



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:35 PM UTC

PDB ID : 3HI1 / pdb\_00003hi1  
Title : Structure of HIV-1 gp120 (core with V3) in Complex with CD4-Binding-Site Antibody F105  
Authors : Kwon, Y.D.; Chen, L.; Zhou, T.; Wu, X.; O'Dell, S.; Cavacini, L.; Hessel, A.J.; Pancera, M.; Tang, M.; Xu, L.; Yang, Z.; Zhang, M.-Y.; Arthos, J.; Burton, D.R.; Dimitrov, D.; Nabel, G.J.; Posner, M.; Sodroski, J.; Wyatt, R.; Mascola, J.R.; Kwong, P.D.  
Deposited on : 2009-05-18  
Resolution : 2.90 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)                                          |

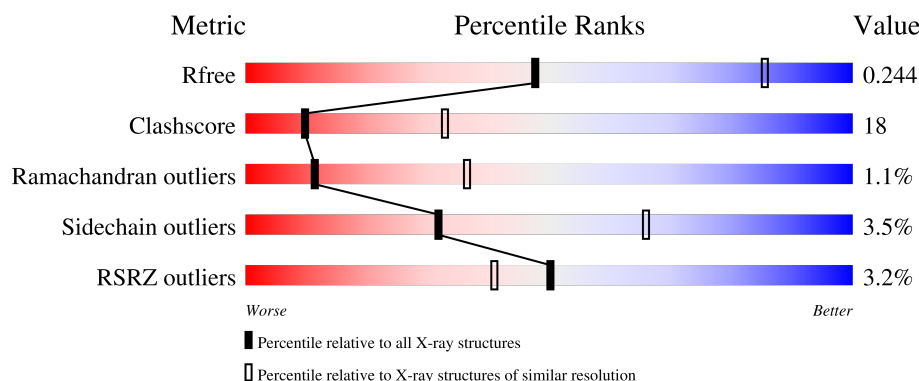
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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                      | 2481 (2.90-2.90)                                      |
| Clashscore            | 190562                      | 2690 (2.90-2.90)                                      |
| Ramachandran outliers | 187476                      | 2623 (2.90-2.90)                                      |
| Sidechain outliers    | 187428                      | 2625 (2.90-2.90)                                      |
| RSRZ outliers         | 180081                      | 2481 (2.90-2.90)                                      |

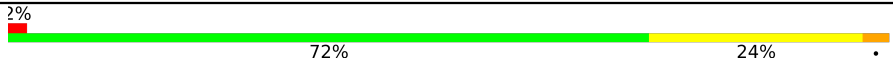
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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   | G     | 321    | <div> <div>5%</div> <div> <div></div> <div>58%</div> <div>29%</div> <div>•</div> <div>10%</div> </div> </div> |
| 1   | J     | 321    | <div> <div>6%</div> <div> <div></div> <div>58%</div> <div>28%</div> <div>•</div> <div>10%</div> </div> </div> |
| 2   | A     | 215    | <div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>••</div> </div> </div>                |
| 2   | L     | 215    | <div> <div></div> <div> <div></div> <div>76%</div> <div>22%</div> <div>•</div> </div> </div>                  |

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Validation Pipeline (wwPDB-VP) : 2.49

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| Mol | Chain | Length | Quality of chain                                                                   |
|-----|-------|--------|------------------------------------------------------------------------------------|
| 3   | B     | 225    |  |
| 3   | H     | 225    |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 4   | NAG  | J     | 801 | X         | -        | -       | -                |
| 4   | NAG  | J     | 894 | X         | -        | -       | -                |
| 4   | NAG  | J     | 913 | X         | -        | -       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11670 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 Glycoprotein 120.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | G     | 289      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2276  | 1428 | 401 | 429 | 18 |         |         |       |
| 1   | J     | 289      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2276  | 1428 | 401 | 429 | 18 |         |         |       |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference  |
|-------|---------|----------|--------|---------|------------|
| G     | 124     | GLY      | -      | linker  | UNP P35961 |
| G     | 198     | GLY      | -      | linker  | UNP P35961 |

- Molecule 2 is a protein called F105 Light Chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2   | L     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1651  | 1027 | 282 | 336 | 6 |         |         |       |
| 2   | A     | 215      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1651  | 1027 | 282 | 336 | 6 |         |         |       |

- Molecule 3 is a protein called F105 Heavy Chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3   | H     | 225      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1680  | 1067 | 276 | 332 | 5 |         |         |       |
| 3   | B     | 225      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1680  | 1067 | 276 | 332 | 5 |         |         |       |

- Molecule 4 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 |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | G     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |

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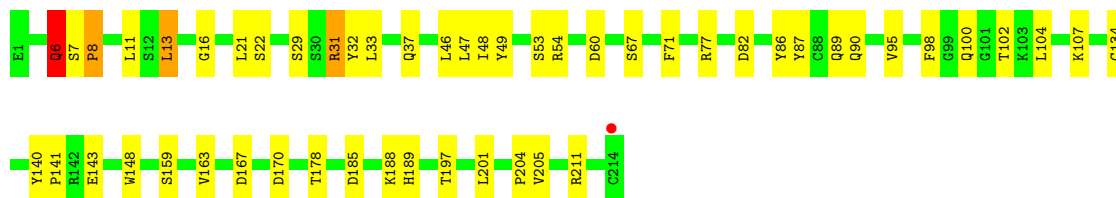
| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 4   | J     | 1        | Total | C | N | O | 0       | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |         |
| 4   | J     | 1        | Total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

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5   | G     | 8        | Total | O  | 0       | 0       |
|     |       |          | 8     | 8  |         |         |
| 5   | L     | 22       | Total | O  | 0       | 0       |
|     |       |          | 22    | 22 |         |         |
| 5   | H     | 42       | Total | O  | 0       | 0       |
|     |       |          | 42    | 42 |         |         |
| 5   | J     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | A     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |
| 5   | B     | 2        | Total | O  | 0       | 0       |
|     |       |          | 2     | 2  |         |         |

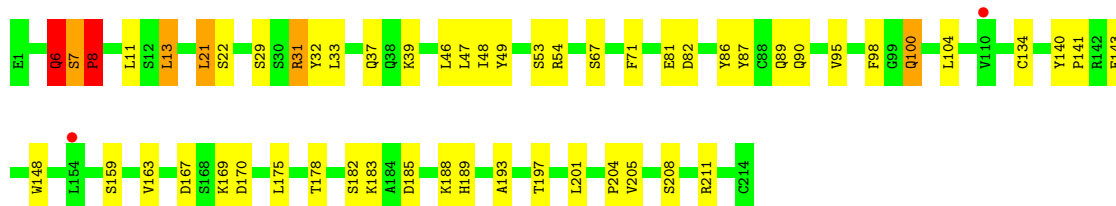


Chain L:  76% 22% .



