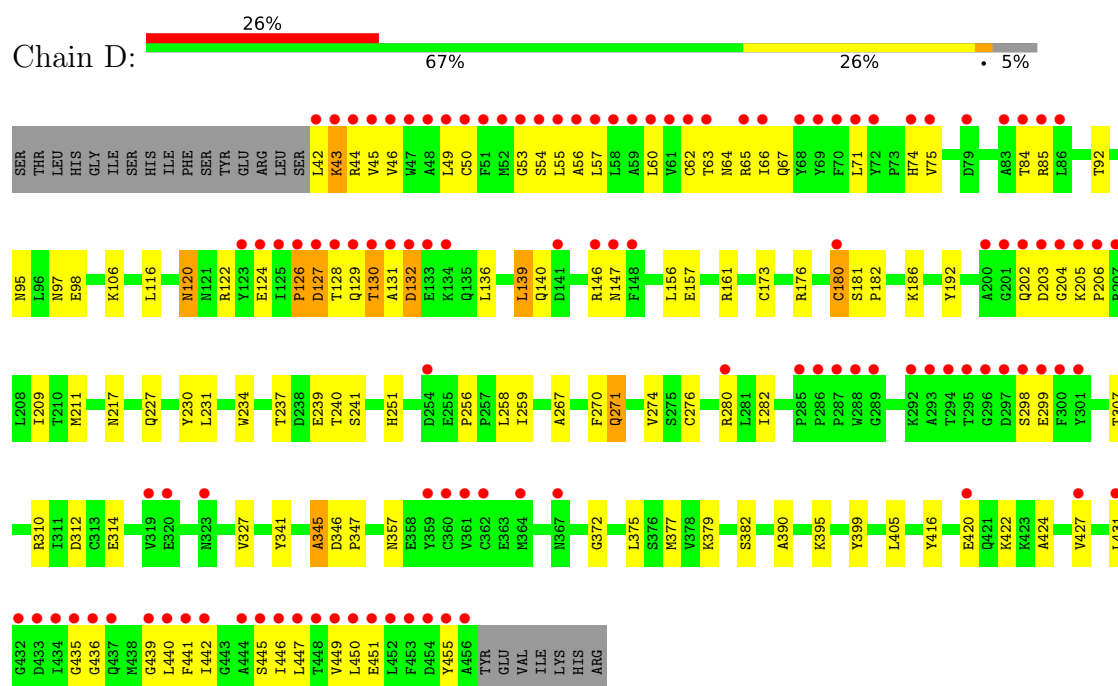




• Molecule 1: Acid-sensing ion channel

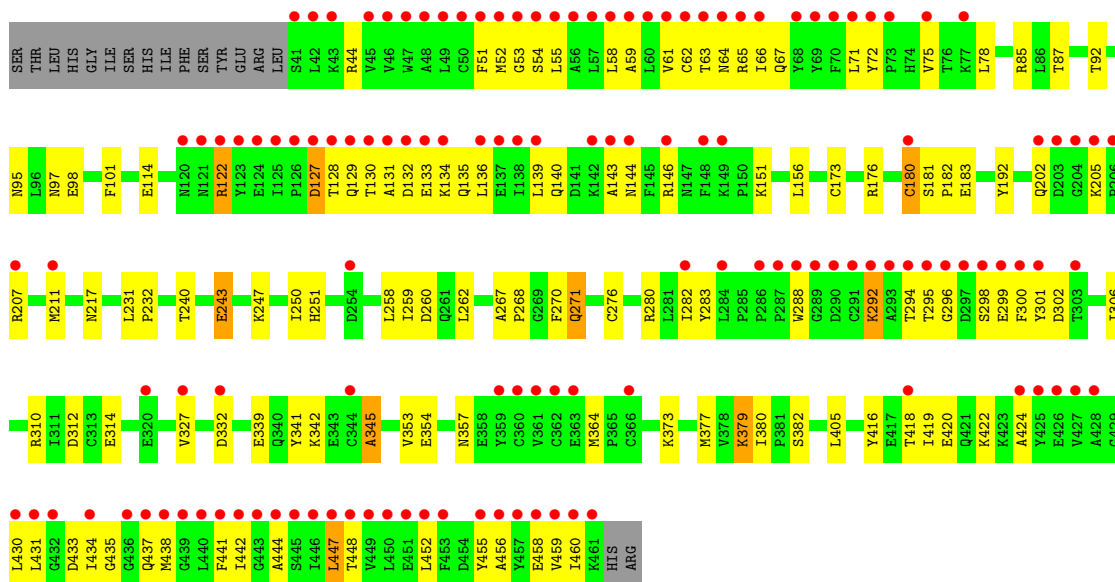


• Molecule 1: Acid-sensing ion channel

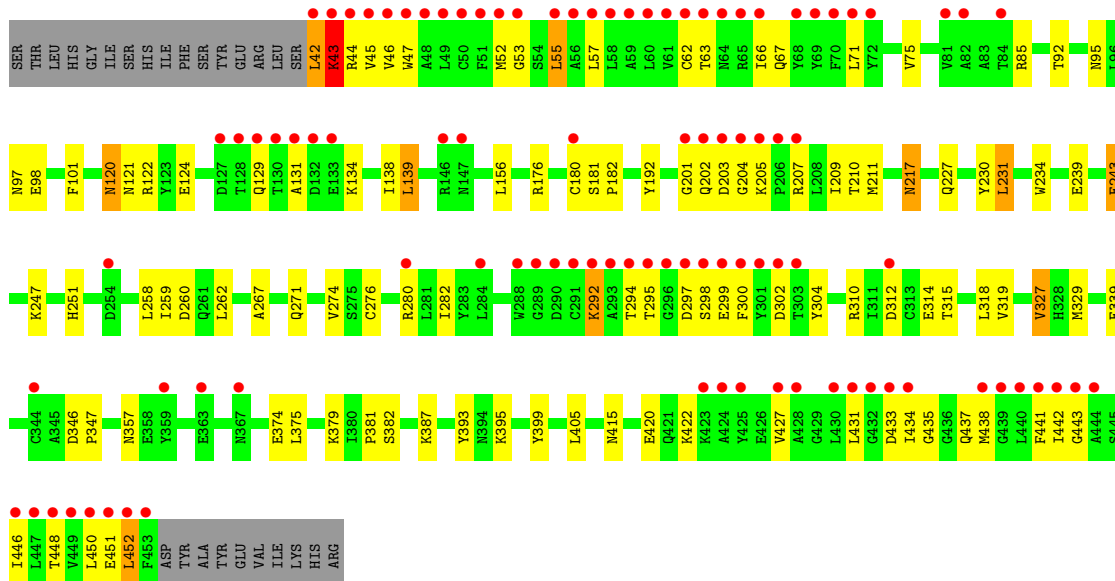


• Molecule 1: Acid-sensing ion channel

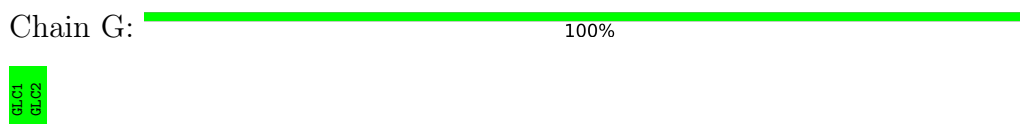




• Molecule 1: Acid-sensing ion channel



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:  50% 50%



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 1 21 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 124.25Å 110.78Å 149.89Å<br>90.00° 97.54° 90.00°             | Depositor        |
| Resolution (Å)                                                          | 30.00 – 1.90<br>30.00 – 1.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 88.4 (30.00-1.90)<br>88.4 (30.00-1.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.06                                                        | Depositor        |
| $R_{sym}$                                                               | 0.07                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 0.78 (at 1.76Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.208 , 0.233<br>0.214 , 0.210                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | No test flags present.                                      | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 20.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.490                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.35 , 49.4                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 22034                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 38.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.17% 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: GLC, NAG, CL

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | A     | 0.35         | 0/3424      | 0.87        | 11/4637 (0.2%)  |
| 1   | B     | 0.36         | 0/3448      | 0.88        | 13/4669 (0.3%)  |
| 1   | C     | 0.37         | 0/3429      | 0.89        | 15/4644 (0.3%)  |
| 1   | D     | 0.36         | 0/3402      | 0.86        | 10/4607 (0.2%)  |
| 1   | E     | 0.36         | 0/3454      | 0.88        | 15/4677 (0.3%)  |
| 1   | F     | 0.35         | 0/3376      | 0.87        | 13/4571 (0.3%)  |
| All | All   | 0.36         | 0/20533     | 0.87        | 77/27805 (0.3%) |

There are no bond length outliers.

All (77) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | E     | 259 | ILE  | N-CA-C | 8.67  | 119.46      | 110.62   |
| 1   | C     | 286 | PRO  | N-CA-C | 8.32  | 120.85      | 110.70   |
| 1   | F     | 259 | ILE  | N-CA-C | 8.25  | 119.04      | 110.62   |
| 1   | C     | 285 | PRO  | CA-C-N | 7.99  | 128.61      | 120.38   |
| 1   | C     | 285 | PRO  | C-N-CA | 7.99  | 128.61      | 120.38   |
| 1   | D     | 259 | ILE  | N-CA-C | 7.62  | 119.30      | 110.62   |
| 1   | A     | 258 | LEU  | N-CA-C | -7.49 | 99.35       | 110.06   |
| 1   | B     | 258 | LEU  | N-CA-C | -7.24 | 98.61       | 109.83   |
| 1   | B     | 71  | LEU  | N-CA-C | -7.19 | 104.51      | 113.28   |
| 1   | C     | 259 | ILE  | N-CA-C | 6.99  | 119.79      | 111.05   |
| 1   | B     | 47  | TRP  | N-CA-C | -6.94 | 106.71      | 114.62   |
| 1   | E     | 382 | SER  | N-CA-C | -6.86 | 101.69      | 110.53   |
| 1   | A     | 259 | ILE  | N-CA-C | 6.83  | 119.58      | 111.05   |
| 1   | B     | 382 | SER  | N-CA-C | -6.82 | 101.73      | 110.53   |
| 1   | F     | 71  | LEU  | N-CA-C | -6.80 | 104.98      | 113.28   |
| 1   | E     | 271 | GLN  | N-CA-C | -6.77 | 97.49       | 108.52   |
| 1   | D     | 382 | SER  | N-CA-C | -6.74 | 101.84      | 110.53   |
| 1   | F     | 382 | SER  | N-CA-C | -6.70 | 101.89      | 110.53   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | E     | 294 | THR  | CB-CA-C | -6.58 | 108.98      | 116.54   |
| 1   | E     | 71  | LEU  | N-CA-C  | -6.57 | 105.30      | 113.38   |
| 1   | D     | 271 | GLN  | N-CA-C  | -6.46 | 98.21       | 108.73   |
| 1   | D     | 258 | LEU  | N-CA-C  | -6.45 | 100.84      | 110.06   |
| 1   | C     | 382 | SER  | N-CA-C  | -6.45 | 101.85      | 110.55   |
| 1   | F     | 327 | VAL  | N-CA-C  | 6.44  | 117.96      | 110.62   |
| 1   | D     | 71  | LEU  | N-CA-C  | -6.40 | 105.47      | 113.28   |
| 1   | B     | 259 | ILE  | N-CA-C  | 6.32  | 118.95      | 111.05   |
| 1   | F     | 271 | GLN  | N-CA-C  | -6.21 | 98.39       | 108.52   |
| 1   | B     | 271 | GLN  | N-CA-C  | -6.20 | 98.63       | 108.73   |
| 1   | C     | 258 | LEU  | N-CA-C  | -6.19 | 100.23      | 109.83   |
| 1   | A     | 382 | SER  | N-CA-C  | -6.17 | 102.57      | 110.53   |
| 1   | C     | 71  | LEU  | N-CA-C  | -6.05 | 105.90      | 113.28   |
| 1   | E     | 295 | THR  | CB-CA-C | -6.03 | 108.61      | 115.79   |
| 1   | B     | 95  | ASN  | N-CA-C  | -6.02 | 101.56      | 110.48   |
| 1   | C     | 276 | CYS  | N-CA-C  | 6.02  | 118.99      | 110.14   |
| 1   | A     | 71  | LEU  | N-CA-C  | -5.95 | 106.02      | 113.28   |
| 1   | A     | 271 | GLN  | N-CA-C  | -5.93 | 98.85       | 108.52   |
| 1   | F     | 95  | ASN  | N-CA-C  | -5.93 | 100.83      | 110.20   |
| 1   | B     | 345 | ALA  | N-CA-C  | 5.84  | 117.32      | 111.07   |
| 1   | C     | 345 | ALA  | N-CA-C  | 5.83  | 117.33      | 110.97   |
| 1   | D     | 276 | CYS  | N-CA-C  | 5.83  | 119.17      | 110.14   |
| 1   | E     | 276 | CYS  | N-CA-C  | 5.82  | 118.70      | 110.14   |
| 1   | C     | 271 | GLN  | N-CA-C  | -5.80 | 99.07       | 108.52   |
| 1   | C     | 214 | GLY  | N-CA-C  | 5.79  | 117.45      | 111.95   |
| 1   | A     | 95  | ASN  | N-CA-C  | -5.79 | 101.92      | 110.48   |
| 1   | B     | 355 | LYS  | N-CA-C  | 5.76  | 120.44      | 113.41   |
| 1   | A     | 345 | ALA  | N-CA-C  | 5.74  | 117.22      | 110.97   |
| 1   | F     | 262 | LEU  | N-CA-C  | 5.72  | 120.38      | 113.17   |
| 1   | E     | 416 | TYR  | N-CA-C  | 5.63  | 117.57      | 108.34   |
| 1   | F     | 276 | CYS  | N-CA-C  | 5.61  | 118.38      | 110.14   |
| 1   | A     | 262 | LEU  | N-CA-C  | 5.60  | 120.27      | 113.38   |
| 1   | E     | 258 | LEU  | N-CA-C  | -5.57 | 99.31       | 109.56   |
| 1   | D     | 267 | ALA  | N-CA-C  | 5.55  | 117.60      | 110.39   |
| 1   | B     | 214 | GLY  | N-CA-C  | 5.54  | 117.21      | 111.95   |
| 1   | D     | 345 | ALA  | N-CA-C  | 5.51  | 116.97      | 110.97   |
| 1   | E     | 262 | LEU  | N-CA-C  | 5.47  | 120.63      | 113.30   |
| 1   | A     | 359 | TYR  | N-CA-C  | 5.43  | 117.00      | 111.14   |
| 1   | E     | 345 | ALA  | N-CA-C  | 5.43  | 116.88      | 111.07   |
| 1   | B     | 276 | CYS  | N-CA-C  | 5.40  | 118.08      | 110.14   |
| 1   | E     | 247 | LYS  | N-CA-C  | -5.38 | 100.93      | 109.59   |
| 1   | F     | 258 | LEU  | N-CA-C  | -5.37 | 99.69       | 109.56   |

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| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | A     | 276 | CYS  | N-CA-C | 5.36  | 118.02      | 110.14   |
| 1   | E     | 267 | ALA  | N-CA-C | 5.32  | 117.63      | 110.29   |
| 1   | C     | 95  | ASN  | N-CA-C | -5.32 | 101.80      | 110.20   |
| 1   | B     | 416 | TYR  | N-CA-C | 5.31  | 117.07      | 108.26   |
| 1   | F     | 267 | ALA  | N-CA-C | 5.29  | 117.59      | 110.29   |
| 1   | C     | 267 | ALA  | N-CA-C | 5.28  | 117.25      | 110.39   |
| 1   | E     | 95  | ASN  | N-CA-C | -5.24 | 101.93      | 110.20   |
| 1   | F     | 415 | ASN  | N-CA-C | 5.22  | 119.50      | 113.18   |
| 1   | A     | 127 | ASP  | N-CA-C | -5.22 | 106.94      | 113.15   |
| 1   | D     | 95  | ASN  | N-CA-C | -5.21 | 101.98      | 110.20   |
| 1   | B     | 420 | GLU  | N-CA-C | 5.19  | 117.36      | 108.90   |
| 1   | D     | 372 | GLY  | N-CA-C | -5.15 | 104.54      | 111.54   |
| 1   | C     | 98  | GLU  | N-CA-C | 5.12  | 118.68      | 112.23   |
| 1   | F     | 44  | ARG  | N-CA-C | -5.06 | 105.47      | 111.69   |
| 1   | C     | 243 | GLU  | N-CA-C | 5.05  | 118.25      | 110.42   |
| 1   | F     | 243 | GLU  | N-CA-C | 5.04  | 118.23      | 110.42   |
| 1   | E     | 243 | GLU  | N-CA-C | 5.02  | 118.21      | 110.42   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3345  | 0        | 3238     | 98      | 0            |
| 1   | B     | 3369  | 0        | 3271     | 112     | 0            |
| 1   | C     | 3350  | 0        | 3248     | 99      | 0            |
| 1   | D     | 3324  | 0        | 3222     | 101     | 0            |
| 1   | E     | 3375  | 0        | 3276     | 107     | 0            |
| 1   | F     | 3299  | 0        | 3205     | 85      | 0            |
| 2   | G     | 23    | 0        | 21       | 0       | 0            |
| 2   | H     | 23    | 0        | 21       | 0       | 0            |
| 2   | I     | 23    | 0        | 21       | 0       | 0            |
| 3   | A     | 28    | 0        | 26       | 0       | 0            |
| 3   | B     | 28    | 0        | 26       | 0       | 0            |
| 3   | C     | 28    | 0        | 26       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3   | D     | 28    | 0        | 26       | 1       | 0            |
| 3   | E     | 28    | 0        | 26       | 0       | 0            |
| 3   | F     | 28    | 0        | 26       | 1       | 0            |
| 4   | A     | 1     | 0        | 0        | 0       | 0            |
| 4   | B     | 1     | 0        | 0        | 0       | 0            |
| 4   | C     | 1     | 0        | 0        | 0       | 0            |
| 4   | D     | 1     | 0        | 0        | 0       | 0            |
| 4   | E     | 1     | 0        | 0        | 0       | 0            |
| 4   | F     | 1     | 0        | 0        | 0       | 0            |
| 5   | A     | 285   | 0        | 0        | 9       | 0            |
| 5   | B     | 280   | 0        | 0        | 3       | 0            |
| 5   | C     | 302   | 0        | 0        | 9       | 0            |
| 5   | D     | 270   | 0        | 0        | 9       | 0            |
| 5   | E     | 292   | 0        | 0        | 7       | 0            |
| 5   | F     | 300   | 0        | 0        | 8       | 0            |
| All | All   | 22034 | 0        | 19679    | 555     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (555) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:D:131:ALA:HA   | 1:F:387:LYS:HD3 | 1.46                     | 0.98              |
| 1:F:294:THR:HG23 | 1:F:304:TYR:H   | 1.28                     | 0.97              |
| 1:F:298:SER:HB2  | 1:F:302:ASP:HA  | 1.47                     | 0.95              |
| 1:B:131:ALA:HB2  | 1:B:234:TRP:HE1 | 1.31                     | 0.93              |
| 1:F:434:ILE:HG22 | 1:F:438:MET:HE2 | 1.53                     | 0.91              |
| 1:C:294:THR:HA   | 1:C:304:TYR:HB3 | 1.50                     | 0.91              |
| 1:B:42:LEU:HD12  | 1:B:44:ARG:HB2  | 1.54                     | 0.88              |
| 1:B:207:ARG:HH21 | 1:B:207:ARG:HB2 | 1.41                     | 0.85              |
| 1:E:122:ARG:HE   | 1:E:122:ARG:HA  | 1.41                     | 0.83              |
| 1:A:154:ASN:HD22 | 1:A:157:GLU:H   | 1.27                     | 0.82              |
| 1:C:186:LYS:HE2  | 1:C:202:GLN:HG2 | 1.60                     | 0.82              |
| 1:D:205:LYS:HB3  | 1:D:206:PRO:HD2 | 1.63                     | 0.80              |
| 1:E:127:ASP:CG   | 1:E:128:THR:H   | 1.90                     | 0.79              |
| 1:D:211:MET:HG3  | 1:E:357:ASN:ND2 | 1.98                     | 0.79              |
| 1:D:98:GLU:HG2   | 1:D:192:TYR:O   | 1.84                     | 0.78              |
| 1:D:357:ASN:ND2  | 1:F:211:MET:HG3 | 1.98                     | 0.77              |
| 1:C:223:LEU:HB2  | 1:C:405:LEU:CD2 | 2.14                     | 0.77              |
| 1:E:146:ARG:HD2  | 5:E:671:HOH:O   | 1.83                     | 0.76              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:395:LYS:HG2  | 1:A:399:TYR:CD1  | 2.19                     | 0.76              |
| 1:C:42:LEU:H     | 1:C:42:LEU:HD22  | 1.52                     | 0.74              |
| 1:D:127:ASP:O    | 1:D:130:THR:HG23 | 1.87                     | 0.73              |
| 1:C:395:LYS:HG2  | 1:C:399:TYR:CD1  | 2.24                     | 0.73              |
| 1:B:97:ASN:HD21  | 1:B:231:LEU:H    | 1.36                     | 0.73              |
| 1:A:130:THR:HB   | 1:C:387:LYS:HB3  | 1.70                     | 0.72              |
| 1:F:98:GLU:HG2   | 1:F:192:TYR:O    | 1.88                     | 0.72              |
| 1:F:435:GLY:HA2  | 1:F:438:MET:HE3  | 1.70                     | 0.72              |
| 1:C:223:LEU:HB2  | 1:C:405:LEU:HD21 | 1.72                     | 0.71              |
| 1:E:65:ARG:HH21  | 1:E:433:ASP:HB3  | 1.56                     | 0.71              |
| 1:E:420:GLU:HG2  | 1:E:422:LYS:HD3  | 1.71                     | 0.71              |
| 1:A:78:LEU:HD13  | 1:A:79:ASP:N     | 2.05                     | 0.70              |
| 1:A:176:ARG:HH22 | 1:B:357:ASN:ND2  | 1.89                     | 0.70              |
| 1:C:98:GLU:HG2   | 1:C:192:TYR:O    | 1.91                     | 0.70              |
| 1:D:395:LYS:HG2  | 1:D:399:TYR:CD1  | 2.27                     | 0.70              |
| 1:F:310:ARG:O    | 1:F:314:GLU:HG3  | 1.92                     | 0.69              |
| 1:D:63:THR:O     | 1:D:67:GLN:HG3   | 1.92                     | 0.69              |
| 1:D:156:LEU:HD13 | 1:D:327:VAL:HG13 | 1.72                     | 0.69              |
| 1:E:63:THR:O     | 1:E:67:GLN:HG3   | 1.92                     | 0.69              |
| 1:B:120:ASN:C    | 1:B:120:ASN:HD22 | 1.98                     | 0.69              |
| 1:B:437:GLN:NE2  | 1:B:437:GLN:H    | 1.90                     | 0.69              |
| 1:E:144:ASN:OD1  | 1:E:146:ARG:HD3  | 1.93                     | 0.69              |
| 1:C:405:LEU:HD23 | 1:C:405:LEU:O    | 1.94                     | 0.67              |
| 1:C:210:THR:HG23 | 1:C:217:ASN:HB3  | 1.75                     | 0.67              |
| 1:D:239:GLU:HB2  | 5:D:705:HOH:O    | 1.94                     | 0.67              |
| 1:E:296:GLY:HA2  | 1:E:302:ASP:HA   | 1.77                     | 0.67              |
| 1:B:45:VAL:C     | 1:B:47:TRP:H     | 2.04                     | 0.66              |
| 1:A:357:ASN:HD21 | 1:C:176:ARG:HH12 | 1.43                     | 0.66              |
| 1:E:332:ASP:HB3  | 5:E:700:HOH:O    | 1.96                     | 0.66              |
| 1:B:120:ASN:ND2  | 1:B:122:ARG:H    | 1.94                     | 0.65              |
| 1:B:341:TYR:HA   | 1:B:345:ALA:HB3  | 1.78                     | 0.65              |
| 1:C:240:THR:HG21 | 5:C:726:HOH:O    | 1.97                     | 0.65              |
| 1:F:42:LEU:N     | 1:F:42:LEU:HD13  | 2.11                     | 0.65              |
| 1:A:86:LEU:HD23  | 1:A:87:THR:N     | 2.12                     | 0.65              |
| 1:A:97:ASN:HD21  | 1:A:231:LEU:H    | 1.43                     | 0.64              |
| 1:A:366:CYS:HB2  | 5:A:692:HOH:O    | 1.97                     | 0.64              |
| 1:D:375:LEU:HD13 | 5:F:591:HOH:O    | 1.98                     | 0.64              |
| 1:D:131:ALA:HB3  | 1:D:234:TRP:HE1  | 1.61                     | 0.64              |
| 1:F:393:TYR:O    | 1:F:395:LYS:HD2  | 1.97                     | 0.64              |
| 1:A:260:ASP:HB3  | 5:A:732:HOH:O    | 1.98                     | 0.64              |
| 1:B:450:LEU:HD21 | 1:C:42:LEU:HB2   | 1.78                     | 0.64              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:310:ARG:O    | 1:D:314:GLU:HG3  | 1.97                     | 0.64              |
| 1:D:341:TYR:HA   | 1:D:345:ALA:HB3  | 1.80                     | 0.64              |
| 1:D:203:ASP:HB3  | 1:D:205:LYS:HG3  | 1.80                     | 0.64              |
| 1:E:122:ARG:HA   | 1:E:122:ARG:NE   | 2.11                     | 0.64              |
| 1:F:298:SER:CB   | 1:F:302:ASP:HA   | 2.25                     | 0.64              |
| 1:A:139:LEU:HD23 | 1:A:234:TRP:CH2  | 2.33                     | 0.63              |
| 1:A:387:LYS:HD3  | 5:A:733:HOH:O    | 1.97                     | 0.63              |
| 1:B:437:GLN:H    | 1:B:437:GLN:HE21 | 1.45                     | 0.63              |
| 1:A:78:LEU:HD23  | 1:A:419:ILE:HG12 | 1.80                     | 0.63              |
| 1:C:75:VAL:HG13  | 1:C:424:ALA:HB2  | 1.79                     | 0.63              |
| 1:D:176:ARG:HH22 | 1:E:357:ASN:ND2  | 1.95                     | 0.63              |
| 1:A:420:GLU:OE1  | 1:A:422:LYS:HE2  | 1.98                     | 0.63              |
| 1:B:156:LEU:HD13 | 1:B:327:VAL:HG13 | 1.79                     | 0.63              |
| 1:B:454:ASP:CG   | 1:C:40:LEU:HD21  | 2.24                     | 0.62              |
| 1:F:97:ASN:HD21  | 1:F:231:LEU:H    | 1.46                     | 0.62              |
| 1:D:120:ASN:C    | 1:D:120:ASN:HD22 | 2.07                     | 0.62              |
| 1:F:120:ASN:C    | 1:F:120:ASN:HD22 | 2.07                     | 0.62              |
| 1:A:67:GLN:O     | 1:A:71:LEU:HD23  | 2.00                     | 0.62              |
| 1:E:55:LEU:HD13  | 1:E:55:LEU:O     | 1.98                     | 0.62              |
| 1:A:120:ASN:C    | 1:A:120:ASN:HD22 | 2.08                     | 0.62              |
| 1:A:295:THR:HG22 | 1:A:296:GLY:N    | 2.14                     | 0.62              |
| 1:B:176:ARG:HH12 | 1:C:357:ASN:HD21 | 1.45                     | 0.62              |
| 1:B:379:LYS:HE3  | 5:B:496:HOH:O    | 1.98                     | 0.62              |
| 1:E:62:CYS:SG    | 1:E:438:MET:HE3  | 2.40                     | 0.62              |
| 1:F:55:LEU:HD23  | 1:F:441:PHE:CE1  | 2.35                     | 0.62              |
| 1:F:239:GLU:HB2  | 5:F:640:HOH:O    | 1.98                     | 0.62              |
| 1:C:156:LEU:HD13 | 1:C:327:VAL:HG13 | 1.81                     | 0.61              |
| 1:A:125:ILE:HD12 | 1:A:140:GLN:HG2  | 1.80                     | 0.61              |
| 1:C:132:ASP:HB3  | 1:C:135:GLN:HG3  | 1.82                     | 0.61              |
| 1:E:53:GLY:C     | 1:E:55:LEU:H     | 2.08                     | 0.61              |
| 1:E:211:MET:HG3  | 1:F:357:ASN:ND2  | 2.16                     | 0.61              |
| 1:B:295:THR:HG22 | 1:B:296:GLY:N    | 2.16                     | 0.61              |
| 1:C:285:PRO:CB   | 1:C:286:PRO:HD2  | 2.30                     | 0.61              |
| 1:B:42:LEU:C     | 1:B:44:ARG:H     | 2.08                     | 0.61              |
| 1:C:418:THR:HG23 | 5:C:532:HOH:O    | 2.01                     | 0.61              |
| 1:E:310:ARG:O    | 1:E:314:GLU:HG3  | 2.00                     | 0.60              |
| 1:B:395:LYS:HG2  | 1:B:399:TYR:CD1  | 2.36                     | 0.60              |
| 1:E:270:PHE:CG   | 1:E:377:MET:HE3  | 2.35                     | 0.60              |
| 1:B:85:ARG:HG3   | 1:B:211:MET:HE1  | 1.83                     | 0.60              |
| 1:D:75:VAL:HG13  | 1:D:424:ALA:HB2  | 1.82                     | 0.60              |
| 1:E:59:ALA:HB2   | 1:E:441:PHE:CE2  | 2.36                     | 0.60              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:438:MET:O    | 1:E:442:ILE:HG13 | 2.00                     | 0.60              |
| 1:C:40:LEU:HD22  | 1:C:43:LYS:HE3   | 1.83                     | 0.60              |
| 1:F:62:CYS:O     | 1:F:66:ILE:HG13  | 2.01                     | 0.60              |
| 1:B:405:LEU:C    | 1:B:405:LEU:HD23 | 2.27                     | 0.60              |
| 1:A:204:GLY:O    | 1:A:205:LYS:C    | 2.45                     | 0.60              |
| 1:D:97:ASN:HD21  | 1:D:231:LEU:H    | 1.50                     | 0.60              |
| 1:F:120:ASN:ND2  | 1:F:122:ARG:H    | 2.00                     | 0.60              |
| 1:B:326:MET:HE3  | 1:B:341:TYR:CE2  | 2.36                     | 0.59              |
| 1:C:133:GLU:CD   | 1:C:133:GLU:H    | 2.09                     | 0.59              |
| 1:E:456:ALA:O    | 1:E:460:ILE:HG13 | 2.02                     | 0.59              |
| 1:C:298:SER:HB2  | 1:C:301:TYR:O    | 2.02                     | 0.59              |
| 1:E:341:TYR:HA   | 1:E:345:ALA:HB3  | 1.84                     | 0.59              |
| 1:C:200:ALA:HB1  | 1:C:202:GLN:NE2  | 2.17                     | 0.59              |
| 1:B:92:THR:OG1   | 1:B:251:HIS:HE1  | 1.85                     | 0.59              |
| 1:D:62:CYS:O     | 1:D:66:ILE:HG12  | 2.02                     | 0.59              |
| 1:A:176:ARG:HH12 | 1:B:357:ASN:HD21 | 1.49                     | 0.59              |
| 1:C:202:GLN:N    | 1:C:202:GLN:HE21 | 2.01                     | 0.59              |
| 1:F:101:PHE:HE1  | 1:F:139:LEU:HD21 | 1.68                     | 0.59              |
| 1:D:157:GLU:CD   | 1:D:161:ARG:HE   | 2.10                     | 0.58              |
| 1:E:139:LEU:O    | 1:E:143:ALA:N    | 2.35                     | 0.58              |
| 1:E:136:LEU:O    | 1:E:140:GLN:HG3  | 2.02                     | 0.58              |
| 1:D:120:ASN:ND2  | 1:D:124:GLU:H    | 2.00                     | 0.58              |
| 1:A:154:ASN:HD21 | 1:A:156:LEU:HB3  | 1.68                     | 0.58              |
| 1:C:47:TRP:HZ3   | 1:C:447:LEU:HB3  | 1.69                     | 0.58              |
| 1:D:50:CYS:HB2   | 1:F:450:LEU:HD21 | 1.84                     | 0.58              |
| 1:E:97:ASN:HD21  | 1:E:231:LEU:H    | 1.52                     | 0.58              |
| 1:E:240:THR:HG21 | 5:E:623:HOH:O    | 2.02                     | 0.58              |
| 1:E:260:ASP:HB3  | 5:E:583:HOH:O    | 2.03                     | 0.58              |
| 1:C:63:THR:O     | 1:C:67:GLN:HG3   | 2.04                     | 0.57              |
| 1:E:127:ASP:CG   | 1:E:128:THR:N    | 2.62                     | 0.57              |
| 1:E:176:ARG:HH12 | 1:F:357:ASN:HD21 | 1.51                     | 0.57              |
| 1:E:181:SER:OG   | 1:E:183:GLU:HG2  | 2.05                     | 0.57              |
| 1:C:405:LEU:HD23 | 1:C:405:LEU:C    | 2.29                     | 0.57              |
| 1:A:98:GLU:HG2   | 1:A:192:TYR:O    | 2.05                     | 0.57              |
| 1:E:62:CYS:O     | 1:E:66:ILE:HG13  | 2.05                     | 0.57              |
| 1:E:207:ARG:NH1  | 1:E:207:ARG:HB2  | 2.20                     | 0.57              |
| 1:A:420:GLU:CD   | 1:A:422:LYS:HE2  | 2.30                     | 0.57              |
| 1:D:120:ASN:ND2  | 1:D:122:ARG:H    | 2.02                     | 0.57              |
| 1:F:207:ARG:HA   | 5:F:551:HOH:O    | 2.03                     | 0.57              |
| 1:B:437:GLN:NE2  | 1:B:437:GLN:N    | 2.53                     | 0.57              |
| 1:B:120:ASN:HD22 | 1:B:122:ARG:H    | 1.52                     | 0.57              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:253:GLN:HG3  | 5:A:578:HOH:O    | 2.05                     | 0.57              |
| 1:B:223:LEU:HB2  | 1:B:405:LEU:HD22 | 1.87                     | 0.57              |
| 1:D:43:LYS:NZ    | 1:D:43:LYS:HB3   | 2.20                     | 0.57              |
| 1:C:341:TYR:HA   | 1:C:345:ALA:HB3  | 1.86                     | 0.57              |
| 1:A:298:SER:HB3  | 1:A:302:ASP:HA   | 1.86                     | 0.56              |
| 1:C:154:ASN:HD22 | 1:C:157:GLU:H    | 1.53                     | 0.56              |
| 1:D:357:ASN:ND2  | 1:F:176:ARG:HH22 | 2.03                     | 0.56              |
| 1:F:203:ASP:O    | 1:F:205:LYS:HG2  | 2.05                     | 0.56              |
| 1:B:207:ARG:HB2  | 1:B:207:ARG:NH2  | 2.17                     | 0.56              |
| 1:D:157:GLU:OE2  | 1:D:161:ARG:NE   | 2.34                     | 0.56              |
| 1:A:131:ALA:C    | 1:A:133:GLU:H    | 2.13                     | 0.56              |
| 1:B:75:VAL:HG23  | 1:B:424:ALA:HB2  | 1.86                     | 0.56              |
| 1:C:167:ARG:NH2  | 1:C:183:GLU:OE1  | 2.39                     | 0.56              |
| 1:C:285:PRO:HB2  | 1:C:286:PRO:HD2  | 1.86                     | 0.56              |
| 1:D:53:GLY:O     | 1:D:57:LEU:HG    | 2.06                     | 0.56              |
| 1:B:128:THR:HB   | 1:B:136:LEU:HD21 | 1.87                     | 0.56              |
| 1:D:202:GLN:C    | 1:D:204:GLY:H    | 2.14                     | 0.56              |
| 1:F:420:GLU:OE1  | 1:F:422:LYS:HE2  | 2.06                     | 0.56              |
| 1:D:209:ILE:HD12 | 1:D:209:ILE:C    | 2.31                     | 0.56              |
| 1:B:127:ASP:O    | 1:B:130:THR:HG23 | 2.06                     | 0.56              |
| 1:B:295:THR:HG22 | 1:B:296:GLY:H    | 1.70                     | 0.56              |
| 1:C:97:ASN:HD21  | 1:C:231:LEU:H    | 1.54                     | 0.56              |
| 1:C:282:ILE:HB   | 1:C:420:GLU:HG3  | 1.88                     | 0.56              |
| 1:D:442:ILE:HG22 | 1:E:54:SER:OG    | 2.05                     | 0.56              |
| 1:F:92:THR:OG1   | 1:F:251:HIS:HE1  | 1.89                     | 0.56              |
| 1:B:206:PRO:HG2  | 5:B:648:HOH:O    | 2.06                     | 0.56              |
| 1:E:176:ARG:HH22 | 1:F:357:ASN:ND2  | 2.04                     | 0.56              |
| 1:A:210:THR:HG22 | 1:A:217:ASN:O    | 2.06                     | 0.55              |
| 1:F:53:GLY:O     | 1:F:57:LEU:HD23  | 2.06                     | 0.55              |
| 1:F:156:LEU:HD13 | 1:F:327:VAL:HG13 | 1.87                     | 0.55              |
| 1:A:42:LEU:N     | 1:A:42:LEU:HD13  | 2.21                     | 0.55              |
| 1:C:270:PHE:CG   | 1:C:377:MET:HE3  | 2.41                     | 0.55              |
| 1:A:65:ARG:NE    | 1:A:65:ARG:HA    | 2.22                     | 0.55              |
| 1:A:50:CYS:HB3   | 1:C:446:ILE:HG23 | 1.89                     | 0.55              |
| 1:D:447:LEU:HD12 | 1:F:450:LEU:HB3  | 1.88                     | 0.55              |
| 1:F:131:ALA:HB2  | 1:F:234:TRP:HE1  | 1.72                     | 0.55              |
| 1:A:211:MET:HG3  | 1:B:357:ASN:ND2  | 2.21                     | 0.55              |
| 1:E:420:GLU:CG   | 1:E:422:LYS:HD3  | 2.37                     | 0.55              |
| 1:A:122:ARG:O    | 1:A:124:GLU:HG3  | 2.07                     | 0.55              |
| 1:A:280:ARG:HG2  | 1:A:280:ARG:HH11 | 1.72                     | 0.55              |
| 1:D:237:THR:OG1  | 1:D:240:THR:HG23 | 2.07                     | 0.55              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:447:LEU:O    | 1:D:451:GLU:HG3  | 2.06                     | 0.55              |
| 1:E:452:LEU:O    | 1:E:452:LEU:HD23 | 2.06                     | 0.55              |
| 1:A:298:SER:HB2  | 1:A:301:TYR:C    | 2.32                     | 0.55              |
| 1:A:295:THR:HG22 | 1:A:296:GLY:H    | 1.71                     | 0.54              |
| 1:B:139:LEU:HD23 | 1:B:234:TRP:CH2  | 2.42                     | 0.54              |
| 1:F:134:LYS:O    | 1:F:138:ILE:HG12 | 2.06                     | 0.54              |
| 1:D:357:ASN:HD22 | 1:F:211:MET:HG3  | 1.72                     | 0.54              |
| 1:D:357:ASN:HD21 | 1:F:176:ARG:HH12 | 1.54                     | 0.54              |
| 1:E:455:TYR:O    | 1:E:459:VAL:HG23 | 2.07                     | 0.54              |
| 3:F:11:NAG:O3    | 3:F:11:NAG:H83   | 2.07                     | 0.54              |
| 1:C:299:GLU:HG2  | 1:C:312:ASP:OD1  | 2.08                     | 0.54              |
| 1:D:146:ARG:O    | 1:D:147:ASN:HB2  | 2.07                     | 0.54              |
| 1:B:130:THR:HA   | 5:B:739:HOH:O    | 2.06                     | 0.54              |
| 1:C:286:PRO:HG2  | 1:C:287:PRO:HD3  | 1.89                     | 0.54              |
| 1:C:420:GLU:CD   | 1:C:422:LYS:HE3  | 2.33                     | 0.54              |
| 1:E:250:ILE:HD12 | 1:E:373:LYS:HD3  | 1.89                     | 0.54              |
| 1:B:236:GLU:HG2  | 1:B:242:PHE:CZ   | 2.42                     | 0.54              |
| 1:C:387:LYS:O    | 1:C:387:LYS:HD3  | 2.07                     | 0.54              |
| 1:D:240:THR:HG21 | 5:D:546:HOH:O    | 2.06                     | 0.54              |
| 1:E:64:ASN:HA    | 1:E:67:GLN:NE2   | 2.23                     | 0.54              |
| 1:F:121:ASN:OD1  | 1:F:122:ARG:HG3  | 2.06                     | 0.54              |
| 1:C:293:ALA:C    | 1:C:295:THR:H    | 2.16                     | 0.54              |
| 1:F:210:THR:HG23 | 1:F:217:ASN:HB3  | 1.90                     | 0.54              |
| 1:C:59:ALA:O     | 1:C:63:THR:HG23  | 2.08                     | 0.54              |
| 1:F:280:ARG:HG2  | 1:F:280:ARG:HH21 | 1.73                     | 0.54              |
| 1:A:154:ASN:ND2  | 1:A:157:GLU:H    | 2.03                     | 0.54              |
| 1:A:294:THR:HG22 | 1:A:295:THR:N    | 2.21                     | 0.54              |
| 1:A:442:ILE:O    | 1:A:446:ILE:HG13 | 2.08                     | 0.54              |
| 1:E:128:THR:HA   | 1:E:136:LEU:HD21 | 1.88                     | 0.54              |
| 1:A:86:LEU:HD21  | 1:A:278:GLU:OE1  | 2.07                     | 0.53              |
| 1:A:130:THR:HG1  | 1:A:234:TRP:CD1  | 2.26                     | 0.53              |
| 1:B:135:GLN:O    | 1:B:139:LEU:HB2  | 2.08                     | 0.53              |
| 1:E:92:THR:OG1   | 1:E:251:HIS:HE1  | 1.92                     | 0.53              |
| 1:A:55:LEU:HB2   | 1:A:441:PHE:HE2  | 1.73                     | 0.53              |
| 1:D:42:LEU:O     | 1:D:45:VAL:HG12  | 2.09                     | 0.53              |
| 1:B:131:ALA:HB2  | 1:B:234:TRP:NE1  | 2.14                     | 0.53              |
| 1:C:420:GLU:OE1  | 1:C:422:LYS:HE3  | 2.09                     | 0.53              |
| 1:A:312:ASP:OD2  | 1:A:316:ARG:NH1  | 2.42                     | 0.53              |
| 1:C:132:ASP:OD1  | 1:C:134:LYS:HG2  | 2.09                     | 0.53              |
| 1:B:42:LEU:HD12  | 1:B:44:ARG:CB    | 2.33                     | 0.53              |
| 1:B:85:ARG:NH2   | 1:B:209:ILE:HD13 | 2.23                     | 0.53              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:270:PHE:CG   | 1:D:377:MET:HE3  | 2.44                     | 0.53              |
| 1:A:341:TYR:HA   | 1:A:345:ALA:HB3  | 1.91                     | 0.53              |
| 1:B:167:ARG:HG2  | 1:B:167:ARG:HH21 | 1.74                     | 0.53              |
| 1:D:139:LEU:HD23 | 1:D:234:TRP:CH2  | 2.44                     | 0.53              |
| 1:D:176:ARG:HH12 | 1:E:357:ASN:HD21 | 1.56                     | 0.53              |
| 1:F:247:LYS:NZ   | 5:F:645:HOH:O    | 2.42                     | 0.52              |
| 1:D:379:LYS:HG3  | 5:D:722:HOH:O    | 2.08                     | 0.52              |
| 1:D:56:ALA:O     | 1:D:60:LEU:HD23  | 2.09                     | 0.52              |
| 1:B:44:ARG:HH11  | 1:B:455:TYR:HE2  | 1.57                     | 0.52              |
| 1:A:63:THR:O     | 1:A:67:GLN:HG3   | 2.09                     | 0.52              |
| 1:A:207:ARG:HA   | 5:A:625:HOH:O    | 2.10                     | 0.52              |
| 1:C:256:PRO:HG2  | 1:C:307:THR:HG22 | 1.91                     | 0.52              |
| 1:C:379:LYS:HE3  | 5:C:480:HOH:O    | 2.10                     | 0.52              |
| 1:D:136:LEU:O    | 1:D:140:GLN:HG3  | 2.09                     | 0.52              |
| 1:A:78:LEU:HD13  | 1:A:78:LEU:C     | 2.34                     | 0.52              |
| 1:A:357:ASN:ND2  | 1:C:176:ARG:HH22 | 2.08                     | 0.52              |
| 1:C:42:LEU:HD22  | 1:C:42:LEU:N     | 2.22                     | 0.52              |
| 1:C:210:THR:HG22 | 5:C:750:HOH:O    | 2.09                     | 0.52              |
| 1:B:310:ARG:O    | 1:B:314:GLU:HG3  | 2.08                     | 0.52              |
| 1:C:92:THR:OG1   | 1:C:251:HIS:HE1  | 1.93                     | 0.52              |
| 1:E:156:LEU:HD13 | 1:E:327:VAL:CG2  | 2.39                     | 0.52              |
| 1:F:55:LEU:HD13  | 1:F:55:LEU:C     | 2.34                     | 0.52              |
| 1:B:46:VAL:HG12  | 1:B:46:VAL:O     | 2.10                     | 0.52              |
| 1:E:442:ILE:C    | 1:E:444:ALA:H    | 2.18                     | 0.52              |
| 1:F:295:THR:HG22 | 1:F:295:THR:O    | 2.10                     | 0.52              |
| 1:D:447:LEU:CD1  | 1:F:450:LEU:HB3  | 2.40                     | 0.51              |
| 1:C:63:THR:O     | 1:C:66:ILE:HG12  | 2.09                     | 0.51              |
| 1:D:44:ARG:HD2   | 1:D:455:TYR:CE2  | 2.45                     | 0.51              |
| 1:D:440:LEU:HD23 | 1:F:443:GLY:HA3  | 1.93                     | 0.51              |
| 1:F:63:THR:O     | 1:F:67:GLN:HG3   | 2.11                     | 0.51              |
| 1:F:312:ASP:HB3  | 5:F:687:HOH:O    | 2.11                     | 0.51              |
| 1:D:274:VAL:HG22 | 1:D:375:LEU:HG   | 1.92                     | 0.51              |
| 1:E:271:GLN:HE21 | 1:F:243:GLU:HG2  | 1.74                     | 0.51              |
| 1:B:271:GLN:HE21 | 1:C:243:GLU:HG2  | 1.76                     | 0.51              |
| 1:E:114:GLU:HG2  | 1:E:342:LYS:HE3  | 1.93                     | 0.51              |
| 1:E:327:VAL:HG12 | 5:E:480:HOH:O    | 2.09                     | 0.51              |
| 1:A:120:ASN:ND2  | 1:A:122:ARG:H    | 2.08                     | 0.51              |
| 1:B:319:VAL:O    | 1:B:323:ASN:HA   | 2.11                     | 0.51              |
| 1:E:52:MET:HE2   | 1:E:448:THR:HG21 | 1.92                     | 0.51              |
| 1:E:299:GLU:C    | 1:E:301:TYR:H    | 2.18                     | 0.51              |
| 1:E:85:ARG:HB3   | 1:E:85:ARG:NH2   | 2.26                     | 0.51              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:256:PRO:HG2  | 1:A:307:THR:HG22 | 1.92                     | 0.51              |
| 1:D:256:PRO:HG2  | 1:D:307:THR:HG22 | 1.92                     | 0.51              |
| 1:A:402:GLU:OE1  | 1:C:383:LYS:HE2  | 2.11                     | 0.50              |
| 1:C:205:LYS:H    | 1:C:206:PRO:HD2  | 1.77                     | 0.50              |
| 1:C:310:ARG:O    | 1:C:314:GLU:HG3  | 2.11                     | 0.50              |
| 1:C:446:ILE:HG22 | 1:C:450:LEU:HD22 | 1.93                     | 0.50              |
| 1:E:418:THR:HG23 | 5:E:543:HOH:O    | 2.12                     | 0.50              |
| 1:B:294:THR:HG21 | 1:B:303:THR:HA   | 1.93                     | 0.50              |
| 1:C:287:PRO:HG2  | 5:C:727:HOH:O    | 2.10                     | 0.50              |
| 1:B:454:ASP:OD2  | 1:C:40:LEU:HD21  | 2.12                     | 0.50              |
| 1:C:442:ILE:O    | 1:C:446:ILE:HG13 | 2.11                     | 0.50              |
| 1:D:49:LEU:C     | 1:D:49:LEU:HD12  | 2.37                     | 0.50              |
| 1:A:292:LYS:HA   | 5:A:644:HOH:O    | 2.12                     | 0.50              |
| 1:D:446:ILE:HG13 | 1:E:54:SER:HB2   | 1.94                     | 0.50              |
| 1:E:420:GLU:CD   | 1:E:422:LYS:HD3  | 2.37                     | 0.50              |
| 1:F:75:VAL:HG13  | 1:F:422:LYS:HB2  | 1.93                     | 0.50              |
| 1:D:186:LYS:HE3  | 5:D:697:HOH:O    | 2.12                     | 0.50              |
| 1:A:43:LYS:NZ    | 1:A:43:LYS:HB3   | 2.27                     | 0.50              |
| 1:A:144:ASN:HD21 | 1:A:146:ARG:HE   | 1.60                     | 0.50              |
| 1:B:120:ASN:C    | 1:B:120:ASN:ND2  | 2.70                     | 0.50              |
| 1:C:395:LYS:HG2  | 1:C:399:TYR:CE1  | 2.47                     | 0.49              |
| 1:A:205:LYS:O    | 1:A:207:ARG:N    | 2.45                     | 0.49              |
| 1:E:129:GLN:C    | 1:E:131:ALA:H    | 2.20                     | 0.49              |
| 1:A:176:ARG:NH1  | 1:B:357:ASN:HD21 | 2.09                     | 0.49              |
| 1:C:154:ASN:ND2  | 1:C:156:LEU:HB3  | 2.27                     | 0.49              |
| 1:E:300:PHE:HD2  | 1:E:312:ASP:CG   | 2.21                     | 0.49              |
| 1:B:176:ARG:HH22 | 1:C:357:ASN:ND2  | 2.10                     | 0.49              |
| 1:F:346:ASP:HB2  | 1:F:347:PRO:HD3  | 1.95                     | 0.49              |
| 1:B:210:THR:HG23 | 1:B:217:ASN:HB3  | 1.95                     | 0.49              |
| 1:E:202:GLN:HB2  | 1:E:205:LYS:CG   | 2.42                     | 0.49              |
| 1:C:274:VAL:HG22 | 1:C:375:LEU:HG   | 1.95                     | 0.49              |
| 1:D:405:LEU:C    | 1:D:405:LEU:HD12 | 2.38                     | 0.49              |
| 1:B:85:ARG:CG    | 1:B:211:MET:HE1  | 2.41                     | 0.49              |
| 1:B:274:VAL:HG22 | 1:B:375:LEU:HG   | 1.95                     | 0.49              |
| 1:B:438:MET:O    | 1:B:442:ILE:HG13 | 2.13                     | 0.49              |
| 1:D:282:ILE:HB   | 1:D:420:GLU:HG3  | 1.95                     | 0.49              |
| 1:E:405:LEU:C    | 1:E:405:LEU:HD12 | 2.38                     | 0.49              |
| 1:B:136:LEU:O    | 1:B:140:GLN:HG3  | 2.13                     | 0.48              |
| 1:C:42:LEU:H     | 1:C:42:LEU:CD2   | 2.23                     | 0.48              |
| 1:C:44:ARG:CZ    | 1:C:455:TYR:HB2  | 2.43                     | 0.48              |
| 1:D:209:ILE:HD12 | 1:D:209:ILE:O    | 2.13                     | 0.48              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:445:SER:O    | 1:D:449:VAL:HG23 | 2.13                     | 0.48              |
| 1:F:101:PHE:CE1  | 1:F:139:LEU:HD21 | 2.47                     | 0.48              |
| 1:D:202:GLN:HG3  | 5:D:697:HOH:O    | 2.13                     | 0.48              |
| 1:D:390:ALA:HB1  | 1:D:395:LYS:O    | 2.14                     | 0.48              |
| 1:F:452:LEU:HD13 | 1:F:452:LEU:O    | 2.13                     | 0.48              |
| 1:A:387:LYS:HE2  | 1:A:397:GLU:OE2  | 2.13                     | 0.48              |
| 1:A:400:ILE:HG23 | 1:A:404:ILE:HG13 | 1.95                     | 0.48              |
| 1:C:292:LYS:HD2  | 1:C:363:GLU:OE1  | 2.13                     | 0.48              |
| 1:E:51:PHE:HD2   | 1:E:447:LEU:HD13 | 1.77                     | 0.48              |
| 1:D:122:ARG:O    | 1:D:124:GLU:HG3  | 2.14                     | 0.48              |
| 1:A:387:LYS:HD3  | 5:A:747:HOH:O    | 2.12                     | 0.48              |
| 1:B:292:LYS:O    | 1:B:292:LYS:HG3  | 2.13                     | 0.48              |
| 1:D:116:LEU:HA   | 5:D:705:HOH:O    | 2.12                     | 0.48              |
| 1:D:211:MET:HG3  | 1:E:357:ASN:HD22 | 1.74                     | 0.48              |
| 1:B:44:ARG:NH1   | 1:B:455:TYR:HE2  | 2.12                     | 0.48              |
| 1:B:346:ASP:HB2  | 1:B:347:PRO:HD3  | 1.96                     | 0.48              |
| 1:C:395:LYS:HE3  | 5:C:635:HOH:O    | 2.13                     | 0.48              |
| 1:E:339:GLU:HG3  | 5:E:694:HOH:O    | 2.13                     | 0.48              |
| 1:F:85:ARG:HD3   | 1:F:209:ILE:HD12 | 1.96                     | 0.48              |
| 1:E:78:LEU:HD13  | 1:E:419:ILE:HG12 | 1.96                     | 0.47              |
| 1:E:202:GLN:HB2  | 1:E:205:LYS:HG2  | 1.95                     | 0.47              |
| 1:A:395:LYS:HG2  | 1:A:399:TYR:CE1  | 2.48                     | 0.47              |
| 1:D:49:LEU:HD12  | 1:D:50:CYS:N     | 2.28                     | 0.47              |
| 1:F:292:LYS:HD3  | 1:F:292:LYS:C    | 2.40                     | 0.47              |
| 1:A:176:ARG:HH22 | 1:B:357:ASN:HD21 | 1.58                     | 0.47              |
| 1:B:236:GLU:HG2  | 1:B:242:PHE:HZ   | 1.80                     | 0.47              |
| 1:D:436:GLY:O    | 1:D:440:LEU:HD13 | 2.14                     | 0.47              |
| 1:E:101:PHE:CE1  | 1:E:139:LEU:HD21 | 2.50                     | 0.47              |
| 1:B:126:PRO:O    | 1:B:127:ASP:C    | 2.58                     | 0.47              |
| 1:B:121:ASN:C    | 1:B:121:ASN:HD22 | 2.22                     | 0.47              |
| 1:C:207:ARG:HA   | 5:C:639:HOH:O    | 2.14                     | 0.47              |
| 1:F:97:ASN:ND2   | 1:F:231:LEU:H    | 2.10                     | 0.47              |
| 1:A:131:ALA:C    | 1:A:133:GLU:N    | 2.71                     | 0.47              |
| 1:B:85:ARG:HG2   | 1:B:209:ILE:HD12 | 1.97                     | 0.47              |
| 1:B:456:ALA:O    | 1:B:459:VAL:HG23 | 2.15                     | 0.47              |
| 1:D:92:THR:OG1   | 1:D:251:HIS:HE1  | 1.96                     | 0.47              |
| 1:F:292:LYS:HD2  | 1:F:304:TYR:CD2  | 2.50                     | 0.47              |
| 1:F:339:GLU:CD   | 1:F:339:GLU:H    | 2.23                     | 0.47              |
| 1:A:405:LEU:C    | 1:A:405:LEU:HD12 | 2.40                     | 0.47              |
| 1:D:181:SER:HB2  | 1:D:182:PRO:CD   | 2.45                     | 0.47              |
| 1:D:420:GLU:OE1  | 1:D:422:LYS:HE2  | 2.15                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:435:GLY:HA3  | 1:E:61:VAL:HG11  | 1.97                     | 0.47              |
| 1:E:59:ALA:O     | 1:E:63:THR:HG23  | 2.15                     | 0.47              |
| 1:E:75:VAL:HG23  | 1:E:424:ALA:HB2  | 1.96                     | 0.47              |
| 1:A:170:LEU:HD11 | 1:A:173:CYS:HB2  | 1.97                     | 0.47              |
| 1:C:205:LYS:H    | 1:C:206:PRO:CD   | 2.27                     | 0.46              |
| 1:F:52:MET:O     | 1:F:55:LEU:HB3   | 2.13                     | 0.46              |
| 1:B:207:ARG:HH21 | 1:B:207:ARG:CB   | 2.20                     | 0.46              |
| 1:B:97:ASN:ND2   | 1:B:231:LEU:H    | 2.09                     | 0.46              |
| 3:C:6:NAG:H83    | 3:C:6:NAG:O3     | 2.15                     | 0.46              |
| 1:F:315:THR:O    | 1:F:319:VAL:HG23 | 2.15                     | 0.46              |
| 1:C:427:VAL:O    | 1:C:431:LEU:HD13 | 2.14                     | 0.46              |
| 1:D:126:PRO:O    | 1:D:127:ASP:C    | 2.59                     | 0.46              |
| 1:A:149:LYS:O    | 1:A:151:LYS:HD3  | 2.16                     | 0.46              |
| 1:A:173:CYS:C    | 1:A:180:CYS:SG   | 2.99                     | 0.46              |
| 1:B:452:LEU:HA   | 1:B:455:TYR:HB3  | 1.96                     | 0.46              |
| 1:F:45:VAL:HG23  | 1:F:46:VAL:N     | 2.30                     | 0.46              |
| 1:A:120:ASN:ND2  | 1:A:124:GLU:H    | 2.14                     | 0.46              |
| 1:C:47:TRP:CZ3   | 1:C:447:LEU:HB3  | 2.51                     | 0.46              |
| 1:D:120:ASN:HD21 | 1:D:124:GLU:H    | 1.64                     | 0.46              |
| 1:E:173:CYS:C    | 1:E:180:CYS:SG   | 2.99                     | 0.46              |
| 1:E:181:SER:HB2  | 1:E:182:PRO:CD   | 2.46                     | 0.46              |
| 1:F:442:ILE:O    | 1:F:446:ILE:HG13 | 2.15                     | 0.46              |
| 1:B:53:GLY:O     | 1:B:57:LEU:HD23  | 2.15                     | 0.46              |
| 1:C:42:LEU:O     | 1:C:45:VAL:HG22  | 2.16                     | 0.46              |
| 1:C:448:THR:HG23 | 1:C:452:LEU:HD12 | 1.98                     | 0.46              |
| 1:D:46:VAL:HA    | 1:D:49:LEU:HG    | 1.98                     | 0.46              |
| 1:E:434:ILE:HA   | 1:E:437:GLN:HB3  | 1.98                     | 0.46              |
| 1:A:453:PHE:HE1  | 1:B:43:LYS:HZ2   | 1.64                     | 0.46              |
| 1:E:65:ARG:NH2   | 1:E:433:ASP:HB3  | 2.28                     | 0.46              |
| 1:C:62:CYS:O     | 1:C:66:ILE:HG23  | 2.16                     | 0.46              |
| 1:A:201:GLY:O    | 1:A:202:GLN:HB2  | 2.16                     | 0.45              |
| 1:A:205:LYS:HA   | 1:A:206:PRO:HD2  | 1.80                     | 0.45              |
| 1:A:240:THR:HG22 | 5:A:618:HOH:O    | 2.16                     | 0.45              |
| 1:B:101:PHE:CE1  | 1:B:139:LEU:HD13 | 2.51                     | 0.45              |
| 3:D:7:NAG:H83    | 3:D:7:NAG:O3     | 2.17                     | 0.45              |
| 1:C:55:LEU:C     | 1:C:55:LEU:HD13  | 2.41                     | 0.45              |
| 1:C:89:PRO:HB3   | 1:C:371:TYR:CZ   | 2.51                     | 0.45              |
| 1:C:139:LEU:HD23 | 1:C:234:TRP:CH2  | 2.51                     | 0.45              |
| 1:D:74:HIS:HD2   | 5:D:588:HOH:O    | 1.99                     | 0.45              |
| 1:F:282:ILE:HB   | 1:F:420:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:63:THR:O     | 1:A:66:ILE:HG22  | 2.17                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:137:GLU:HG2  | 5:C:632:HOH:O    | 2.17                     | 0.45              |
| 1:E:282:ILE:HB   | 1:E:420:GLU:HG3  | 1.98                     | 0.45              |
| 1:A:390:ALA:HB1  | 1:A:395:LYS:O    | 2.15                     | 0.45              |
| 1:D:446:ILE:O    | 1:D:450:LEU:HG   | 2.17                     | 0.45              |
| 1:E:283:TYR:CZ   | 1:E:364:MET:HE1  | 2.52                     | 0.45              |
| 1:A:58:LEU:HD13  | 1:A:438:MET:HA   | 1.99                     | 0.45              |
| 1:E:132:ASP:OD2  | 1:E:134:LYS:HB3  | 2.17                     | 0.45              |
| 1:B:181:SER:HB2  | 1:B:182:PRO:CD   | 2.47                     | 0.45              |
| 1:D:280:ARG:HG3  | 1:D:416:TYR:CE1  | 2.51                     | 0.45              |
| 1:A:227:GLN:HA   | 1:A:230:TYR:CD1  | 2.52                     | 0.45              |
| 1:B:61:VAL:HG11  | 1:B:437:GLN:HG2  | 1.97                     | 0.45              |
| 1:C:205:LYS:HB3  | 1:C:206:PRO:HD3  | 1.97                     | 0.45              |
| 1:F:192:TYR:CE2  | 1:F:260:ASP:HA   | 2.52                     | 0.45              |
| 1:A:176:ARG:NH2  | 1:B:357:ASN:HD21 | 2.15                     | 0.45              |
| 1:B:300:PHE:HD2  | 1:B:312:ASP:CG   | 2.25                     | 0.45              |
| 1:B:436:GLY:O    | 1:B:440:LEU:HG   | 2.17                     | 0.45              |
| 1:C:154:ASN:HD21 | 1:C:156:LEU:HB3  | 1.82                     | 0.45              |
| 1:E:97:ASN:ND2   | 1:E:231:LEU:H    | 2.13                     | 0.45              |
| 1:E:130:THR:HG22 | 1:E:130:THR:O    | 2.17                     | 0.45              |
| 1:B:434:ILE:O    | 1:B:438:MET:HG2  | 2.17                     | 0.45              |
| 1:E:292:LYS:HD3  | 1:E:292:LYS:C    | 2.41                     | 0.45              |
| 1:A:42:LEU:C     | 1:A:42:LEU:HD22  | 2.41                     | 0.44              |
| 1:A:204:GLY:O    | 1:A:206:PRO:N    | 2.49                     | 0.44              |
| 1:F:274:VAL:HG22 | 1:F:375:LEU:HG   | 1.99                     | 0.44              |
| 1:D:202:GLN:C    | 1:D:204:GLY:N    | 2.75                     | 0.44              |
| 1:F:395:LYS:HG2  | 1:F:399:TYR:CD1  | 2.51                     | 0.44              |
| 1:F:405:LEU:C    | 1:F:405:LEU:HD12 | 2.43                     | 0.44              |
| 1:B:449:VAL:HA   | 1:B:452:LEU:CD2  | 2.47                     | 0.44              |
| 1:C:43:LYS:O     | 1:C:47:TRP:HD1   | 2.00                     | 0.44              |
| 1:D:132:ASP:HB2  | 5:D:651:HOH:O    | 2.17                     | 0.44              |
| 1:E:53:GLY:O     | 1:E:54:SER:HB3   | 2.18                     | 0.44              |
| 1:F:433:ASP:O    | 1:F:437:GLN:HG2  | 2.17                     | 0.44              |
| 1:A:134:LYS:O    | 1:A:138:ILE:HG22 | 2.18                     | 0.44              |
| 1:B:42:LEU:C     | 1:B:44:ARG:N     | 2.76                     | 0.44              |
| 1:E:53:GLY:C     | 1:E:55:LEU:N     | 2.70                     | 0.44              |
| 1:B:405:LEU:HD23 | 1:B:405:LEU:O    | 2.17                     | 0.44              |
| 1:D:176:ARG:HH22 | 1:E:357:ASN:HD21 | 1.60                     | 0.44              |
| 1:E:51:PHE:HB2   | 1:E:448:THR:OG1  | 2.17                     | 0.44              |
| 1:F:318:LEU:HD22 | 1:F:329:MET:HE1  | 2.00                     | 0.44              |
| 1:A:377:MET:HE3  | 1:B:377:MET:HE1  | 2.00                     | 0.44              |
| 1:C:109:LEU:HG   | 1:C:119:LEU:HD11 | 1.99                     | 0.44              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:E:133:GLU:HG3  | 1:E:134:LYS:N    | 2.33                     | 0.44              |
| 1:E:452:LEU:HD23 | 1:E:452:LEU:C    | 2.43                     | 0.44              |
| 1:A:53:GLY:O     | 1:A:57:LEU:HD23  | 2.17                     | 0.44              |
| 1:B:405:LEU:C    | 1:B:405:LEU:CD2  | 2.90                     | 0.44              |
| 1:D:84:THR:O     | 1:D:85:ARG:HB2   | 2.17                     | 0.44              |
| 1:A:120:ASN:C    | 1:A:120:ASN:ND2  | 2.76                     | 0.44              |
| 1:C:42:LEU:O     | 1:C:46:VAL:HG23  | 2.17                     | 0.44              |
| 1:E:55:LEU:HD11  | 1:E:58:LEU:HD22  | 2.00                     | 0.44              |
| 1:A:295:THR:CG2  | 1:A:296:GLY:N    | 2.81                     | 0.43              |
| 1:D:227:GLN:HA   | 1:D:230:TYR:CD1  | 2.53                     | 0.43              |
| 1:F:120:ASN:ND2  | 1:F:124:GLU:H    | 2.17                     | 0.43              |
| 1:E:353:VAL:HG23 | 1:E:354:GLU:HG3  | 2.01                     | 0.43              |
| 1:C:346:ASP:HB2  | 1:C:347:PRO:HD3  | 2.00                     | 0.43              |
| 1:E:58:LEU:N     | 1:E:58:LEU:HD12  | 2.34                     | 0.43              |
| 1:F:42:LEU:O     | 1:F:42:LEU:HD22  | 2.19                     | 0.43              |
| 1:D:395:LYS:HG2  | 1:D:399:TYR:CE1  | 2.54                     | 0.43              |
| 1:E:271:GLN:NE2  | 1:F:243:GLU:HG2  | 2.33                     | 0.43              |
| 1:C:173:CYS:C    | 1:C:180:CYS:SG   | 3.01                     | 0.43              |
| 1:F:55:LEU:HD22  | 1:F:55:LEU:O     | 2.18                     | 0.43              |
| 1:F:227:GLN:HA   | 1:F:230:TYR:CD1  | 2.54                     | 0.43              |
| 1:A:445:SER:O    | 1:A:449:VAL:HG23 | 2.18                     | 0.43              |
| 1:B:165:ASP:OD1  | 1:B:167:ARG:HG3  | 2.18                     | 0.43              |
| 1:B:395:LYS:HG2  | 1:B:399:TYR:CE1  | 2.53                     | 0.43              |
| 1:C:293:ALA:O    | 1:C:295:THR:N    | 2.49                     | 0.43              |
| 1:F:300:PHE:HD2  | 1:F:312:ASP:OD1  | 2.01                     | 0.43              |
| 1:B:45:VAL:C     | 1:B:47:TRP:N     | 2.72                     | 0.43              |
| 1:B:45:VAL:O     | 1:B:49:LEU:HG    | 2.19                     | 0.43              |
| 1:D:120:ASN:C    | 1:D:120:ASN:ND2  | 2.75                     | 0.43              |
| 1:D:271:GLN:HE21 | 1:E:243:GLU:HG2  | 1.84                     | 0.43              |
| 1:E:135:GLN:NE2  | 1:E:232:PRO:HG3  | 2.34                     | 0.43              |
| 1:E:181:SER:HB2  | 1:E:182:PRO:HD2  | 2.01                     | 0.43              |
| 1:A:86:LEU:HD23  | 1:A:86:LEU:C     | 2.44                     | 0.43              |
| 1:B:139:LEU:HD12 | 1:B:139:LEU:HA   | 1.86                     | 0.43              |
| 1:C:128:THR:HB   | 1:C:234:TRP:CE2  | 2.53                     | 0.43              |
| 1:D:173:CYS:C    | 1:D:180:CYS:SG   | 3.02                     | 0.43              |
| 1:D:346:ASP:HB2  | 1:D:347:PRO:HD3  | 2.01                     | 0.43              |
| 1:E:98:GLU:HG2   | 1:E:192:TYR:O    | 2.19                     | 0.43              |
| 1:F:43:LYS:NZ    | 1:F:43:LYS:HB3   | 2.34                     | 0.43              |
| 1:F:427:VAL:O    | 1:F:431:LEU:HD13 | 2.20                     | 0.42              |
| 1:B:449:VAL:O    | 1:B:453:PHE:HB2  | 2.20                     | 0.42              |
| 1:C:205:LYS:N    | 1:C:206:PRO:CD   | 2.81                     | 0.42              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:280:ARG:HG2 | 1:C:280:ARG:HH11 | 1.84                     | 0.42              |
| 1:D:106:LYS:HE3 | 1:D:106:LYS:HB2  | 1.88                     | 0.42              |
| 1:D:176:ARG:NH1 | 1:E:357:ASN:HD21 | 2.17                     | 0.42              |
| 1:D:427:VAL:O   | 1:D:431:LEU:HD13 | 2.18                     | 0.42              |
| 1:A:346:ASP:N   | 1:A:347:PRO:HD2  | 2.34                     | 0.42              |
| 1:D:447:LEU:O   | 1:D:447:LEU:HD13 | 2.19                     | 0.42              |
| 1:E:268:PRO:HA  | 1:E:405:LEU:HB3  | 2.01                     | 0.42              |
| 1:B:135:GLN:O   | 1:B:138:ILE:HG23 | 2.19                     | 0.42              |
| 1:A:256:PRO:O   | 1:A:307:THR:HG21 | 2.19                     | 0.42              |
| 1:B:121:ASN:ND2 | 1:B:122:ARG:HG3  | 2.33                     | 0.42              |
| 1:B:134:LYS:O   | 1:B:138:ILE:HG22 | 2.19                     | 0.42              |
| 1:D:146:ARG:HG3 | 1:D:146:ARG:HH11 | 1.84                     | 0.42              |
| 1:D:241:SER:HB2 | 5:D:518:HOH:O    | 2.19                     | 0.42              |
| 1:F:201:GLY:O   | 1:F:202:GLN:NE2  | 2.53                     | 0.42              |
| 1:B:121:ASN:C   | 1:B:121:ASN:ND2  | 2.75                     | 0.42              |
| 1:B:227:GLN:HA  | 1:B:230:TYR:CD1  | 2.55                     | 0.42              |
| 1:B:394:ASN:O   | 1:B:395:LYS:HD2  | 2.18                     | 0.42              |
| 1:E:58:LEU:O    | 1:E:62:CYS:HB2   | 2.20                     | 0.42              |
| 1:B:120:ASN:ND2 | 1:B:124:GLU:H    | 2.17                     | 0.42              |
| 1:F:47:TRP:HH2  | 1:F:448:THR:HG1  | 1.60                     | 0.42              |
| 1:B:455:TYR:C   | 1:B:457:TYR:N    | 2.77                     | 0.42              |
| 1:C:85:ARG:HH21 | 1:C:209:ILE:HD13 | 1.83                     | 0.42              |
| 1:D:55:LEU:HB2  | 1:D:441:PHE:HE2  | 1.84                     | 0.42              |
| 1:A:97:ASN:ND2  | 1:A:231:LEU:H    | 2.14                     | 0.42              |
| 1:D:202:GLN:OE1 | 1:D:202:GLN:HA   | 2.20                     | 0.42              |
| 1:B:128:THR:O   | 1:B:130:THR:N    | 2.53                     | 0.41              |
| 1:B:454:ASP:OD1 | 1:C:40:LEU:HD21  | 2.20                     | 0.41              |
| 1:D:46:VAL:O    | 1:D:49:LEU:HG    | 2.19                     | 0.41              |
| 1:D:64:ASN:OD1  | 1:D:65:ARG:HD2   | 2.20                     | 0.41              |
| 1:F:181:SER:HB3 | 1:F:182:PRO:CD   | 2.50                     | 0.41              |
| 1:A:120:ASN:C   | 1:A:122:ARG:H    | 2.29                     | 0.41              |
| 5:A:728:HOH:O   | 1:B:437:GLN:HG3  | 2.19                     | 0.41              |
| 1:B:42:LEU:CD1  | 1:B:44:ARG:HB2   | 2.38                     | 0.41              |
| 1:B:448:THR:O   | 1:B:452:LEU:HD22 | 2.20                     | 0.41              |
| 1:D:54:SER:OG   | 1:D:441:PHE:HA   | 2.20                     | 0.41              |
| 1:D:97:ASN:ND2  | 1:D:231:LEU:H    | 2.16                     | 0.41              |
| 1:F:374:GLU:HB3 | 5:F:591:HOH:O    | 2.19                     | 0.41              |
| 1:B:44:ARG:O    | 1:B:47:TRP:HB3   | 2.21                     | 0.41              |
| 1:C:227:GLN:HA  | 1:C:230:TYR:CD1  | 2.55                     | 0.41              |
| 1:A:235:GLY:O   | 1:A:240:THR:HG21 | 2.20                     | 0.41              |
| 1:A:364:MET:HA  | 1:A:365:PRO:HD3  | 1.97                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:188:VAL:O    | 1:B:188:VAL:HG13 | 2.21                     | 0.41              |
| 1:C:85:ARG:HD3   | 1:C:209:ILE:CD1  | 2.50                     | 0.41              |
| 1:D:128:THR:HG22 | 1:D:129:GLN:N    | 2.36                     | 0.41              |
| 1:C:296:GLY:O    | 1:C:297:ASP:C    | 2.63                     | 0.41              |
| 1:D:44:ARG:HG2   | 1:D:44:ARG:HH11  | 1.85                     | 0.41              |
| 1:E:176:ARG:NH1  | 1:F:357:ASN:HD21 | 2.17                     | 0.41              |
| 1:E:270:PHE:CD1  | 1:E:377:MET:HE3  | 2.55                     | 0.41              |
| 1:A:450:LEU:HD11 | 1:B:50:CYS:SG    | 2.61                     | 0.41              |
| 1:F:204:GLY:N    | 5:F:654:HOH:O    | 2.54                     | 0.41              |
| 1:A:99:PHE:CE2   | 1:A:116:LEU:HD21 | 2.55                     | 0.41              |
| 1:B:295:THR:CG2  | 1:B:296:GLY:N    | 2.83                     | 0.41              |
| 1:E:72:TYR:HB3   | 1:E:288:TRP:CD1  | 2.56                     | 0.41              |
| 1:E:306:ILE:O    | 1:E:310:ARG:HG3  | 2.20                     | 0.41              |
| 1:E:379:LYS:HD2  | 1:E:380:ILE:N    | 2.36                     | 0.41              |
| 1:F:120:ASN:HD22 | 1:F:122:ARG:H    | 1.67                     | 0.41              |
| 1:A:144:ASN:OD1  | 1:A:146:ARG:HG2  | 2.21                     | 0.41              |
| 1:A:181:SER:HB2  | 1:A:182:PRO:HD2  | 2.03                     | 0.41              |
| 1:B:292:LYS:HD2  | 1:B:304:TYR:CZ   | 2.55                     | 0.41              |
| 1:C:433:ASP:O    | 1:C:437:GLN:HG2  | 2.21                     | 0.41              |
| 1:F:420:GLU:CD   | 1:F:422:LYS:HE2  | 2.46                     | 0.41              |
| 1:A:301:TYR:OH   | 1:A:311:ILE:HG21 | 2.19                     | 0.41              |
| 1:B:67:GLN:HE21  | 1:B:67:GLN:HB2   | 1.67                     | 0.41              |
| 1:C:210:THR:HG21 | 5:C:738:HOH:O    | 2.21                     | 0.41              |
| 1:E:55:LEU:CD1   | 1:E:58:LEU:HD22  | 2.51                     | 0.40              |
| 1:E:298:SER:C    | 1:E:300:PHE:H    | 2.29                     | 0.40              |
| 1:E:431:LEU:HD12 | 1:E:431:LEU:N    | 2.36                     | 0.40              |
| 1:F:181:SER:HB3  | 1:F:182:PRO:HD2  | 2.01                     | 0.40              |
| 1:F:379:LYS:HD3  | 5:F:757:HOH:O    | 2.21                     | 0.40              |
| 1:A:57:LEU:HB3   | 1:A:437:GLN:OE1  | 2.21                     | 0.40              |
| 1:A:236:GLU:HG2  | 1:A:242:PHE:CZ   | 2.55                     | 0.40              |
| 1:D:439:GLY:HA3  | 1:E:58:LEU:CD1   | 2.52                     | 0.40              |
| 1:E:128:THR:HA   | 1:E:136:LEU:CD2  | 2.50                     | 0.40              |
| 1:E:280:ARG:HH21 | 1:E:280:ARG:HG2  | 1.86                     | 0.40              |
| 1:F:448:THR:O    | 1:F:452:LEU:HB2  | 2.21                     | 0.40              |
| 1:B:135:GLN:HA   | 1:B:138:ILE:CG2  | 2.52                     | 0.40              |
| 1:B:387:LYS:HE2  | 1:C:131:ALA:HA   | 2.04                     | 0.40              |
| 1:D:357:ASN:HD21 | 1:F:176:ARG:NH1  | 2.19                     | 0.40              |
| 1:E:52:MET:HG3   | 1:E:448:THR:OG1  | 2.21                     | 0.40              |
| 1:B:104:VAL:HG21 | 1:B:231:LEU:HD21 | 2.03                     | 0.40              |
| 1:B:303:THR:HG22 | 1:B:304:TYR:N    | 2.37                     | 0.40              |
| 1:C:42:LEU:C     | 1:C:44:ARG:H     | 2.29                     | 0.40              |