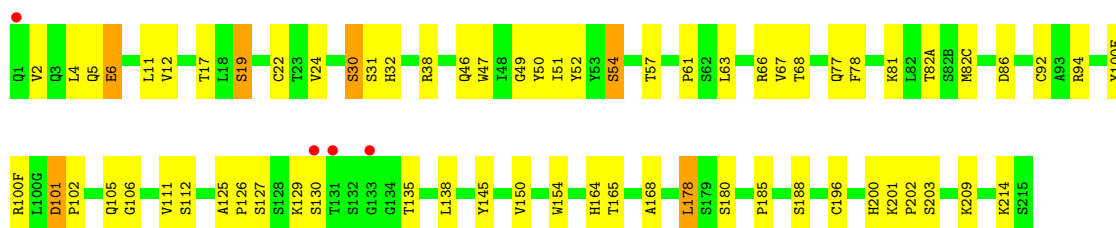
• Molecule 2: F105 Light Chain

Chain A:  74% 22% ..



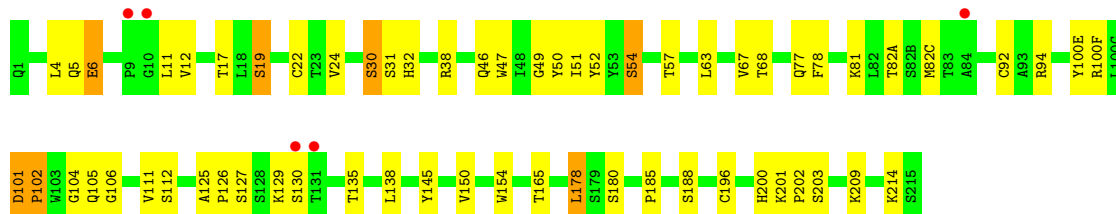
• Molecule 3: F105 Heavy Chain

Chain H:  70% 27% .



• Molecule 3: F105 Heavy Chain

Chain B:  72% 24% .



## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | H 3 2                                                       | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 412.40Å 412.40Å 83.21Å<br>90.00° 90.00° 120.00°             | Depositor        |
| Resolution (Å)                                                          | 43.48 – 2.90<br>43.48 – 2.90                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 75.5 (43.48-2.90)<br>75.4 (43.48-2.90)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.12                                                        | Depositor        |
| $R_{sym}$                                                               | 0.09                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.56 (at 2.81Å)                                             | Xtriage          |
| Refinement program                                                      | REFMAC 5.2.0019                                             | Depositor        |
| R, $R_{free}$                                                           | 0.202 , 0.243<br>0.208 , 0.244                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2414 reflections (4.97%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 70.5                                                        | Xtriage          |
| Anisotropy                                                              | 0.312                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 70.6                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Estimated twinning fraction                                             | No twinning to report.                                      | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.94                                                        | EDS              |
| Total number of atoms                                                   | 11670                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 109.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths |         | Bond angles |                |
|-----|-------|--------------|---------|-------------|----------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5        |
| 1   | G     | 0.39         | 0/2321  | 0.77        | 1/3142 (0.0%)  |
| 1   | J     | 0.34         | 0/2321  | 0.74        | 2/3142 (0.1%)  |
| 2   | A     | 0.36         | 0/1684  | 0.79        | 1/2283 (0.0%)  |
| 2   | L     | 0.42         | 0/1684  | 0.81        | 0/2283         |
| 3   | B     | 0.37         | 0/1725  | 0.78        | 0/2357         |
| 3   | H     | 0.45         | 0/1725  | 0.82        | 0/2357         |
| All | All   | 0.39         | 0/11460 | 0.78        | 4/15564 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1   | G     | 0                   | 1                   |
| 1   | J     | 0                   | 1                   |
| 2   | A     | 0                   | 1                   |
| 2   | L     | 0                   | 1                   |
| 3   | B     | 0                   | 1                   |
| 3   | H     | 0                   | 1                   |
| All | All   | 0                   | 6                   |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 277 | PHE  | N-CA-C  | -7.77 | 104.32      | 113.88   |
| 1   | J     | 447 | SER  | N-CA-C  | 5.78  | 115.73      | 108.45   |
| 1   | J     | 330 | HIS  | N-CA-CB | -5.30 | 101.53      | 110.49   |
| 2   | A     | 8   | PRO  | N-CA-C  | -5.01 | 102.14      | 112.47   |

There are no chirality outliers.

All (6) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 2   | A     | 6   | GLN  | Peptide |
| 3   | B     | 101 | ASP  | Peptide |
| 1   | G     | 469 | ARG  | Peptide |
| 3   | H     | 101 | ASP  | Peptide |
| 1   | J     | 469 | ARG  | Peptide |
| 2   | L     | 6   | GLN  | Peptide |

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | G     | 2276  | 0        | 2221     | 113     | 0            |
| 1   | J     | 2276  | 0        | 2217     | 104     | 0            |
| 2   | A     | 1651  | 0        | 1602     | 49      | 0            |
| 2   | L     | 1651  | 0        | 1602     | 43      | 0            |
| 3   | B     | 1680  | 0        | 1661     | 56      | 0            |
| 3   | H     | 1680  | 0        | 1661     | 62      | 0            |
| 4   | G     | 182   | 0        | 169      | 9       | 0            |
| 4   | J     | 196   | 0        | 182      | 10      | 0            |
| 5   | A     | 2     | 0        | 0        | 0       | 0            |
| 5   | B     | 2     | 0        | 0        | 0       | 0            |
| 5   | G     | 8     | 0        | 0        | 0       | 0            |
| 5   | H     | 42    | 0        | 0        | 4       | 0            |
| 5   | J     | 2     | 0        | 0        | 1       | 0            |
| 5   | L     | 22    | 0        | 0        | 1       | 0            |
| All | All   | 11670 | 0        | 11315    | 402     | 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 18.