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| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:D:176:ARG:NH2 | 1:E:357:ASN:HD21 | 2.20                     | 0.40              |
| 1:E:44:ARG:HG2  | 1:E:44:ARG:HH21  | 1.87                     | 0.40              |
| 1:A:455:TYR:CD1 | 1:A:455:TYR:C    | 2.99                     | 0.40              |
| 1:C:85:ARG:HD3  | 1:C:209:ILE:HD12 | 2.03                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|---------|----------|-------------|----|
| 1   | A     | 415/438 (95%)   | 396 (95%)  | 12 (3%) | 7 (2%)   | 7           | 2  |
| 1   | B     | 418/438 (95%)   | 397 (95%)  | 18 (4%) | 3 (1%)   | 18          | 10 |
| 1   | C     | 416/438 (95%)   | 398 (96%)  | 12 (3%) | 6 (1%)   | 9           | 3  |
| 1   | D     | 413/438 (94%)   | 390 (94%)  | 18 (4%) | 5 (1%)   | 10          | 4  |
| 1   | E     | 419/438 (96%)   | 397 (95%)  | 20 (5%) | 2 (0%)   | 24          | 16 |
| 1   | F     | 410/438 (94%)   | 394 (96%)  | 13 (3%) | 3 (1%)   | 18          | 10 |
| All | All   | 2491/2628 (95%) | 2372 (95%) | 93 (4%) | 26 (1%)  | 12          | 5  |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 202 | GLN  |
| 1   | A     | 203 | ASP  |
| 1   | A     | 206 | PRO  |
| 1   | C     | 205 | LYS  |
| 1   | D     | 132 | ASP  |
| 1   | D     | 298 | SER  |
| 1   | D     | 299 | GLU  |
| 1   | E     | 127 | ASP  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | F     | 43  | LYS  |
| 1   | D     | 127 | ASP  |
| 1   | F     | 299 | GLU  |
| 1   | A     | 207 | ARG  |
| 1   | B     | 46  | VAL  |
| 1   | B     | 129 | GLN  |
| 1   | C     | 286 | PRO  |
| 1   | C     | 294 | THR  |
| 1   | C     | 455 | TYR  |
| 1   | F     | 297 | ASP  |
| 1   | A     | 205 | LYS  |
| 1   | C     | 206 | PRO  |
| 1   | C     | 297 | ASP  |
| 1   | E     | 435 | GLY  |
| 1   | A     | 296 | GLY  |
| 1   | B     | 126 | PRO  |
| 1   | D     | 126 | PRO  |
| 1   | A     | 126 | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |    |
|-----|-------|-----------------|------------|----------|-------------|----|
| 1   | A     | 363/383 (95%)   | 352 (97%)  | 11 (3%)  | 36          | 30 |
| 1   | B     | 366/383 (96%)   | 354 (97%)  | 12 (3%)  | 33          | 26 |
| 1   | C     | 364/383 (95%)   | 356 (98%)  | 8 (2%)   | 45          | 42 |
| 1   | D     | 361/383 (94%)   | 354 (98%)  | 7 (2%)   | 50          | 47 |
| 1   | E     | 367/383 (96%)   | 357 (97%)  | 10 (3%)  | 39          | 34 |
| 1   | F     | 359/383 (94%)   | 346 (96%)  | 13 (4%)  | 31          | 23 |
| All | All   | 2180/2298 (95%) | 2119 (97%) | 61 (3%)  | 38          | 32 |

All (61) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 42  | LEU  |
| 1   | A     | 43  | LYS  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 147 | ASN  |
| 1   | A     | 151 | LYS  |
| 1   | A     | 180 | CYS  |
| 1   | A     | 217 | ASN  |
| 1   | A     | 240 | THR  |
| 1   | A     | 299 | GLU  |
| 1   | A     | 381 | PRO  |
| 1   | A     | 430 | LEU  |
| 1   | B     | 42  | LEU  |
| 1   | B     | 120 | ASN  |
| 1   | B     | 121 | ASN  |
| 1   | B     | 138 | ILE  |
| 1   | B     | 180 | CYS  |
| 1   | B     | 207 | ARG  |
| 1   | B     | 217 | ASN  |
| 1   | B     | 312 | ASP  |
| 1   | B     | 320 | GLU  |
| 1   | B     | 405 | LEU  |
| 1   | B     | 437 | GLN  |
| 1   | B     | 458 | GLU  |
| 1   | C     | 42  | LEU  |
| 1   | C     | 139 | LEU  |
| 1   | C     | 180 | CYS  |
| 1   | C     | 202 | GLN  |
| 1   | C     | 217 | ASN  |
| 1   | C     | 405 | LEU  |
| 1   | C     | 450 | LEU  |
| 1   | C     | 457 | TYR  |
| 1   | D     | 43  | LYS  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 130 | THR  |
| 1   | D     | 139 | LEU  |
| 1   | D     | 180 | CYS  |
| 1   | D     | 217 | ASN  |
| 1   | D     | 312 | ASP  |
| 1   | E     | 87  | THR  |
| 1   | E     | 122 | ARG  |
| 1   | E     | 151 | LYS  |
| 1   | E     | 180 | CYS  |
| 1   | E     | 217 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | E     | 292 | LYS  |
| 1   | E     | 379 | LYS  |
| 1   | E     | 430 | LEU  |
| 1   | E     | 447 | LEU  |
| 1   | E     | 458 | GLU  |
| 1   | F     | 42  | LEU  |
| 1   | F     | 43  | LYS  |
| 1   | F     | 55  | LEU  |
| 1   | F     | 120 | ASN  |
| 1   | F     | 129 | GLN  |
| 1   | F     | 139 | LEU  |
| 1   | F     | 180 | CYS  |
| 1   | F     | 217 | ASN  |
| 1   | F     | 231 | LEU  |
| 1   | F     | 292 | LYS  |
| 1   | F     | 381 | PRO  |
| 1   | F     | 451 | GLU  |
| 1   | F     | 452 | LEU  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 67  | GLN  |
| 1   | A     | 97  | ASN  |
| 1   | A     | 111 | HIS  |
| 1   | A     | 120 | ASN  |
| 1   | A     | 129 | GLN  |
| 1   | A     | 144 | ASN  |
| 1   | A     | 154 | ASN  |
| 1   | A     | 202 | GLN  |
| 1   | A     | 357 | ASN  |
| 1   | B     | 67  | GLN  |
| 1   | B     | 97  | ASN  |
| 1   | B     | 120 | ASN  |
| 1   | B     | 121 | ASN  |
| 1   | B     | 129 | GLN  |
| 1   | B     | 147 | ASN  |
| 1   | B     | 251 | HIS  |
| 1   | B     | 271 | GLN  |
| 1   | B     | 323 | ASN  |
| 1   | B     | 357 | ASN  |
| 1   | B     | 437 | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 64  | ASN  |
| 1   | C     | 67  | GLN  |
| 1   | C     | 97  | ASN  |
| 1   | C     | 135 | GLN  |
| 1   | C     | 140 | GLN  |
| 1   | C     | 144 | ASN  |
| 1   | C     | 154 | ASN  |
| 1   | C     | 202 | GLN  |
| 1   | C     | 251 | HIS  |
| 1   | C     | 321 | ASN  |
| 1   | C     | 357 | ASN  |
| 1   | D     | 74  | HIS  |
| 1   | D     | 97  | ASN  |
| 1   | D     | 120 | ASN  |
| 1   | D     | 140 | GLN  |
| 1   | D     | 144 | ASN  |
| 1   | D     | 147 | ASN  |
| 1   | D     | 251 | HIS  |
| 1   | D     | 271 | GLN  |
| 1   | D     | 357 | ASN  |
| 1   | E     | 64  | ASN  |
| 1   | E     | 67  | GLN  |
| 1   | E     | 135 | GLN  |
| 1   | E     | 251 | HIS  |
| 1   | E     | 271 | GLN  |
| 1   | E     | 357 | ASN  |
| 1   | E     | 398 | GLN  |
| 1   | F     | 64  | ASN  |
| 1   | F     | 67  | GLN  |
| 1   | F     | 97  | ASN  |
| 1   | F     | 120 | ASN  |
| 1   | F     | 135 | GLN  |
| 1   | F     | 140 | GLN  |
| 1   | F     | 202 | GLN  |
| 1   | F     | 251 | HIS  |
| 1   | F     | 323 | ASN  |
| 1   | F     | 357 | ASN  |
| 1   | F     | 398 | 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 ⓘ