All (402) 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:J:426:MET:SD | 2:A:32:TYR:OH | 1.98                     | 1.20              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 2:A:7:SER:HB3    | 2:A:8:PRO:HD3      | 1.32                     | 1.07              |
| 2:A:7:SER:HB3    | 2:A:8:PRO:CD       | 1.87                     | 1.04              |
| 2:A:7:SER:CB     | 2:A:8:PRO:HD3      | 1.87                     | 1.04              |
| 1:G:99:ASN:HB2   | 1:J:202:THR:HG23   | 1.37                     | 1.03              |
| 2:L:7:SER:CB     | 2:L:22:SER:H       | 1.71                     | 1.02              |
| 1:G:469:ARG:HB3  | 1:G:470:PRO:CD     | 1.89                     | 1.02              |
| 2:L:7:SER:HB2    | 2:L:22:SER:H       | 1.20                     | 1.02              |
| 2:A:7:SER:HB2    | 2:A:22:SER:H       | 1.21                     | 1.00              |
| 1:G:428:GLN:HE22 | 1:G:432:LYS:HG2    | 1.27                     | 0.99              |
| 1:G:425:ASN:HB3  | 1:G:426:MET:HA     | 1.46                     | 0.95              |
| 1:G:463:ASN:HB2  | 4:G:963:NAG:H2     | 1.47                     | 0.95              |
| 1:G:202:THR:HG23 | 1:J:99:ASN:HB2     | 1.48                     | 0.95              |
| 1:G:425:ASN:CB   | 1:G:426:MET:HA     | 1.97                     | 0.95              |
| 2:A:7:SER:CB     | 2:A:22:SER:H       | 1.79                     | 0.95              |
| 1:G:469:ARG:CB   | 1:G:470:PRO:HD3    | 1.96                     | 0.93              |
| 1:J:441:GLY:H    | 1:J:442:GLN:HA     | 1.34                     | 0.93              |
| 2:L:7:SER:HB2    | 2:L:22:SER:N       | 1.84                     | 0.92              |
| 1:G:469:ARG:HB3  | 1:G:470:PRO:HD3    | 1.45                     | 0.92              |
| 1:J:444:ARG:H    | 1:J:444:ARG:HD3    | 1.34                     | 0.90              |
| 2:A:7:SER:HB2    | 2:A:22:SER:N       | 1.87                     | 0.89              |
| 1:G:425:ASN:HB3  | 1:G:426:MET:CA     | 2.04                     | 0.87              |
| 1:G:201:ILE:HG22 | 1:J:99:ASN:HB3     | 1.53                     | 0.86              |
| 1:G:99:ASN:HB3   | 1:J:201:ILE:HG22   | 1.59                     | 0.85              |
| 3:H:17:THR:HG22  | 5:H:243:HOH:O      | 1.78                     | 0.84              |
| 1:J:441:GLY:N    | 1:J:442:GLN:HA     | 1.88                     | 0.84              |
| 2:L:7:SER:HB3    | 2:L:8:PRO:HD2      | 1.57                     | 0.84              |
| 1:G:368:ASP:H    | 3:H:32:HIS:HE1     | 1.25                     | 0.84              |
| 1:G:436:ALA:HB1  | 1:G:437:PRO:CD     | 2.07                     | 0.84              |
| 1:J:336:THR:OG1  | 1:J:412:ARG:HG2    | 1.78                     | 0.83              |
| 1:G:463:ASN:C    | 1:G:465:THR:H      | 1.86                     | 0.83              |
| 2:L:189:HIS:O    | 2:L:211:ARG:NH1    | 2.11                     | 0.82              |
| 1:G:435:TYR:HD2  | 1:G:436:ALA:H      | 1.25                     | 0.82              |
| 2:A:189:HIS:O    | 2:A:211:ARG:NH1    | 2.13                     | 0.82              |
| 2:L:31:ARG:NH2   | 3:H:100(E):TYR:HE1 | 1.78                     | 0.82              |
| 1:G:216:HIS:CE1  | 1:J:440:ARG:HG2    | 2.15                     | 0.81              |
| 3:H:38:ARG:HE    | 3:H:46:GLN:NE2     | 1.78                     | 0.81              |
| 1:J:463:ASN:C    | 1:J:465:THR:H      | 1.89                     | 0.81              |
| 1:G:428:GLN:NE2  | 1:G:432:LYS:HG2    | 1.96                     | 0.80              |
| 1:J:429:GLU:HG2  | 1:J:430:VAL:H      | 1.46                     | 0.80              |
| 3:B:38:ARG:HE    | 3:B:46:GLN:NE2     | 1.79                     | 0.80              |
| 2:L:7:SER:CB     | 2:L:8:PRO:CD       | 2.61                     | 0.79              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:436:ALA:HB1  | 1:G:437:PRO:HD2    | 1.65                     | 0.77              |
| 1:G:274:SER:OG   | 1:G:276:ASN:O      | 2.03                     | 0.76              |
| 2:A:7:SER:CB     | 2:A:8:PRO:CD       | 2.54                     | 0.76              |
| 2:L:7:SER:OG     | 2:L:8:PRO:HD3      | 1.87                     | 0.75              |
| 1:J:435:TYR:HD2  | 1:J:436:ALA:H      | 1.33                     | 0.75              |
| 3:H:17:THR:CG2   | 5:H:243:HOH:O      | 2.35                     | 0.74              |
| 1:J:444:ARG:HD3  | 1:J:444:ARG:N      | 2.00                     | 0.74              |
| 3:B:19:SER:HB3   | 3:B:81:LYS:NZ      | 2.02                     | 0.74              |
| 2:A:33:LEU:HD22  | 2:A:71:PHE:CD2     | 2.23                     | 0.73              |
| 1:G:216:HIS:HE1  | 1:J:440:ARG:HG2    | 1.51                     | 0.73              |
| 1:G:469:ARG:CB   | 1:G:470:PRO:CD     | 2.57                     | 0.71              |
| 2:A:33:LEU:HD22  | 2:A:71:PHE:CG      | 2.24                     | 0.71              |
| 1:G:447:SER:HB3  | 4:G:762:NAG:HN2    | 1.55                     | 0.71              |
| 3:H:178:LEU:HD12 | 3:H:178:LEU:C      | 2.16                     | 0.70              |
| 1:G:94:ASN:HD22  | 1:G:236:THR:HG22   | 1.57                     | 0.70              |
| 3:H:52:TYR:CD2   | 3:H:54:SER:HB3     | 2.27                     | 0.70              |
| 1:J:469:ARG:HB3  | 1:J:470:PRO:HD2    | 1.74                     | 0.70              |
| 3:H:19:SER:HB3   | 3:H:81:LYS:NZ      | 2.06                     | 0.69              |
| 2:L:33:LEU:HD22  | 2:L:71:PHE:CG      | 2.27                     | 0.69              |
| 2:L:67:SER:HA    | 2:L:71:PHE:CE2     | 2.27                     | 0.69              |
| 2:L:31:ARG:NH2   | 3:H:100(E):TYR:CE1 | 2.60                     | 0.69              |
| 1:J:469:ARG:HB3  | 1:J:470:PRO:CD     | 2.23                     | 0.69              |
| 1:G:424:ILE:O    | 1:G:425:ASN:HB2    | 1.93                     | 0.68              |
| 2:L:7:SER:HB3    | 2:L:8:PRO:CD       | 2.23                     | 0.68              |
| 2:L:33:LEU:HD22  | 2:L:71:PHE:CD2     | 2.27                     | 0.68              |
| 1:G:463:ASN:C    | 1:G:465:THR:N      | 2.49                     | 0.68              |
| 1:G:469:ARG:HB3  | 1:G:470:PRO:HD2    | 1.74                     | 0.67              |
| 1:J:463:ASN:C    | 1:J:465:THR:N      | 2.51                     | 0.67              |
| 1:J:94:ASN:HD22  | 1:J:236:THR:HG22   | 1.60                     | 0.67              |
| 3:B:178:LEU:C    | 3:B:178:LEU:HD12   | 2.19                     | 0.67              |
| 1:G:277:PHE:O    | 1:G:456:ARG:NH2    | 2.29                     | 0.66              |
| 3:B:126:PRO:HG3  | 3:B:138:LEU:HB3    | 1.78                     | 0.66              |
| 3:B:52:TYR:CD2   | 3:B:54:SER:HB3     | 2.30                     | 0.66              |
| 1:G:370:GLU:HG3  | 1:G:384:TYR:CE2    | 2.30                     | 0.66              |
| 1:G:368:ASP:H    | 3:H:32:HIS:CE1     | 2.11                     | 0.66              |
| 4:J:795:NAG:H62  | 4:J:913:NAG:H62    | 1.77                     | 0.66              |
| 1:J:370:GLU:HG3  | 1:J:384:TYR:CE2    | 2.31                     | 0.65              |
| 2:A:67:SER:HA    | 2:A:71:PHE:CE2     | 2.32                     | 0.65              |
| 1:J:357:LYS:HB3  | 1:J:464:GLY:O      | 1.97                     | 0.64              |
| 1:J:251:ILE:O    | 1:J:253:PRO:HD3    | 1.98                     | 0.64              |
| 1:G:463:ASN:O    | 1:G:465:THR:N      | 2.31                     | 0.64              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:G:99:ASN:CB    | 1:J:202:THR:HG23   | 2.21                     | 0.64              |
| 3:H:126:PRO:HG3  | 3:H:138:LEU:HB3    | 1.79                     | 0.63              |
| 1:J:329:ALA:O    | 1:J:418:CYS:HB2    | 1.98                     | 0.63              |
| 2:L:197:THR:HG22 | 2:L:204:PRO:HG3    | 1.78                     | 0.63              |
| 3:H:38:ARG:HE    | 3:H:46:GLN:HE21    | 1.47                     | 0.63              |
| 2:L:7:SER:HB2    | 2:L:22:SER:CA      | 2.28                     | 0.63              |
| 1:J:299:PRO:HB3  | 1:J:328:GLN:HB2    | 1.80                     | 0.62              |
| 3:B:19:SER:HB3   | 3:B:81:LYS:HZ3     | 1.63                     | 0.62              |
| 1:G:357:LYS:HB3  | 1:G:464:GLY:O      | 2.00                     | 0.62              |
| 3:B:68:THR:HB    | 3:B:81:LYS:HB3     | 1.82                     | 0.62              |
| 1:J:424:ILE:O    | 1:J:425:ASN:C      | 2.42                     | 0.62              |
| 2:A:31:ARG:NH2   | 3:B:100(E):TYR:HE1 | 1.98                     | 0.61              |
| 1:J:463:ASN:O    | 1:J:465:THR:N      | 2.34                     | 0.61              |
| 2:A:197:THR:HG22 | 2:A:204:PRO:HG3    | 1.83                     | 0.61              |
| 3:H:19:SER:HB3   | 3:H:81:LYS:HZ2     | 1.66                     | 0.60              |
| 1:J:380:GLY:O    | 1:J:423:ILE:HG13   | 2.01                     | 0.60              |
| 2:A:7:SER:OG     | 2:A:8:PRO:HD3      | 2.01                     | 0.60              |
| 3:B:17:THR:HG22  | 3:B:82(A):THR:HA   | 1.83                     | 0.60              |
| 1:J:336:THR:H    | 1:J:412:ARG:HB3    | 1.65                     | 0.60              |
| 1:J:364:SER:HB2  | 1:J:470:PRO:HG2    | 1.83                     | 0.60              |
| 1:G:251:ILE:O    | 1:G:253:PRO:HD3    | 2.01                     | 0.60              |
| 3:H:138:LEU:N    | 3:H:138:LEU:HD23   | 2.17                     | 0.59              |
| 3:H:200:HIS:ND1  | 3:H:203:SER:OG     | 2.25                     | 0.59              |
| 1:J:118:PRO:HG3  | 1:J:428:GLN:HG3    | 1.85                     | 0.59              |
| 2:L:21:LEU:HD12  | 2:L:21:LEU:N       | 2.19                     | 0.58              |
| 1:G:357:LYS:HZ3  | 4:G:856:NAG:HN2    | 1.52                     | 0.58              |
| 2:A:31:ARG:NH2   | 3:B:100(E):TYR:CE1 | 2.71                     | 0.58              |
| 3:H:17:THR:HG22  | 3:H:82(A):THR:HA   | 1.85                     | 0.58              |
| 1:G:474:ASP:OD2  | 1:G:476:ARG:HB2    | 2.03                     | 0.58              |
| 1:J:239:CYS:SG   | 1:J:242:VAL:HG22   | 2.43                     | 0.58              |
| 2:L:201:LEU:HD13 | 2:L:205:VAL:HG23   | 1.84                     | 0.58              |
| 1:J:444:ARG:N    | 1:J:444:ARG:CD     | 2.67                     | 0.57              |
| 3:B:47:TRP:CZ2   | 3:B:49:GLY:HA2     | 2.40                     | 0.57              |
| 3:H:68:THR:HB    | 3:H:81:LYS:HB3     | 1.85                     | 0.57              |
| 1:G:474:ASP:HB3  | 3:H:52:TYR:OH      | 2.04                     | 0.57              |
| 2:L:7:SER:OG     | 2:L:8:PRO:CD       | 2.53                     | 0.56              |
| 3:B:38:ARG:HE    | 3:B:46:GLN:HE21    | 1.53                     | 0.56              |
| 1:J:476:ARG:HH22 | 3:B:54:SER:HB2     | 1.69                     | 0.56              |
| 1:G:239:CYS:SG   | 1:G:242:VAL:HG22   | 2.46                     | 0.56              |
| 1:J:350:LYS:HB3  | 1:J:355:ASN:HA     | 1.88                     | 0.56              |