6 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 2   | GLC  | G     | 1   | 2    | 12,12,12     | 1.00 | 0           | 17,17,17    | 0.71 | 0           |
| 2   | GLC  | G     | 2   | 2    | 11,11,12     | 1.07 | 0           | 15,15,17    | 0.75 | 0           |
| 2   | GLC  | H     | 1   | 2    | 12,12,12     | 1.01 | 0           | 17,17,17    | 0.73 | 0           |
| 2   | GLC  | H     | 2   | 2    | 11,11,12     | 1.13 | 1 (9%)      | 15,15,17    | 0.74 | 0           |
| 2   | GLC  | I     | 1   | 2    | 12,12,12     | 1.00 | 0           | 17,17,17    | 0.72 | 0           |
| 2   | GLC  | I     | 2   | 2    | 11,11,12     | 1.11 | 1 (9%)      | 15,15,17    | 0.73 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 2   | GLC  | G     | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | GLC  | G     | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | GLC  | H     | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | GLC  | H     | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | GLC  | I     | 1   | 2    | -       | 0/2/22/22 | 0/1/1/1 |
| 2   | GLC  | I     | 2   | 2    | -       | 0/2/19/22 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | I     | 2   | GLC  | O5-C1 | 2.09 | 1.47        | 1.43     |
| 2   | H     | 2   | GLC  | O5-C1 | 2.07 | 1.47        | 1.43     |

There are no bond angle outliers.

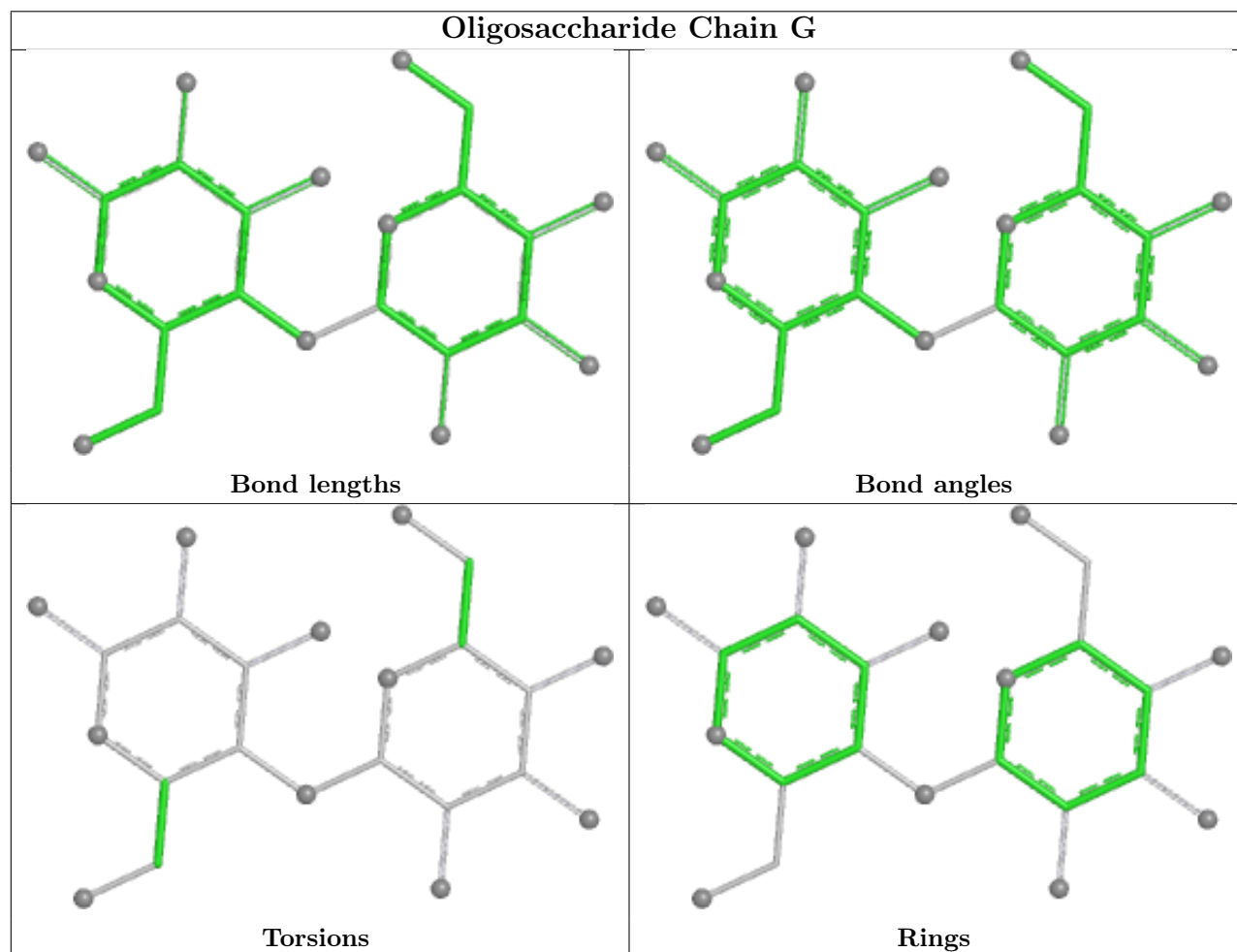
There are no chirality outliers.

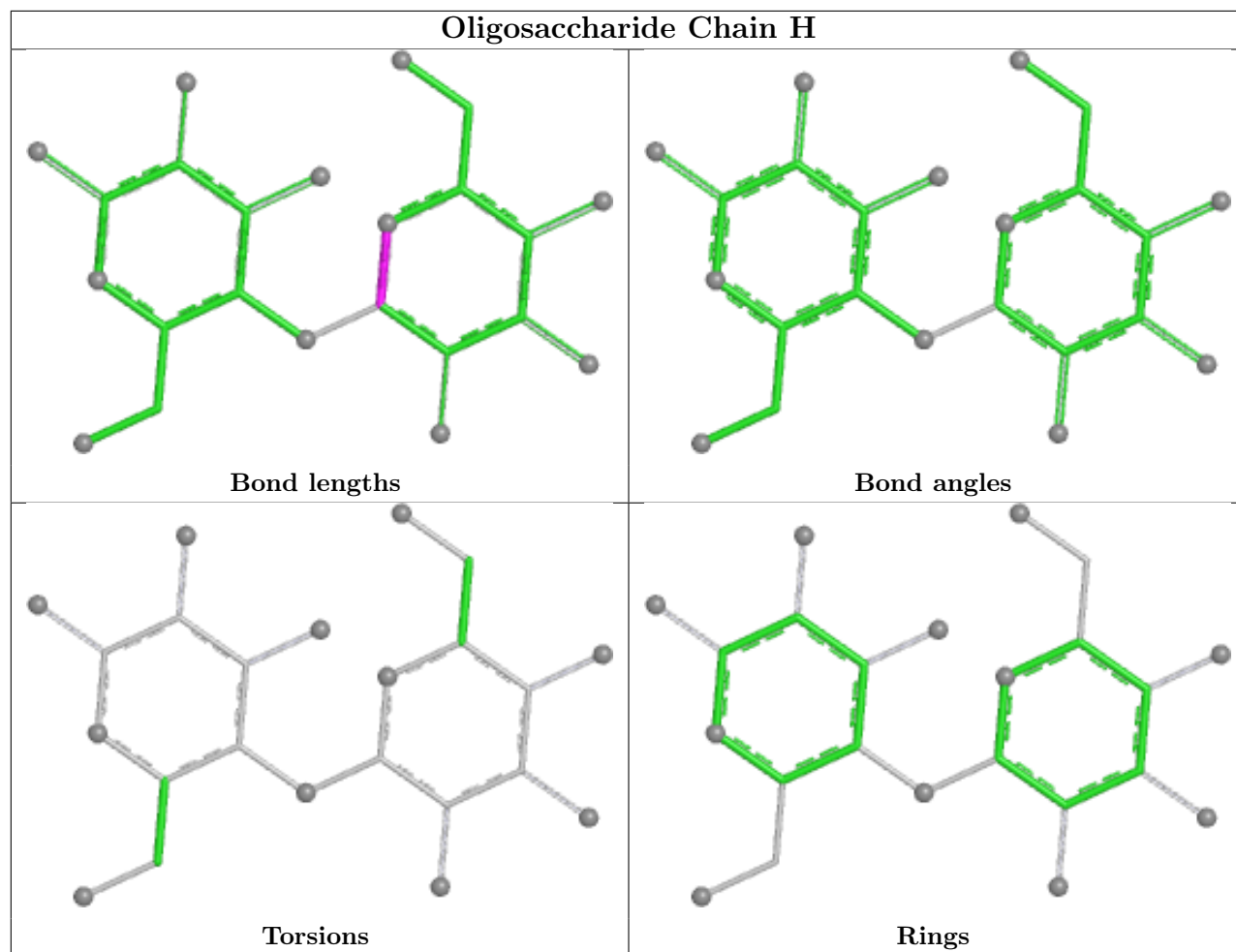
There are no torsion outliers.

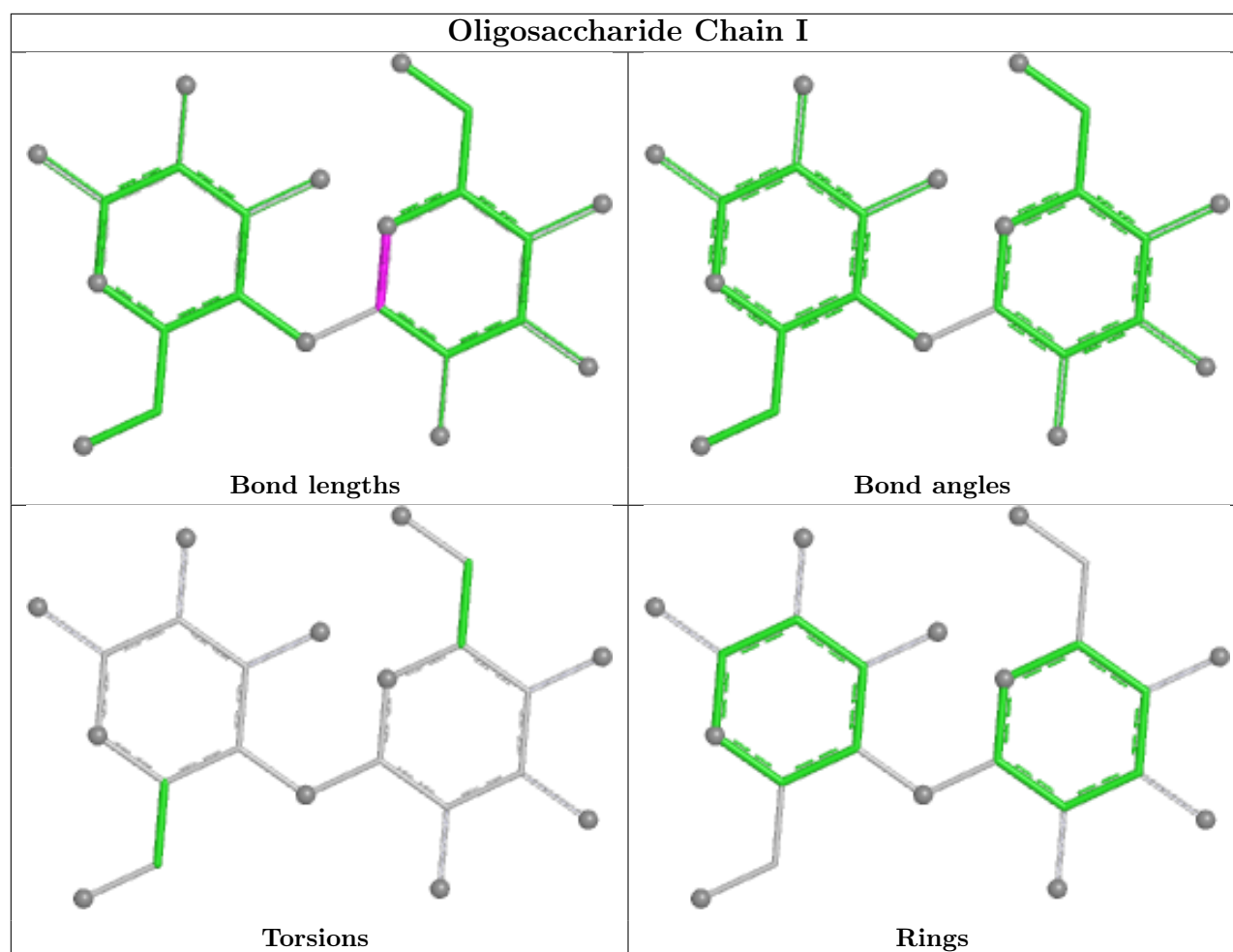
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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 | $\# Z  > 2$ |
| 3   | NAG  | F     | 11  | 1    | 14,14,15     | 0.57 | 0           | 17,19,21    | 0.64 | 0           |
| 3   | NAG  | D     | 8   | 1    | 14,14,15     | 0.62 | 0           | 17,19,21    | 0.70 | 1 (5%)      |
| 3   | NAG  | A     | 1   | 1    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.71 | 1 (5%)      |
| 3   | NAG  | F     | 12  | 1    | 14,14,15     | 0.60 | 0           | 17,19,21    | 0.61 | 0           |
| 3   | NAG  | E     | 10  | 1    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.66 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | D     | 7   | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.69 | 1 (5%)   |
| 3   | NAG  | E     | 9   | 1    | 14,14,15     | 0.49 | 0        | 17,19,21    | 0.70 | 1 (5%)   |
| 3   | NAG  | B     | 3   | 1    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.69 | 1 (5%)   |
| 3   | NAG  | B     | 4   | 1    | 14,14,15     | 0.53 | 0        | 17,19,21    | 0.63 | 0        |
| 3   | NAG  | C     | 5   | 1    | 14,14,15     | 0.53 | 0        | 17,19,21    | 0.59 | 0        |
| 3   | NAG  | C     | 6   | 1    | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.65 | 0        |
| 3   | NAG  | A     | 2   | 1    | 14,14,15     | 0.60 | 0        | 17,19,21    | 0.68 | 1 (5%)   |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | F     | 11  | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 8   | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 1   | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | F     | 12  | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 10  | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | D     | 7   | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 9   | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 3   | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | B     | 4   | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 5   | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | C     | 6   | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | A     | 2   | 1    | -       | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (6) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | D     | 8   | NAG  | C2-N2-C7 | -2.23 | 119.92      | 122.90   |
| 3   | E     | 9   | NAG  | C2-N2-C7 | -2.21 | 119.93      | 122.90   |
| 3   | A     | 1   | NAG  | C2-N2-C7 | -2.20 | 119.96      | 122.90   |
| 3   | D     | 7   | NAG  | C2-N2-C7 | -2.17 | 119.99      | 122.90   |
| 3   | B     | 3   | NAG  | C2-N2-C7 | -2.08 | 120.11      | 122.90   |
| 3   | A     | 2   | NAG  | C2-N2-C7 | -2.07 | 120.13      | 122.90   |

There are no chirality outliers.

All (32) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | C     | 5   | NAG  | C3-C2-N2-C7 |
| 3   | C     | 5   | NAG  | C8-C7-N2-C2 |
| 3   | C     | 5   | NAG  | O7-C7-N2-C2 |
| 3   | C     | 6   | NAG  | C8-C7-N2-C2 |
| 3   | C     | 6   | NAG  | O7-C7-N2-C2 |
| 3   | D     | 7   | NAG  | C8-C7-N2-C2 |
| 3   | D     | 7   | NAG  | O7-C7-N2-C2 |
| 3   | E     | 9   | NAG  | C8-C7-N2-C2 |
| 3   | E     | 9   | NAG  | O7-C7-N2-C2 |
| 3   | E     | 10  | NAG  | C8-C7-N2-C2 |
| 3   | E     | 10  | NAG  | O7-C7-N2-C2 |
| 3   | F     | 11  | NAG  | C8-C7-N2-C2 |
| 3   | F     | 11  | NAG  | O7-C7-N2-C2 |
| 3   | F     | 12  | NAG  | C8-C7-N2-C2 |
| 3   | F     | 12  | NAG  | O7-C7-N2-C2 |
| 3   | E     | 9   | NAG  | O5-C5-C6-O6 |
| 3   | E     | 10  | NAG  | C4-C5-C6-O6 |
| 3   | F     | 12  | NAG  | O5-C5-C6-O6 |
| 3   | E     | 9   | NAG  | C4-C5-C6-O6 |
| 3   | E     | 10  | NAG  | O5-C5-C6-O6 |
| 3   | F     | 12  | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | D     | 7   | NAG  | O5-C5-C6-O6 |
| 3   | D     | 7   | NAG  | C4-C5-C6-O6 |
| 3   | A     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | B     | 4   | NAG  | C8-C7-N2-C2 |
| 3   | F     | 11  | NAG  | O5-C5-C6-O6 |
| 3   | B     | 4   | NAG  | C4-C5-C6-O6 |
| 3   | B     | 4   | NAG  | O7-C7-N2-C2 |
| 3   | B     | 4   | NAG  | O5-C5-C6-O6 |
| 3   | F     | 12  | NAG  | C3-C2-N2-C7 |
| 3   | F     | 12  | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

3 monomers are involved in 3 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 3   | F     | 11  | NAG  | 1       | 0            |
| 3   | D     | 7   | NAG  | 1       | 0            |
| 3   | C     | 6   | NAG  | 1       | 0            |

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2                     | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|-----------------------------|-----------------------|-------|
| 1   | A     | 417/438 (95%)   | 1.07   | 102 (24%) <b>2</b> <b>1</b> | 13, 30, 80, 91        | 0     |
| 1   | B     | 420/438 (95%)   | 1.01   | 93 (22%) <b>2</b> <b>2</b>  | 12, 31, 85, 97        | 0     |
| 1   | C     | 418/438 (95%)   | 0.81   | 94 (22%) <b>2</b> <b>2</b>  | 13, 28, 73, 88        | 0     |
| 1   | D     | 415/438 (94%)   | 1.23   | 113 (27%) <b>1</b> <b>1</b> | 12, 31, 80, 91        | 0     |
| 1   | E     | 421/438 (96%)   | 1.31   | 131 (31%) <b>1</b> <b>1</b> | 11, 31, 87, 96        | 0     |
| 1   | F     | 412/438 (94%)   | 1.09   | 98 (23%) <b>2</b> <b>1</b>  | 13, 30, 81, 94        | 0     |
| All | All   | 2503/2628 (95%) | 1.09   | 631 (25%) <b>1</b> <b>1</b> | 11, 30, 82, 97        | 0     |

All (631) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 293 | ALA  | 9.0  |
| 1   | F     | 42  | LEU  | 8.8  |
| 1   | B     | 457 | TYR  | 8.0  |
| 1   | D     | 456 | ALA  | 7.6  |
| 1   | E     | 447 | LEU  | 7.6  |
| 1   | F     | 202 | GLN  | 7.6  |
| 1   | F     | 293 | ALA  | 7.4  |
| 1   | E     | 293 | ALA  | 7.4  |
| 1   | B     | 128 | THR  | 7.4  |
| 1   | A     | 206 | PRO  | 7.2  |
| 1   | F     | 450 | LEU  | 7.1  |
| 1   | E     | 446 | ILE  | 7.0  |
| 1   | D     | 447 | LEU  | 6.9  |
| 1   | E     | 298 | SER  | 6.9  |
| 1   | E     | 295 | THR  | 6.9  |
| 1   | A     | 293 | ALA  | 6.8  |
| 1   | F     | 45  | VAL  | 6.7  |
| 1   | A     | 450 | LEU  | 6.6  |
| 1   | D     | 453 | PHE  | 6.6  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 294 | THR  | 6.5  |
| 1   | A     | 295 | THR  | 6.4  |
| 1   | E     | 48  | ALA  | 6.3  |
| 1   | A     | 128 | THR  | 6.3  |
| 1   | F     | 46  | VAL  | 6.3  |
| 1   | A     | 453 | PHE  | 6.2  |
| 1   | E     | 130 | THR  | 6.2  |
| 1   | D     | 42  | LEU  | 6.2  |
| 1   | E     | 54  | SER  | 6.1  |
| 1   | B     | 447 | LEU  | 6.1  |
| 1   | F     | 48  | ALA  | 6.1  |
| 1   | B     | 460 | ILE  | 6.0  |
| 1   | A     | 294 | THR  | 6.0  |
| 1   | D     | 128 | THR  | 6.0  |
| 1   | D     | 130 | THR  | 6.0  |
| 1   | B     | 300 | PHE  | 6.0  |
| 1   | E     | 131 | ALA  | 5.9  |
| 1   | D     | 297 | ASP  | 5.9  |
| 1   | B     | 453 | PHE  | 5.9  |
| 1   | E     | 125 | ILE  | 5.9  |
| 1   | F     | 296 | GLY  | 5.8  |
| 1   | C     | 457 | TYR  | 5.8  |
| 1   | D     | 298 | SER  | 5.8  |
| 1   | F     | 300 | PHE  | 5.8  |
| 1   | B     | 296 | GLY  | 5.8  |
| 1   | E     | 449 | VAL  | 5.8  |
| 1   | D     | 45  | VAL  | 5.7  |
| 1   | D     | 295 | THR  | 5.7  |
| 1   | E     | 128 | THR  | 5.7  |
| 1   | B     | 295 | THR  | 5.7  |
| 1   | F     | 295 | THR  | 5.7  |
| 1   | A     | 42  | LEU  | 5.7  |
| 1   | F     | 56  | ALA  | 5.7  |
| 1   | F     | 61  | VAL  | 5.6  |
| 1   | B     | 450 | LEU  | 5.6  |
| 1   | D     | 58  | LEU  | 5.6  |
| 1   | A     | 131 | ALA  | 5.6  |
| 1   | F     | 49  | LEU  | 5.5  |
| 1   | C     | 293 | ALA  | 5.4  |
| 1   | A     | 130 | THR  | 5.4  |
| 1   | F     | 453 | PHE  | 5.4  |
| 1   | A     | 447 | LEU  | 5.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 453 | PHE  | 5.3  |
| 1   | C     | 66  | ILE  | 5.2  |
| 1   | D     | 292 | LYS  | 5.2  |
| 1   | B     | 42  | LEU  | 5.2  |
| 1   | E     | 450 | LEU  | 5.2  |
| 1   | F     | 452 | LEU  | 5.2  |
| 1   | E     | 456 | ALA  | 5.2  |
| 1   | D     | 296 | GLY  | 5.2  |
| 1   | E     | 457 | TYR  | 5.2  |
| 1   | D     | 49  | LEU  | 5.2  |
| 1   | A     | 141 | ASP  | 5.1  |
| 1   | A     | 300 | PHE  | 5.1  |
| 1   | E     | 452 | LEU  | 5.1  |
| 1   | D     | 446 | ILE  | 5.1  |
| 1   | E     | 50  | CYS  | 5.1  |
| 1   | B     | 359 | TYR  | 5.1  |
| 1   | E     | 70  | PHE  | 5.1  |
| 1   | A     | 452 | LEU  | 5.0  |
| 1   | D     | 452 | LEU  | 5.0  |
| 1   | B     | 455 | TYR  | 5.0  |
| 1   | A     | 449 | VAL  | 5.0  |
| 1   | C     | 294 | THR  | 5.0  |
| 1   | A     | 204 | GLY  | 5.0  |
| 1   | E     | 294 | THR  | 5.0  |
| 1   | F     | 449 | VAL  | 5.0  |
| 1   | D     | 434 | ILE  | 5.0  |
| 1   | C     | 47  | TRP  | 4.9  |
| 1   | C     | 51  | PHE  | 4.9  |
| 1   | E     | 57  | LEU  | 4.9  |
| 1   | E     | 460 | ILE  | 4.9  |
| 1   | D     | 450 | LEU  | 4.9  |
| 1   | A     | 127 | ASP  | 4.9  |
| 1   | E     | 300 | PHE  | 4.9  |
| 1   | E     | 459 | VAL  | 4.9  |
| 1   | E     | 442 | ILE  | 4.9  |
| 1   | C     | 295 | THR  | 4.8  |
| 1   | F     | 294 | THR  | 4.8  |
| 1   | A     | 442 | ILE  | 4.8  |
| 1   | F     | 298 | SER  | 4.8  |
| 1   | E     | 49  | LEU  | 4.8  |
| 1   | F     | 55  | LEU  | 4.8  |
| 1   | A     | 46  | VAL  | 4.8  |