| 3:B:138:LEU:N    | 3:B:138:LEU:HD23   | 2.21                     | 0.56              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:21:LEU:N     | 2:A:21:LEU:HD12  | 2.21                     | 0.55              |
| 3:B:19:SER:HB3   | 3:B:81:LYS:HZ2   | 1.71                     | 0.55              |
| 1:J:427:TRP:O    | 1:J:428:GLN:HB2  | 2.06                     | 0.55              |
| 2:A:48:ILE:HD13  | 2:A:54:ARG:HA    | 1.88                     | 0.55              |
| 1:J:344:GLN:OE1  | 4:J:789:NAG:H62  | 2.06                     | 0.55              |
| 1:J:96:TRP:CE3   | 1:J:236:THR:CG2  | 2.90                     | 0.55              |
| 3:B:125:ALA:CB   | 3:B:214:LYS:HE3  | 2.37                     | 0.55              |
| 4:J:795:NAG:H62  | 4:J:913:NAG:C6   | 2.37                     | 0.54              |
| 1:G:103:GLN:HA   | 1:G:103:GLN:NE2  | 2.21                     | 0.54              |
| 1:J:103:GLN:HA   | 1:J:103:GLN:NE2  | 2.22                     | 0.54              |
| 3:B:201:LYS:HB2  | 3:B:202:PRO:HD3  | 1.88                     | 0.54              |
| 1:G:202:THR:HG23 | 1:J:99:ASN:CB    | 2.31                     | 0.54              |
| 3:H:138:LEU:HD23 | 3:H:138:LEU:H    | 1.72                     | 0.54              |
| 1:G:96:TRP:CE3   | 1:G:236:THR:HG21 | 2.43                     | 0.54              |
| 1:G:99:ASN:HB2   | 1:J:202:THR:CG2  | 2.26                     | 0.54              |
| 1:G:96:TRP:CE3   | 1:G:236:THR:CG2  | 2.89                     | 0.54              |
| 1:G:350:LYS:HB3  | 1:G:355:ASN:HA   | 1.90                     | 0.54              |
| 3:H:125:ALA:CB   | 3:H:214:LYS:HE3  | 2.38                     | 0.54              |
| 3:H:201:LYS:HB2  | 3:H:202:PRO:HD3  | 1.90                     | 0.53              |
| 1:G:344:GLN:HA   | 1:G:347:ILE:HD12 | 1.90                     | 0.53              |
| 1:J:259:LEU:HB2  | 1:J:374:HIS:CE1  | 2.44                     | 0.53              |
| 3:B:101:ASP:C    | 3:B:102:PRO:O    | 2.51                     | 0.53              |
| 1:G:259:LEU:HB2  | 1:G:374:HIS:CE1  | 2.43                     | 0.53              |
| 2:A:37:GLN:HG3   | 2:A:86:TYR:CE2   | 2.44                     | 0.53              |
| 1:G:108:ILE:HD13 | 1:G:479:TRP:CZ2  | 2.43                     | 0.53              |
| 1:G:344:GLN:OE1  | 4:G:789:NAG:H61  | 2.09                     | 0.53              |
| 1:G:96:TRP:CZ3   | 1:G:236:THR:HG23 | 2.44                     | 0.53              |
| 1:G:370:GLU:H    | 1:G:370:GLU:CD   | 2.17                     | 0.53              |
| 1:J:96:TRP:CE3   | 1:J:236:THR:HG21 | 2.44                     | 0.53              |
| 1:G:283:THR:HG23 | 1:G:472:GLY:HA3  | 1.90                     | 0.53              |
| 2:L:48:ILE:HD13  | 2:L:54:ARG:HA    | 1.90                     | 0.53              |
| 3:H:178:LEU:C    | 3:H:178:LEU:CD1  | 2.81                     | 0.52              |
| 1:J:430:VAL:HG12 | 1:J:430:VAL:O    | 2.09                     | 0.52              |
| 1:J:276:ASN:HB3  | 1:J:279:ASN:HB3  | 1.91                     | 0.52              |
| 2:L:67:SER:HA    | 2:L:71:PHE:CZ    | 2.44                     | 0.52              |
| 3:H:47:TRP:CZ2   | 3:H:49:GLY:HA2   | 2.45                     | 0.52              |
| 1:J:370:GLU:CD   | 1:J:370:GLU:H    | 2.18                     | 0.52              |
| 2:L:143:GLU:CD   | 2:L:143:GLU:H    | 2.18                     | 0.52              |
| 1:J:91:GLU:O     | 1:J:238:PRO:HA   | 2.10                     | 0.52              |
| 1:J:370:GLU:HG3  | 1:J:384:TYR:HE2  | 1.73                     | 0.52              |
| 1:J:474:ASP:OD2  | 1:J:476:ARG:HB2  | 2.09                     | 0.52              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:A:143:GLU:H    | 2:A:143:GLU:CD   | 2.17                     | 0.51              |
| 1:G:104:MET:HA   | 1:G:217:TYR:OH   | 2.10                     | 0.51              |
| 1:G:233:PHE:O    | 1:G:273:ARG:NH1  | 2.43                     | 0.51              |
| 1:G:370:GLU:HG3  | 1:G:384:TYR:HE2  | 1.73                     | 0.51              |
| 3:H:19:SER:HB3   | 3:H:81:LYS:HZ3   | 1.75                     | 0.51              |
| 1:G:213:ILE:HD12 | 1:J:213:ILE:HD12 | 1.93                     | 0.51              |
| 2:L:170:ASP:C    | 2:L:170:ASP:OD1  | 2.52                     | 0.51              |
| 1:J:299:PRO:HD3  | 1:J:329:ALA:HB2  | 1.93                     | 0.51              |
| 1:G:428:GLN:HE22 | 1:G:432:LYS:CG   | 2.11                     | 0.51              |
| 2:A:11:LEU:HD21  | 2:A:13:LEU:HD11  | 1.93                     | 0.51              |
| 1:J:233:PHE:O    | 1:J:273:ARG:NH1  | 2.44                     | 0.51              |
| 1:G:96:TRP:HE3   | 1:G:236:THR:HG21 | 1.75                     | 0.50              |
| 1:G:295:ASN:HA   | 1:G:446:SER:HB3  | 1.93                     | 0.50              |
| 1:G:491:ILE:O    | 1:G:492:GLU:HB3  | 2.10                     | 0.50              |
| 2:L:37:GLN:HG3   | 2:L:86:TYR:CE2   | 2.46                     | 0.50              |
| 3:H:51:ILE:HG13  | 3:H:57:THR:HG22  | 1.93                     | 0.50              |
| 1:J:491:ILE:O    | 1:J:492:GLU:HB3  | 2.11                     | 0.50              |
| 1:G:91:GLU:O     | 1:G:238:PRO:HA   | 2.10                     | 0.50              |
| 1:G:201:ILE:HD12 | 1:J:103:GLN:NE2  | 2.27                     | 0.50              |
| 1:J:108:ILE:HD13 | 1:J:479:TRP:CZ2  | 2.47                     | 0.50              |
| 3:B:6:GLU:CD     | 3:B:106:GLY:H    | 2.19                     | 0.50              |
| 1:G:384:TYR:O    | 1:G:418:CYS:HA   | 2.12                     | 0.50              |