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| <b>Mol</b> | <b>Chain</b> | <b>Res</b> | <b>Type</b> | <b>RSRZ</b> |
|------------|--------------|------------|-------------|-------------|
| 1          | D            | 47         | TRP         | 4.8         |
| 1          | D            | 444        | ALA         | 4.8         |
| 1          | E            | 56         | ALA         | 4.7         |
| 1          | E            | 66         | ILE         | 4.7         |
| 1          | F            | 58         | LEU         | 4.7         |
| 1          | A            | 298        | SER         | 4.7         |
| 1          | F            | 301        | TYR         | 4.7         |
| 1          | E            | 61         | VAL         | 4.7         |
| 1          | C            | 50         | CYS         | 4.7         |
| 1          | E            | 55         | LEU         | 4.7         |
| 1          | A            | 132        | ASP         | 4.7         |
| 1          | E            | 47         | TRP         | 4.7         |
| 1          | A            | 297        | ASP         | 4.6         |
| 1          | A            | 66         | ILE         | 4.6         |
| 1          | F            | 47         | TRP         | 4.6         |
| 1          | E            | 204        | GLY         | 4.6         |
| 1          | A            | 45         | VAL         | 4.6         |
| 1          | B            | 45         | VAL         | 4.5         |
| 1          | E            | 431        | LEU         | 4.5         |
| 1          | D            | 131        | ALA         | 4.5         |
| 1          | D            | 202        | GLN         | 4.5         |
| 1          | C            | 296        | GLY         | 4.5         |
| 1          | D            | 206        | PRO         | 4.5         |
| 1          | E            | 42         | LEU         | 4.5         |
| 1          | E            | 434        | ILE         | 4.5         |
| 1          | E            | 129        | GLN         | 4.4         |
| 1          | E            | 65         | ARG         | 4.4         |
| 1          | A            | 49         | LEU         | 4.4         |
| 1          | C            | 450        | LEU         | 4.4         |
| 1          | B            | 301        | TYR         | 4.4         |
| 1          | B            | 452        | LEU         | 4.4         |
| 1          | F            | 60         | LEU         | 4.4         |
| 1          | D            | 455        | TYR         | 4.4         |
| 1          | E            | 123        | TYR         | 4.4         |
| 1          | A            | 290        | ASP         | 4.4         |
| 1          | D            | 203        | ASP         | 4.4         |
| 1          | B            | 461        | LYS         | 4.3         |
| 1          | B            | 456        | ALA         | 4.3         |
| 1          | D            | 441        | PHE         | 4.3         |
| 1          | E            | 291        | CYS         | 4.3         |
| 1          | E            | 359        | TYR         | 4.3         |
| 1          | E            | 445        | SER         | 4.3         |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 57  | LEU  | 4.3  |
| 1   | B     | 130 | THR  | 4.3  |
| 1   | E     | 46  | VAL  | 4.3  |
| 1   | D     | 125 | ILE  | 4.3  |
| 1   | C     | 359 | TYR  | 4.3  |
| 1   | A     | 296 | GLY  | 4.3  |
| 1   | F     | 204 | GLY  | 4.3  |
| 1   | A     | 299 | GLU  | 4.3  |
| 1   | A     | 58  | LEU  | 4.2  |
| 1   | B     | 294 | THR  | 4.2  |
| 1   | C     | 300 | PHE  | 4.2  |
| 1   | A     | 180 | CYS  | 4.2  |
| 1   | F     | 446 | ILE  | 4.2  |
| 1   | F     | 439 | GLY  | 4.2  |
| 1   | F     | 443 | GLY  | 4.2  |
| 1   | A     | 205 | LYS  | 4.2  |
| 1   | F     | 43  | LYS  | 4.2  |
| 1   | F     | 441 | PHE  | 4.2  |
| 1   | D     | 51  | PHE  | 4.1  |
| 1   | E     | 62  | CYS  | 4.1  |
| 1   | F     | 66  | ILE  | 4.1  |
| 1   | C     | 287 | PRO  | 4.1  |
| 1   | E     | 146 | ARG  | 4.1  |
| 1   | B     | 131 | ALA  | 4.1  |
| 1   | C     | 290 | ASP  | 4.1  |
| 1   | B     | 49  | LEU  | 4.1  |
| 1   | B     | 47  | TRP  | 4.1  |
| 1   | C     | 46  | VAL  | 4.1  |
| 1   | E     | 45  | VAL  | 4.1  |
| 1   | A     | 455 | TYR  | 4.1  |
| 1   | A     | 292 | LYS  | 4.1  |
| 1   | B     | 298 | SER  | 4.1  |
| 1   | D     | 57  | LEU  | 4.1  |
| 1   | B     | 446 | ILE  | 4.0  |
| 1   | E     | 332 | ASP  | 4.0  |
| 1   | D     | 55  | LEU  | 4.0  |
| 1   | E     | 448 | THR  | 4.0  |
| 1   | F     | 69  | TYR  | 4.0  |
| 1   | E     | 122 | ARG  | 4.0  |
| 1   | D     | 132 | ASP  | 4.0  |
| 1   | F     | 51  | PHE  | 4.0  |
| 1   | C     | 286 | PRO  | 4.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 455 | TYR  | 4.0  |
| 1   | A     | 57  | LEU  | 4.0  |
| 1   | B     | 292 | LYS  | 4.0  |
| 1   | D     | 454 | ASP  | 4.0  |
| 1   | C     | 206 | PRO  | 4.0  |
| 1   | A     | 47  | TRP  | 3.9  |
| 1   | B     | 55  | LEU  | 3.9  |
| 1   | D     | 442 | ILE  | 3.9  |
| 1   | D     | 299 | GLU  | 3.9  |
| 1   | F     | 299 | GLU  | 3.9  |
| 1   | B     | 454 | ASP  | 3.9  |
| 1   | D     | 445 | SER  | 3.9  |
| 1   | D     | 448 | THR  | 3.9  |
| 1   | D     | 451 | GLU  | 3.9  |
| 1   | E     | 53  | GLY  | 3.9  |
| 1   | B     | 51  | PHE  | 3.9  |
| 1   | F     | 438 | MET  | 3.9  |
| 1   | A     | 129 | GLN  | 3.9  |
| 1   | D     | 440 | LEU  | 3.9  |
| 1   | F     | 440 | LEU  | 3.9  |
| 1   | B     | 48  | ALA  | 3.9  |
| 1   | B     | 293 | ALA  | 3.9  |
| 1   | C     | 204 | GLY  | 3.9  |
| 1   | F     | 50  | CYS  | 3.9  |
| 1   | B     | 46  | VAL  | 3.9  |
| 1   | C     | 449 | VAL  | 3.9  |
| 1   | E     | 438 | MET  | 3.9  |
| 1   | D     | 359 | TYR  | 3.8  |
| 1   | F     | 288 | TRP  | 3.8  |
| 1   | D     | 46  | VAL  | 3.8  |
| 1   | E     | 75  | VAL  | 3.8  |
| 1   | C     | 42  | LEU  | 3.8  |
| 1   | E     | 430 | LEU  | 3.8  |
| 1   | E     | 63  | THR  | 3.8  |
| 1   | F     | 64  | ASN  | 3.8  |
| 1   | F     | 434 | ILE  | 3.8  |
| 1   | D     | 61  | VAL  | 3.8  |
| 1   | D     | 43  | LYS  | 3.8  |
| 1   | F     | 203 | ASP  | 3.8  |
| 1   | A     | 457 | TYR  | 3.7  |
| 1   | E     | 124 | GLU  | 3.7  |
| 1   | C     | 41  | SER  | 3.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 75  | VAL  | 3.7  |
| 1   | E     | 443 | GLY  | 3.7  |
| 1   | B     | 134 | LYS  | 3.7  |
| 1   | E     | 127 | ASP  | 3.7  |
| 1   | F     | 52  | MET  | 3.7  |
| 1   | B     | 291 | CYS  | 3.7  |
| 1   | F     | 289 | GLY  | 3.7  |
| 1   | D     | 70  | PHE  | 3.7  |
| 1   | E     | 440 | LEU  | 3.6  |
| 1   | F     | 444 | ALA  | 3.6  |
| 1   | E     | 69  | TYR  | 3.6  |
| 1   | D     | 129 | GLN  | 3.6  |
| 1   | C     | 40  | LEU  | 3.6  |
| 1   | C     | 440 | LEU  | 3.6  |
| 1   | C     | 203 | ASP  | 3.6  |
| 1   | A     | 59  | ALA  | 3.6  |
| 1   | C     | 205 | LYS  | 3.6  |
| 1   | E     | 292 | LYS  | 3.6  |
| 1   | F     | 292 | LYS  | 3.6  |
| 1   | E     | 297 | ASP  | 3.6  |
| 1   | A     | 207 | ARG  | 3.6  |
| 1   | E     | 43  | LYS  | 3.6  |
| 1   | E     | 425 | TYR  | 3.6  |
| 1   | B     | 362 | CYS  | 3.6  |
| 1   | B     | 203 | ASP  | 3.6  |
| 1   | E     | 51  | PHE  | 3.6  |
| 1   | D     | 72  | TYR  | 3.5  |
| 1   | A     | 434 | ILE  | 3.5  |
| 1   | C     | 453 | PHE  | 3.5  |
| 1   | A     | 55  | LEU  | 3.5  |
| 1   | A     | 440 | LEU  | 3.5  |
| 1   | E     | 296 | GLY  | 3.5  |
| 1   | B     | 52  | MET  | 3.5  |
| 1   | E     | 360 | CYS  | 3.5  |
| 1   | A     | 61  | VAL  | 3.5  |
| 1   | B     | 458 | GLU  | 3.5  |
| 1   | E     | 299 | GLU  | 3.5  |
| 1   | E     | 202 | GLN  | 3.5  |
| 1   | C     | 444 | ALA  | 3.5  |
| 1   | C     | 452 | LEU  | 3.5  |
| 1   | E     | 60  | LEU  | 3.5  |
| 1   | B     | 127 | ASP  | 3.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 433 | ASP  | 3.5  |
| 1   | D     | 50  | CYS  | 3.5  |
| 1   | B     | 299 | GLU  | 3.5  |
| 1   | A     | 446 | ILE  | 3.5  |
| 1   | D     | 300 | PHE  | 3.5  |
| 1   | E     | 366 | CYS  | 3.4  |
| 1   | F     | 72  | TYR  | 3.4  |
| 1   | C     | 292 | LYS  | 3.4  |
| 1   | F     | 205 | LYS  | 3.4  |
| 1   | A     | 71  | LEU  | 3.4  |
| 1   | E     | 362 | CYS  | 3.4  |
| 1   | D     | 60  | LEU  | 3.4  |
| 1   | A     | 126 | PRO  | 3.4  |
| 1   | A     | 125 | ILE  | 3.4  |
| 1   | C     | 297 | ASP  | 3.4  |
| 1   | D     | 204 | GLY  | 3.4  |
| 1   | A     | 70  | PHE  | 3.4  |
| 1   | C     | 49  | LEU  | 3.4  |
| 1   | E     | 133 | GLU  | 3.3  |
| 1   | F     | 359 | TYR  | 3.3  |
| 1   | D     | 48  | ALA  | 3.3  |
| 1   | F     | 447 | LEU  | 3.3  |
| 1   | A     | 448 | THR  | 3.3  |
| 1   | B     | 320 | GLU  | 3.3  |
| 1   | D     | 133 | GLU  | 3.3  |
| 1   | A     | 44  | ARG  | 3.3  |
| 1   | B     | 323 | ASN  | 3.3  |
| 1   | C     | 431 | LEU  | 3.3  |
| 1   | B     | 441 | PHE  | 3.3  |
| 1   | B     | 129 | GLN  | 3.3  |
| 1   | F     | 297 | ASP  | 3.3  |
| 1   | B     | 438 | MET  | 3.3  |
| 1   | E     | 139 | LEU  | 3.3  |
| 1   | A     | 203 | ASP  | 3.3  |
| 1   | B     | 332 | ASP  | 3.3  |
| 1   | D     | 432 | GLY  | 3.3  |
| 1   | C     | 54  | SER  | 3.3  |
| 1   | E     | 134 | LYS  | 3.2  |
| 1   | B     | 138 | ILE  | 3.2  |
| 1   | C     | 57  | LEU  | 3.2  |
| 1   | F     | 206 | PRO  | 3.2  |
| 1   | D     | 323 | ASN  | 3.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 298 | SER  | 3.2  |
| 1   | B     | 434 | ILE  | 3.2  |
| 1   | E     | 59  | ALA  | 3.2  |
| 1   | D     | 56  | ALA  | 3.2  |
| 1   | E     | 301 | TYR  | 3.2  |
| 1   | B     | 60  | LEU  | 3.2  |
| 1   | A     | 54  | SER  | 3.2  |
| 1   | C     | 441 | PHE  | 3.2  |
| 1   | E     | 132 | ASP  | 3.2  |
| 1   | E     | 203 | ASP  | 3.2  |
| 1   | B     | 344 | CYS  | 3.2  |
| 1   | D     | 180 | CYS  | 3.2  |
| 1   | E     | 458 | GLU  | 3.2  |
| 1   | A     | 43  | LYS  | 3.1  |
| 1   | B     | 43  | LYS  | 3.1  |
| 1   | F     | 131 | ALA  | 3.1  |
| 1   | F     | 71  | LEU  | 3.1  |
| 1   | A     | 51  | PHE  | 3.1  |
| 1   | F     | 70  | PHE  | 3.1  |
| 1   | C     | 439 | GLY  | 3.1  |
| 1   | B     | 459 | VAL  | 3.1  |
| 1   | F     | 427 | VAL  | 3.1  |
| 1   | A     | 451 | GLU  | 3.1  |
| 1   | C     | 312 | ASP  | 3.1  |
| 1   | F     | 451 | GLU  | 3.1  |
| 1   | D     | 437 | GLN  | 3.1  |
| 1   | E     | 344 | CYS  | 3.1  |
| 1   | D     | 84  | THR  | 3.1  |
| 1   | B     | 444 | ALA  | 3.1  |
| 1   | D     | 83  | ALA  | 3.1  |
| 1   | F     | 68  | TYR  | 3.1  |
| 1   | F     | 425 | TYR  | 3.1  |
| 1   | F     | 430 | LEU  | 3.1  |
| 1   | C     | 45  | VAL  | 3.1  |
| 1   | A     | 441 | PHE  | 3.1  |
| 1   | B     | 126 | PRO  | 3.1  |
| 1   | E     | 363 | GLU  | 3.1  |
| 1   | A     | 138 | ILE  | 3.0  |
| 1   | A     | 454 | ASP  | 3.0  |
| 1   | C     | 43  | LYS  | 3.0  |
| 1   | E     | 461 | LYS  | 3.0  |
| 1   | C     | 62  | CYS  | 3.0  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | E     | 126 | PRO  | 3.0  |
| 1   | E     | 439 | GLY  | 3.0  |
| 1   | D     | 59  | ALA  | 3.0  |
| 1   | A     | 202 | GLN  | 3.0  |
| 1   | E     | 52  | MET  | 3.0  |
| 1   | F     | 431 | LEU  | 3.0  |
| 1   | D     | 124 | GLU  | 3.0  |
| 1   | C     | 445 | SER  | 3.0  |
| 1   | B     | 366 | CYS  | 3.0  |
| 1   | F     | 424 | ALA  | 3.0  |
| 1   | D     | 146 | ARG  | 3.0  |
| 1   | D     | 205 | LYS  | 3.0  |
| 1   | D     | 436 | GLY  | 3.0  |
| 1   | B     | 360 | CYS  | 3.0  |
| 1   | F     | 62  | CYS  | 3.0  |
| 1   | E     | 444 | ALA  | 3.0  |
| 1   | B     | 440 | LEU  | 2.9  |
| 1   | E     | 455 | TYR  | 2.9  |
| 1   | A     | 436 | GLY  | 2.9  |
| 1   | B     | 448 | THR  | 2.9  |
| 1   | C     | 320 | GLU  | 2.9  |
| 1   | A     | 48  | ALA  | 2.9  |
| 1   | C     | 442 | ILE  | 2.9  |
| 1   | A     | 430 | LEU  | 2.9  |
| 1   | A     | 122 | ARG  | 2.9  |
| 1   | A     | 301 | TYR  | 2.9  |
| 1   | E     | 68  | TYR  | 2.9  |
| 1   | A     | 52  | MET  | 2.9  |
| 1   | A     | 438 | MET  | 2.9  |
| 1   | B     | 339 | GLU  | 2.9  |
| 1   | D     | 148 | PHE  | 2.9  |
| 1   | E     | 441 | PHE  | 2.9  |
| 1   | A     | 362 | CYS  | 2.9  |
| 1   | E     | 288 | TRP  | 2.9  |
| 1   | A     | 134 | LYS  | 2.9  |
| 1   | C     | 426 | GLU  | 2.9  |
| 1   | B     | 449 | VAL  | 2.9  |
| 1   | C     | 289 | GLY  | 2.9  |
| 1   | E     | 361 | VAL  | 2.9  |
| 1   | C     | 425 | TYR  | 2.9  |
| 1   | E     | 72  | TYR  | 2.9  |
| 1   | C     | 456 | ALA  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 44  | ARG  | 2.9  |
| 1   | C     | 141 | ASP  | 2.9  |
| 1   | D     | 54  | SER  | 2.9  |
| 1   | D     | 127 | ASP  | 2.9  |
| 1   | E     | 71  | LEU  | 2.9  |
| 1   | B     | 61  | VAL  | 2.8  |
| 1   | E     | 427 | VAL  | 2.8  |
| 1   | B     | 50  | CYS  | 2.8  |
| 1   | D     | 52  | MET  | 2.8  |
| 1   | D     | 86  | LEU  | 2.8  |
| 1   | D     | 288 | TRP  | 2.8  |
| 1   | C     | 434 | ILE  | 2.8  |
| 1   | F     | 53  | GLY  | 2.8  |
| 1   | F     | 44  | ARG  | 2.8  |
| 1   | B     | 56  | ALA  | 2.8  |
| 1   | C     | 438 | MET  | 2.8  |
| 1   | D     | 360 | CYS  | 2.8  |
| 1   | F     | 291 | CYS  | 2.8  |
| 1   | D     | 44  | ARG  | 2.8  |
| 1   | D     | 71  | LEU  | 2.8  |
| 1   | F     | 130 | THR  | 2.8  |
| 1   | F     | 312 | ASP  | 2.8  |
| 1   | E     | 424 | ALA  | 2.8  |
| 1   | A     | 50  | CYS  | 2.8  |
| 1   | C     | 180 | CYS  | 2.8  |
| 1   | B     | 289 | GLY  | 2.8  |
| 1   | A     | 358 | GLU  | 2.8  |
| 1   | C     | 58  | LEU  | 2.8  |
| 1   | F     | 63  | THR  | 2.8  |
| 1   | F     | 442 | ILE  | 2.8  |
| 1   | B     | 59  | ALA  | 2.7  |
| 1   | F     | 367 | ASN  | 2.7  |
| 1   | D     | 62  | CYS  | 2.7  |
| 1   | B     | 451 | GLU  | 2.7  |
| 1   | E     | 137 | GLU  | 2.7  |
| 1   | A     | 456 | ALA  | 2.7  |
| 1   | C     | 48  | ALA  | 2.7  |
| 1   | C     | 134 | LYS  | 2.7  |
| 1   | A     | 291 | CYS  | 2.7  |
| 1   | B     | 297 | ASP  | 2.7  |
| 1   | C     | 79  | ASP  | 2.7  |
| 1   | F     | 132 | ASP  | 2.7  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 58  | LEU  | 2.7  |
| 1   | E     | 287 | PRO  | 2.7  |
| 1   | B     | 442 | ILE  | 2.7  |
| 1   | E     | 138 | ILE  | 2.7  |
| 1   | B     | 445 | SER  | 2.7  |
| 1   | C     | 131 | ALA  | 2.7  |
| 1   | D     | 289 | GLY  | 2.7  |
| 1   | D     | 301 | TYR  | 2.7  |
| 1   | B     | 66  | ILE  | 2.7  |
| 1   | D     | 449 | VAL  | 2.7  |
| 1   | B     | 53  | GLY  | 2.6  |
| 1   | C     | 454 | ASP  | 2.6  |
| 1   | B     | 322 | CYS  | 2.6  |
| 1   | D     | 63  | THR  | 2.6  |
| 1   | C     | 299 | GLU  | 2.6  |
| 1   | C     | 451 | GLU  | 2.6  |
| 1   | C     | 60  | LEU  | 2.6  |
| 1   | B     | 132 | ASP  | 2.6  |
| 1   | C     | 302 | ASP  | 2.6  |
| 1   | B     | 202 | GLN  | 2.6  |
| 1   | E     | 437 | GLN  | 2.6  |
| 1   | F     | 129 | GLN  | 2.6  |
| 1   | D     | 69  | TYR  | 2.6  |
| 1   | A     | 62  | CYS  | 2.6  |
| 1   | C     | 344 | CYS  | 2.6  |
| 1   | F     | 147 | ASN  | 2.6  |
| 1   | E     | 58  | LEU  | 2.6  |
| 1   | C     | 127 | ASP  | 2.6  |
| 1   | E     | 432 | GLY  | 2.6  |
| 1   | F     | 82  | ALA  | 2.6  |
| 1   | C     | 301 | TYR  | 2.6  |
| 1   | A     | 60  | LEU  | 2.6  |
| 1   | D     | 364 | MET  | 2.6  |
| 1   | C     | 254 | ASP  | 2.6  |
| 1   | E     | 451 | GLU  | 2.6  |
| 1   | B     | 75  | VAL  | 2.6  |
| 1   | E     | 143 | ALA  | 2.6  |
| 1   | C     | 207 | ARG  | 2.5  |
| 1   | D     | 123 | TYR  | 2.5  |
| 1   | B     | 358 | GLU  | 2.5  |
| 1   | D     | 141 | ASP  | 2.5  |
| 1   | E     | 254 | ASP  | 2.5  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | F     | 201 | GLY  | 2.5  |
| 1   | F     | 133 | GLU  | 2.5  |
| 1   | E     | 149 | LYS  | 2.5  |
| 1   | C     | 55  | LEU  | 2.5  |
| 1   | D     | 435 | GLY  | 2.5  |
| 1   | F     | 432 | GLY  | 2.5  |
| 1   | E     | 64  | ASN  | 2.5  |
| 1   | F     | 207 | ARG  | 2.5  |
| 1   | F     | 59  | ALA  | 2.5  |
| 1   | A     | 133 | GLU  | 2.5  |
| 1   | C     | 366 | CYS  | 2.5  |
| 1   | A     | 78  | LEU  | 2.5  |
| 1   | C     | 430 | LEU  | 2.5  |
| 1   | C     | 147 | ASN  | 2.5  |
| 1   | E     | 120 | ASN  | 2.5  |
| 1   | A     | 146 | ARG  | 2.5  |
| 1   | D     | 85  | ARG  | 2.5  |
| 1   | A     | 445 | SER  | 2.5  |
| 1   | A     | 137 | GLU  | 2.5  |
| 1   | C     | 358 | GLU  | 2.5  |
| 1   | F     | 428 | ALA  | 2.5  |
| 1   | F     | 84  | THR  | 2.5  |
| 1   | F     | 448 | THR  | 2.5  |
| 1   | D     | 427 | VAL  | 2.5  |
| 1   | F     | 127 | ASP  | 2.5  |
| 1   | D     | 285 | PRO  | 2.5  |
| 1   | E     | 289 | GLY  | 2.4  |
| 1   | A     | 72  | TYR  | 2.4  |
| 1   | C     | 447 | LEU  | 2.4  |
| 1   | A     | 84  | THR  | 2.4  |
| 1   | D     | 126 | PRO  | 2.4  |
| 1   | C     | 44  | ARG  | 2.4  |
| 1   | D     | 134 | LYS  | 2.4  |
| 1   | D     | 79  | ASP  | 2.4  |
| 1   | A     | 444 | ALA  | 2.4  |
| 1   | B     | 428 | ALA  | 2.4  |
| 1   | E     | 426 | GLU  | 2.4  |
| 1   | A     | 53  | GLY  | 2.4  |
| 1   | F     | 344 | CYS  | 2.4  |
| 1   | A     | 123 | TYR  | 2.4  |
| 1   | E     | 148 | PHE  | 2.4  |
| 1   | F     | 302 | ASP  | 2.4  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 125 | ILE  | 2.4  |
| 1   | D     | 65  | ARG  | 2.4  |
| 1   | A     | 135 | GLN  | 2.4  |
| 1   | C     | 285 | PRO  | 2.4  |
| 1   | E     | 121 | ASN  | 2.4  |
| 1   | D     | 53  | GLY  | 2.4  |
| 1   | F     | 290 | ASP  | 2.3  |
| 1   | A     | 136 | LEU  | 2.3  |
| 1   | D     | 431 | LEU  | 2.3  |
| 1   | F     | 146 | ARG  | 2.3  |
| 1   | E     | 320 | GLU  | 2.3  |
| 1   | E     | 418 | THR  | 2.3  |
| 1   | C     | 56  | ALA  | 2.3  |
| 1   | C     | 150 | PRO  | 2.3  |
| 1   | D     | 361 | VAL  | 2.3  |
| 1   | D     | 362 | CYS  | 2.3  |
| 1   | A     | 124 | GLU  | 2.3  |
| 1   | A     | 86  | LEU  | 2.3  |
| 1   | A     | 140 | GLN  | 2.3  |
| 1   | C     | 67  | GLN  | 2.3  |
| 1   | E     | 303 | THR  | 2.3  |
| 1   | F     | 303 | THR  | 2.3  |
| 1   | D     | 74  | HIS  | 2.3  |
| 1   | D     | 367 | ASN  | 2.3  |
| 1   | A     | 82  | ALA  | 2.3  |
| 1   | C     | 83  | ALA  | 2.3  |
| 1   | A     | 437 | GLN  | 2.3  |
| 1   | B     | 313 | CYS  | 2.3  |
| 1   | B     | 57  | LEU  | 2.3  |
| 1   | A     | 147 | ASN  | 2.3  |
| 1   | B     | 333 | ALA  | 2.3  |
| 1   | E     | 73  | PRO  | 2.3  |
| 1   | A     | 439 | GLY  | 2.3  |
| 1   | F     | 254 | ASP  | 2.3  |
| 1   | C     | 61  | VAL  | 2.3  |
| 1   | C     | 427 | VAL  | 2.3  |
| 1   | C     | 52  | MET  | 2.3  |
| 1   | F     | 284 | LEU  | 2.3  |
| 1   | A     | 458 | GLU  | 2.2  |
| 1   | B     | 435 | GLY  | 2.2  |
| 1   | D     | 286 | PRO  | 2.2  |
| 1   | D     | 287 | PRO  | 2.2  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 446 | ILE  | 2.2  |
| 1   | E     | 290 | ASP  | 2.2  |
| 1   | B     | 140 | GLN  | 2.2  |
| 1   | D     | 147 | ASN  | 2.2  |
| 1   | E     | 77  | LYS  | 2.2  |
| 1   | E     | 211 | MET  | 2.2  |
| 1   | B     | 180 | CYS  | 2.2  |
| 1   | C     | 448 | THR  | 2.2  |
| 1   | F     | 128 | THR  | 2.2  |
| 1   | F     | 280 | ARG  | 2.2  |
| 1   | F     | 363 | GLU  | 2.2  |
| 1   | A     | 56  | ALA  | 2.2  |
| 1   | A     | 143 | ALA  | 2.2  |
| 1   | D     | 254 | ASP  | 2.2  |
| 1   | E     | 428 | ALA  | 2.2  |
| 1   | D     | 207 | ARG  | 2.2  |
| 1   | E     | 327 | VAL  | 2.2  |
| 1   | F     | 180 | CYS  | 2.2  |
| 1   | B     | 141 | ASP  | 2.2  |
| 1   | C     | 332 | ASP  | 2.2  |
| 1   | E     | 206 | PRO  | 2.2  |
| 1   | A     | 69  | TYR  | 2.2  |
| 1   | C     | 70  | PHE  | 2.2  |
| 1   | D     | 68  | TYR  | 2.2  |
| 1   | A     | 85  | ARG  | 2.2  |
| 1   | A     | 211 | MET  | 2.2  |
| 1   | D     | 280 | ARG  | 2.2  |
| 1   | E     | 144 | ASN  | 2.2  |
| 1   | E     | 207 | ARG  | 2.2  |
| 1   | B     | 361 | VAL  | 2.2  |
| 1   | D     | 319 | VAL  | 2.2  |
| 1   | F     | 433 | ASP  | 2.2  |
| 1   | C     | 65  | ARG  | 2.2  |
| 1   | E     | 282 | ILE  | 2.1  |
| 1   | B     | 54  | SER  | 2.1  |
| 1   | C     | 53  | GLY  | 2.1  |
| 1   | D     | 201 | GLY  | 2.1  |
| 1   | A     | 366 | CYS  | 2.1  |
| 1   | E     | 136 | LEU  | 2.1  |
| 1   | E     | 284 | LEU  | 2.1  |
| 1   | F     | 423 | LYS  | 2.1  |
| 1   | C     | 133 | GLU  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | C     | 64  | ASN  | 2.1  |
| 1   | D     | 200 | ALA  | 2.1  |
| 1   | B     | 72  | TYR  | 2.1  |
| 1   | D     | 66  | ILE  | 2.1  |
| 1   | E     | 436 | GLY  | 2.1  |
| 1   | F     | 65  | ARG  | 2.1  |
| 1   | E     | 205 | LYS  | 2.1  |
| 1   | A     | 285 | PRO  | 2.1  |
| 1   | B     | 67  | GLN  | 2.1  |
| 1   | B     | 133 | GLU  | 2.1  |
| 1   | D     | 439 | GLY  | 2.1  |
| 1   | C     | 202 | GLN  | 2.1  |
| 1   | C     | 132 | ASP  | 2.1  |
| 1   | A     | 114 | GLU  | 2.0  |
| 1   | B     | 148 | PHE  | 2.0  |
| 1   | E     | 41  | SER  | 2.0  |
| 1   | B     | 287 | PRO  | 2.0  |
| 1   | E     | 180 | CYS  | 2.0  |
| 1   | C     | 428 | ALA  | 2.0  |
| 1   | D     | 320 | GLU  | 2.0  |
| 1   | D     | 420 | GLU  | 2.0  |
| 1   | E     | 142 | LYS  | 2.0  |
| 1   | E     | 286 | PRO  | 2.0  |
| 1   | F     | 81  | VAL  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

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.

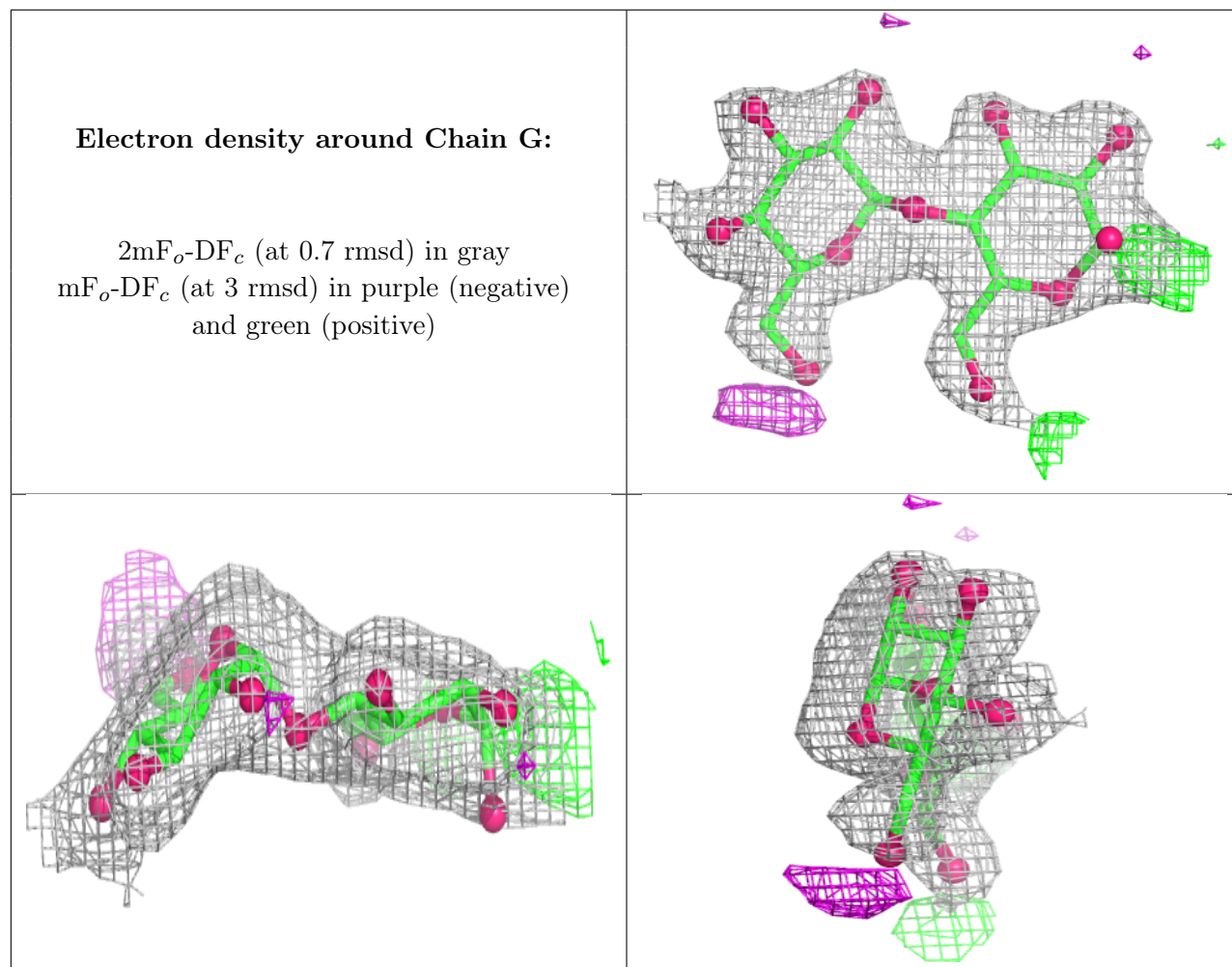
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 2   | GLC  | I     | 1   | 12/12 | 0.70 | 0.20 | 78,78,79,79                | 0     |
| 2   | GLC  | I     | 2   | 11/12 | 0.73 | 0.17 | 76,77,78,78                | 0     |
| 2   | GLC  | H     | 1   | 12/12 | 0.75 | 0.16 | 71,73,74,74                | 0     |
| 2   | GLC  | H     | 2   | 11/12 | 0.78 | 0.16 | 73,73,75,76                | 0     |

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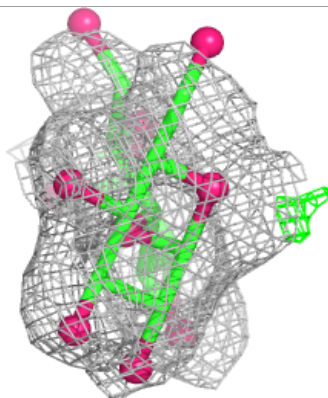
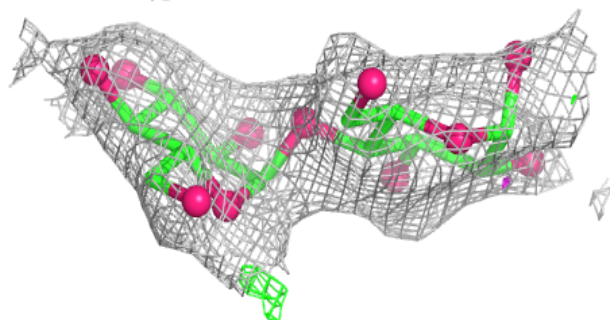
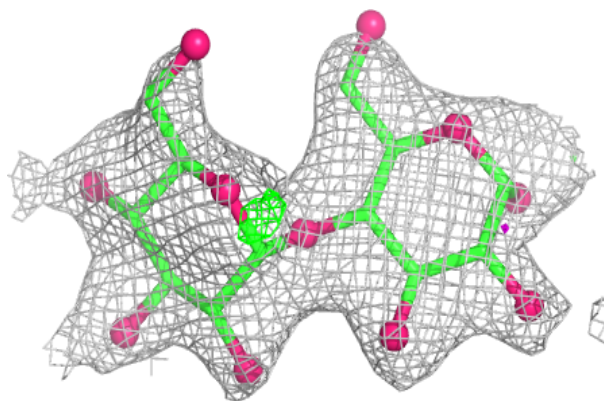
| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 2   | GLC  | G     | 2   | 11/12 | 0.81 | 0.17 | 63,63,64,64                 | 0     |
| 2   | GLC  | G     | 1   | 12/12 | 0.82 | 0.18 | 63,64,64,65                 | 0     |

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

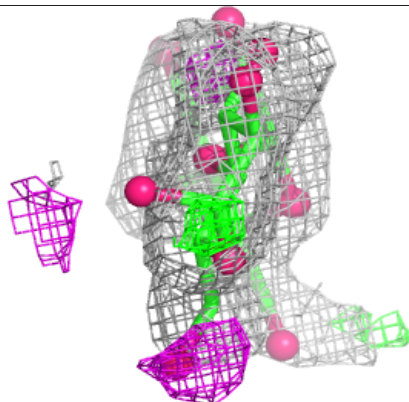
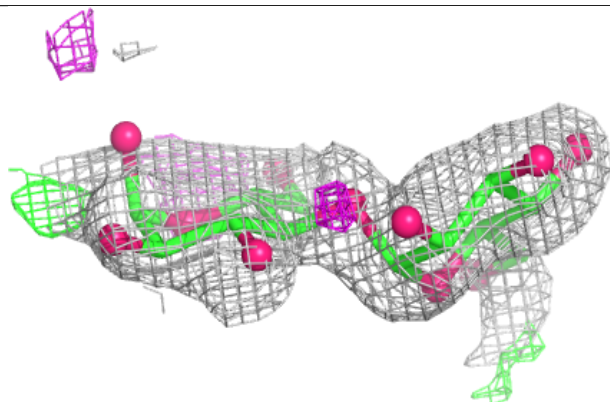
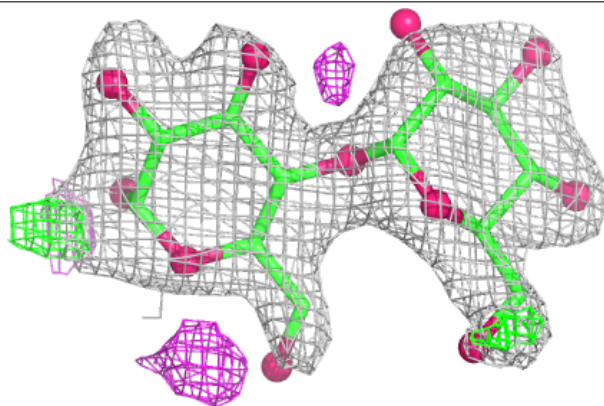


**Electron density around Chain H:**

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

**Electron density around Chain I:**

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



## 6.4 Ligands

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 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 3   | NAG  | F     | 12  | 14/15 | 0.10 | 0.22 | 67,72,74,74                 | 0     |
| 3   | NAG  | D     | 7   | 14/15 | 0.35 | 0.20 | 69,73,74,75                 | 0     |
| 3   | NAG  | F     | 11  | 14/15 | 0.36 | 0.21 | 70,74,76,76                 | 0     |
| 3   | NAG  | E     | 10  | 14/15 | 0.45 | 0.19 | 61,67,69,70                 | 0     |
| 3   | NAG  | C     | 5   | 14/15 | 0.46 | 0.16 | 61,66,68,69                 | 0     |
| 3   | NAG  | C     | 6   | 14/15 | 0.56 | 0.18 | 65,71,73,73                 | 0     |
| 3   | NAG  | B     | 4   | 14/15 | 0.72 | 0.14 | 52,55,59,61                 | 0     |
| 3   | NAG  | A     | 2   | 14/15 | 0.76 | 0.13 | 44,46,50,51                 | 0     |
| 3   | NAG  | E     | 9   | 14/15 | 0.78 | 0.15 | 53,57,59,61                 | 0     |
| 3   | NAG  | A     | 1   | 14/15 | 0.81 | 0.13 | 50,54,56,57                 | 0     |
| 3   | NAG  | B     | 3   | 14/15 | 0.85 | 0.11 | 42,45,48,50                 | 0     |
| 3   | NAG  | D     | 8   | 14/15 | 0.87 | 0.10 | 32,36,42,45                 | 0     |
| 4   | CL   | B     | 464 | 1/1   | 0.97 | 0.06 | 29,29,29,29                 | 0     |
| 4   | CL   | D     | 4   | 1/1   | 0.97 | 0.07 | 31,31,31,31                 | 0     |
| 4   | CL   | F     | 6   | 1/1   | 0.98 | 0.08 | 28,28,28,28                 | 0     |
| 4   | CL   | A     | 464 | 1/1   | 0.99 | 0.03 | 26,26,26,26                 | 0     |
| 4   | CL   | E     | 5   | 1/1   | 0.99 | 0.04 | 31,31,31,31                 | 0     |
| 4   | CL   | C     | 464 | 1/1   | 0.99 | 0.03 | 24,24,24,24                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.