| 2:L:11:LEU:HD21  | 2:L:13:LEU:HD11  | 1.92                     | 0.50              |
| 2:A:7:SER:HB3    | 2:A:8:PRO:HD2    | 1.87                     | 0.50              |
| 3:H:11:LEU:HD11  | 3:H:112:SER:HB3  | 1.93                     | 0.50              |
| 1:J:432:LYS:C    | 1:J:434:MET:H    | 2.20                     | 0.50              |
| 1:J:96:TRP:HE3   | 1:J:236:THR:HG21 | 1.76                     | 0.50              |
| 1:J:96:TRP:CZ3   | 1:J:236:THR:HG23 | 2.46                     | 0.50              |
| 2:A:37:GLN:HB2   | 2:A:47:LEU:HD22  | 1.94                     | 0.50              |
| 3:B:101:ASP:O    | 3:B:102:PRO:O    | 2.30                     | 0.50              |
| 1:G:298:ARG:HG3  | 1:G:443:ILE:HG13 | 1.94                     | 0.49              |
| 3:H:4:LEU:HB3    | 3:H:22:CYS:SG    | 2.52                     | 0.49              |
| 1:J:443:ILE:HG22 | 1:J:444:ARG:H    | 1.77                     | 0.49              |
| 3:B:22:CYS:O     | 3:B:77:GLN:HB2   | 2.12                     | 0.49              |
| 1:G:463:ASN:OD1  | 1:G:463:ASN:N    | 2.43                     | 0.49              |
| 1:J:104:MET:HA   | 1:J:217:TYR:OH   | 2.12                     | 0.49              |
| 2:A:49:TYR:O     | 2:A:53:SER:HB2   | 2.12                     | 0.49              |
| 1:G:430:VAL:HG12 | 1:G:430:VAL:O    | 2.13                     | 0.49              |
| 2:L:89:GLN:HB2   | 2:L:98:PHE:CD2   | 2.47                     | 0.49              |
| 1:J:344:GLN:HA   | 1:J:347:ILE:HD12 | 1.93                     | 0.49              |
| 1:J:463:ASN:N    | 1:J:463:ASN:OD1  | 2.46                     | 0.49              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:386:ASN:O    | 1:G:416:LEU:HD22 | 2.13                     | 0.49              |
| 2:L:140:TYR:CG   | 2:L:141:PRO:HA   | 2.47                     | 0.49              |
| 3:B:30:SER:O     | 3:B:32:HIS:HD2   | 1.95                     | 0.49              |
| 2:L:37:GLN:HB2   | 2:L:47:LEU:HD22  | 1.94                     | 0.49              |
| 1:J:357:LYS:CB   | 1:J:464:GLY:O    | 2.60                     | 0.49              |
| 3:B:129:LYS:O    | 3:B:130:SER:C    | 2.56                     | 0.49              |
| 3:B:178:LEU:C    | 3:B:178:LEU:CD1  | 2.84                     | 0.49              |
| 3:H:94:ARG:HB3   | 3:H:101:ASP:O    | 2.13                     | 0.49              |
| 3:H:178:LEU:HD12 | 3:H:178:LEU:O    | 2.13                     | 0.49              |
| 1:J:258:GLN:HA   | 1:J:470:PRO:O    | 2.12                     | 0.49              |
| 2:A:89:GLN:HB2   | 2:A:98:PHE:CD2   | 2.48                     | 0.49              |
| 1:G:390:LEU:HD11 | 1:G:416:LEU:HD11 | 1.95                     | 0.49              |
| 1:G:436:ALA:CB   | 1:G:437:PRO:CD   | 2.80                     | 0.49              |
| 3:H:129:LYS:O    | 3:H:130:SER:C    | 2.56                     | 0.49              |
| 1:J:278:THR:HB   | 4:J:776:NAG:H5   | 1.95                     | 0.48              |
| 1:J:336:THR:HG1  | 1:J:412:ARG:HG2  | 1.77                     | 0.48              |
| 1:G:420:ILE:O    | 1:G:420:ILE:HG22 | 2.13                     | 0.48              |
| 3:B:12:VAL:O     | 3:B:111:VAL:HA   | 2.13                     | 0.48              |
| 3:B:154:TRP:CZ3  | 3:B:196:CYS:HB3  | 2.48                     | 0.48              |
| 1:G:270:ILE:HG12 | 4:G:789:NAG:H62  | 1.95                     | 0.48              |
| 3:H:12:VAL:O     | 3:H:111:VAL:HA   | 2.12                     | 0.48              |
| 2:A:170:ASP:OD1  | 2:A:170:ASP:C    | 2.56                     | 0.48              |
| 1:G:234:ASN:HB2  | 4:G:734:NAG:C7   | 2.43                     | 0.48              |
| 3:B:200:HIS:ND1  | 3:B:203:SER:OG   | 2.30                     | 0.48              |
| 2:L:167:ASP:HB3  | 2:L:170:ASP:OD1  | 2.13                     | 0.48              |
| 3:B:22:CYS:HB3   | 3:B:78:PHE:CE2   | 2.48                     | 0.48              |
| 3:B:50:TYR:C     | 3:B:50:TYR:CD2   | 2.91                     | 0.48              |
| 3:H:30:SER:O     | 3:H:32:HIS:HD2   | 1.96                     | 0.47              |
| 3:H:6:GLU:CD     | 3:H:106:GLY:H    | 2.22                     | 0.47              |
| 1:J:429:GLU:CG   | 1:J:430:VAL:H    | 2.22                     | 0.47              |
| 3:H:30:SER:O     | 3:H:31:SER:HB2   | 2.14                     | 0.47              |
| 2:A:140:TYR:CG   | 2:A:141:PRO:HA   | 2.48                     | 0.47              |
| 1:G:94:ASN:HA    | 1:G:236:THR:HG22 | 1.96                     | 0.47              |
| 3:H:154:TRP:CZ3  | 3:H:196:CYS:HB3  | 2.50                     | 0.47              |
| 1:G:96:TRP:CZ3   | 1:G:236:THR:CG2  | 2.98                     | 0.47              |
| 1:J:229:ASN:HB2  | 1:J:241:ASN:O    | 2.15                     | 0.47              |
| 1:J:368:ASP:H    | 3:B:32:HIS:HE1   | 1.63                     | 0.47              |
| 3:B:52:TYR:HD2   | 3:B:54:SER:HB3   | 1.77                     | 0.47              |
| 1:G:103:GLN:NE2  | 1:J:201:ILE:HD12 | 2.30                     | 0.47              |
| 1:G:357:LYS:CB   | 1:G:464:GLY:O    | 2.62                     | 0.47              |
| 2:L:6:GLN:HE21   | 2:L:6:GLN:HB3    | 1.52                     | 0.47              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 3:H:22:CYS:O     | 3:H:77:GLN:HB2     | 2.14                     | 0.47              |
| 2:A:67:SER:HA    | 2:A:71:PHE:CZ      | 2.49                     | 0.47              |
| 1:G:375:SER:HA   | 1:G:383:PHE:O      | 2.15                     | 0.47              |
| 1:G:438:PRO:HG2  | 1:G:439:ILE:H      | 1.78                     | 0.47              |
| 1:J:234:ASN:HB2  | 4:J:734:NAG:C7     | 2.44                     | 0.47              |
| 1:J:375:SER:HA   | 1:J:383:PHE:O      | 2.15                     | 0.47              |
| 3:B:11:LEU:HD11  | 3:B:112:SER:HB3    | 1.96                     | 0.47              |
| 3:B:138:LEU:HD23 | 3:B:138:LEU:H      | 1.78                     | 0.47              |
| 1:G:94:ASN:HD22  | 1:G:236:THR:CG2    | 2.27                     | 0.47              |
| 3:B:78:PHE:CZ    | 3:B:92:CYS:HB2     | 2.50                     | 0.47              |
| 1:G:270:ILE:HD13 | 1:G:289:ASN:H      | 1.80                     | 0.47              |
| 1:G:435:TYR:CD2  | 1:G:436:ALA:N      | 2.79                     | 0.47              |
| 1:J:94:ASN:HA    | 1:J:236:THR:HG22   | 1.97                     | 0.47              |
| 1:J:429:GLU:HG2  | 1:J:430:VAL:N      | 2.21                     | 0.47              |
| 1:G:215:ILE:HG12 | 1:J:208:VAL:HG22   | 1.97                     | 0.46              |
| 1:J:356:ASN:HB3  | 4:J:856:NAG:H83    | 1.97                     | 0.46              |
| 1:G:423:ILE:HD11 | 1:G:440:ARG:HH22   | 1.81                     | 0.46              |
| 2:A:201:LEU:HD13 | 2:A:205:VAL:HG23   | 1.97                     | 0.46              |
| 3:B:30:SER:O     | 3:B:31:SER:HB2     | 2.16                     | 0.46              |
| 2:L:107:LYS:O    | 5:L:232:HOH:O      | 2.20                     | 0.46              |
| 1:J:386:ASN:OD1  | 4:J:886:NAG:H2     | 2.13                     | 0.46              |
| 1:G:463:ASN:CB   | 4:G:963:NAG:H2     | 2.27                     | 0.46              |
| 3:H:50:TYR:C     | 3:H:50:TYR:CD2     | 2.93                     | 0.46              |
| 3:B:4:LEU:HB3    | 3:B:22:CYS:SG      | 2.54                     | 0.46              |
| 1:G:298:ARG:HB2  | 1:G:443:ILE:H      | 1.81                     | 0.46              |
| 2:L:8:PRO:O      | 2:L:102:THR:HG23   | 2.15                     | 0.46              |
| 3:H:135:THR:HG22 | 3:H:185:PRO:HA     | 1.98                     | 0.46              |
| 1:J:94:ASN:HD22  | 1:J:236:THR:CG2    | 2.28                     | 0.46              |
| 1:G:295:ASN:O    | 1:G:331:CYS:HA     | 2.16                     | 0.46              |
| 1:J:343:GLU:HG2  | 1:J:393:TRP:HZ2    | 1.81                     | 0.46              |
| 1:J:270:ILE:HD13 | 1:J:289:ASN:H      | 1.81                     | 0.46              |
| 4:J:913:NAG:N2   | 4:J:913:NAG:H5     | 2.31                     | 0.46              |
| 3:B:51:ILE:HG13  | 3:B:57:THR:HG22    | 1.97                     | 0.46              |
| 2:L:46:LEU:HD22  | 3:H:100(F):ARG:HG3 | 1.98                     | 0.46              |
| 3:B:6:GLU:OE2    | 3:B:105:GLN:N      | 2.47                     | 0.45              |
| 3:B:165:THR:HG23 | 3:B:180:SER:HB2    | 1.98                     | 0.45              |
| 1:G:364:SER:N    | 1:G:470:PRO:HG2    | 2.31                     | 0.45              |
| 3:H:145:TYR:CE2  | 3:H:150:VAL:HG13   | 2.51                     | 0.45              |
| 1:G:435:TYR:HD2  | 1:G:436:ALA:N      | 2.02                     | 0.45              |
| 3:H:22:CYS:HB3   | 3:H:78:PHE:CE2     | 2.52                     | 0.45              |
| 3:H:164:HIS:HD2  | 5:H:246:HOH:O      | 1.99                     | 0.45              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 1:J:96:TRP:HE3   | 1:J:236:THR:CG2    | 2.29                     | 0.45              |
| 1:J:451:GLY:C    | 1:J:452:LEU:HD12   | 2.41                     | 0.45              |
| 2:L:49:TYR:O     | 2:L:53:SER:HB2     | 2.17                     | 0.45              |
| 3:H:125:ALA:HA   | 3:H:126:PRO:HD3    | 1.82                     | 0.45              |
| 2:A:193:ALA:HA   | 2:A:208:SER:HB3    | 1.98                     | 0.45              |
| 1:G:96:TRP:CE3   | 1:G:236:THR:HG23   | 2.52                     | 0.45              |
| 1:J:277:PHE:O    | 1:J:456:ARG:NH2    | 2.50                     | 0.45              |
| 2:A:167:ASP:HB3  | 2:A:170:ASP:OD1    | 2.17                     | 0.45              |
| 1:G:229:ASN:HB2  | 1:G:241:ASN:O      | 2.16                     | 0.45              |
| 3:B:94:ARG:HB3   | 3:B:101:ASP:O      | 2.15                     | 0.45              |
| 1:J:96:TRP:CE3   | 1:J:236:THR:HG23   | 2.52                     | 0.45              |
| 1:J:107:ASP:OD1  | 1:J:217:TYR:OH     | 2.23                     | 0.45              |
| 3:B:63:LEU:O     | 3:B:67:VAL:HG23    | 2.17                     | 0.45              |
| 1:J:96:TRP:CZ3   | 1:J:236:THR:CG2    | 3.00                     | 0.45              |
| 2:A:46:LEU:HD22  | 3:B:100(F):ARG:HG3 | 1.99                     | 0.45              |
| 2:A:6:GLN:HE21   | 2:A:6:GLN:HB3      | 1.53                     | 0.44              |
| 3:H:125:ALA:HB3  | 3:H:214:LYS:HE3    | 1.97                     | 0.44              |
| 3:H:185:PRO:O    | 3:H:188:SER:OG     | 2.34                     | 0.44              |
| 3:H:4:LEU:HD22   | 3:H:24:VAL:HG22    | 1.98                     | 0.44              |
| 3:H:63:LEU:O     | 3:H:67:VAL:HG23    | 2.17                     | 0.44              |
| 2:A:29:SER:HB3   | 2:A:32:TYR:CD1     | 2.53                     | 0.44              |
| 1:G:96:TRP:HE3   | 1:G:236:THR:CG2    | 2.29                     | 0.44              |
| 2:L:82:ASP:O     | 2:L:104:LEU:HD23   | 2.17                     | 0.44              |
| 3:B:4:LEU:HD22   | 3:B:24:VAL:HG22    | 1.99                     | 0.44              |
| 3:H:154:TRP:CH2  | 3:H:196:CYS:HB3    | 2.53                     | 0.44              |
| 3:B:125:ALA:HB3  | 3:B:214:LYS:HE3    | 2.00                     | 0.44              |
| 1:G:274:SER:C    | 1:G:276:ASN:N      | 2.75                     | 0.44              |
| 2:L:185:ASP:O    | 2:L:188:LYS:HG2    | 2.17                     | 0.44              |
| 2:A:82:ASP:O     | 2:A:104:LEU:HD23   | 2.18                     | 0.44              |
| 1:J:434:MET:O    | 1:J:435:TYR:CB     | 2.65                     | 0.44              |
| 2:A:32:TYR:O     | 2:A:90:GLN:HA      | 2.16                     | 0.44              |
| 3:B:154:TRP:CH2  | 3:B:196:CYS:HB3    | 2.52                     | 0.44              |
| 1:J:283:THR:HG22 | 1:J:284:ILE:N      | 2.33                     | 0.43              |
| 1:G:300:ASN:CG   | 1:G:442:GLN:HE21   | 2.26                     | 0.43              |
| 2:A:134:CYS:HB2  | 2:A:148:TRP:CZ2    | 2.53                     | 0.43              |
| 3:B:78:PHE:HZ    | 3:B:92:CYS:HB2     | 1.83                     | 0.43              |
| 1:G:275:GLU:O    | 1:G:276:ASN:HB2    | 2.18                     | 0.43              |
| 1:G:490:LYS:HG2  | 1:G:491:ILE:N      | 2.33                     | 0.43              |
| 3:H:52:TYR:HD2   | 3:H:54:SER:HB3     | 1.78                     | 0.43              |
| 2:A:185:ASP:O    | 2:A:188:LYS:HG2    | 2.17                     | 0.43              |
| 3:H:61:PRO:HG2   | 5:H:236:HOH:O      | 2.18                     | 0.43              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:G:216:HIS:CE1  | 1:J:440:ARG:CG    | 2.97                     | 0.43              |
| 1:J:440:ARG:HA   | 1:J:441:GLY:HA2   | 1.67                     | 0.43              |
| 1:G:103:GLN:O    | 1:G:106:GLU:HB2   | 2.19                     | 0.43              |
| 1:G:283:THR:HG22 | 1:G:284:ILE:N     | 2.33                     | 0.43              |
| 2:L:134:CYS:HB2  | 2:L:148:TRP:CZ2   | 2.54                     | 0.43              |
| 1:G:274:SER:C    | 1:G:276:ASN:H     | 2.27                     | 0.43              |
| 1:J:276:ASN:HB3  | 1:J:279:ASN:CB    | 2.49                     | 0.43              |
| 1:G:451:GLY:C    | 1:G:452:LEU:HD12  | 2.44                     | 0.43              |
| 1:G:258:GLN:HA   | 1:G:470:PRO:O     | 2.19                     | 0.43              |
| 2:L:6:GLN:OE1    | 2:L:87:TYR:HA     | 2.19                     | 0.42              |
| 3:H:165:THR:HG23 | 3:H:180:SER:HB2   | 2.01                     | 0.42              |
| 1:J:114:GLN:HA   | 5:J:63:HOH:O      | 2.18                     | 0.42              |
| 3:H:127:SER:HB2  | 3:H:130:SER:H     | 1.83                     | 0.42              |
| 2:A:29:SER:HB3   | 2:A:32:TYR:HD1    | 1.84                     | 0.42              |
| 1:J:350:LYS:HB3  | 1:J:355:ASN:CB    | 2.49                     | 0.42              |
| 2:A:33:LEU:CD2   | 2:A:71:PHE:CD2    | 3.00                     | 0.42              |
| 3:B:145:TYR:CE2  | 3:B:150:VAL:HG13  | 2.54                     | 0.42              |
| 1:G:219:ALA:HA   | 1:G:220:PRO:HD3   | 1.94                     | 0.42              |
| 3:H:12:VAL:HG11  | 3:H:82(C):MET:HG3 | 2.02                     | 0.42              |
| 1:J:439:ILE:H    | 1:J:439:ILE:HG13  | 1.55                     | 0.42              |
| 2:A:175:LEU:C    | 2:A:175:LEU:HD23  | 2.43                     | 0.42              |
| 3:B:135:THR:HG22 | 3:B:185:PRO:HA    | 2.01                     | 0.42              |
| 1:G:350:LYS:HB3  | 1:G:355:ASN:CB    | 2.50                     | 0.42              |
| 1:J:234:ASN:HB2  | 4:J:734:NAG:O7    | 2.19                     | 0.42              |
| 1:J:436:ALA:O    | 1:J:438:PRO:HD3   | 2.20                     | 0.42              |
| 1:J:490:LYS:HG2  | 1:J:491:ILE:N     | 2.35                     | 0.42              |
| 1:G:395:ASP:OD1  | 1:G:395:ASP:N     | 2.53                     | 0.42              |
| 3:H:6:GLU:OE2    | 3:H:105:GLN:N     | 2.50                     | 0.42              |
| 1:J:463:ASN:H    | 1:J:465:THR:HG22  | 1.85                     | 0.42              |
| 3:B:12:VAL:HG11  | 3:B:82(C):MET:HG3 | 2.02                     | 0.42              |
| 1:J:234:ASN:CB   | 4:J:734:NAG:H2    | 2.50                     | 0.42              |
| 1:G:98:ASN:O     | 1:G:100:MET:N     | 2.53                     | 0.41              |
| 1:G:436:ALA:HB1  | 1:G:437:PRO:HD3   | 1.99                     | 0.41              |
| 2:L:16:GLY:HA2   | 2:L:77:ARG:HG2    | 2.02                     | 0.41              |
| 2:L:60:ASP:OD1   | 2:L:60:ASP:N      | 2.53                     | 0.41              |
| 1:J:381:GLU:HG2  | 1:J:422:GLN:HG2   | 2.01                     | 0.41              |
| 3:B:6:GLU:OE2    | 3:B:104:GLY:HA3   | 2.20                     | 0.41              |
| 3:B:185:PRO:O    | 3:B:188:SER:OG    | 2.35                     | 0.41              |
| 2:A:159:SER:HA   | 2:A:178:THR:O     | 2.20                     | 0.41              |
| 2:L:140:TYR:CD1  | 2:L:141:PRO:HA    | 2.55                     | 0.41              |
| 3:H:30:SER:O     | 3:H:31:SER:CB     | 2.69                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:G:208:VAL:HG22 | 1:J:215:ILE:HG12 | 2.03                     | 0.41              |
| 3:H:168:ALA:HA   | 3:H:178:LEU:HB3  | 2.03                     | 0.41              |
| 1:G:257:THR:O    | 1:G:259:LEU:N    | 2.49                     | 0.41              |
| 3:H:138:LEU:N    | 3:H:138:LEU:CD2  | 2.84                     | 0.41              |
| 1:J:283:THR:HG23 | 1:J:472:GLY:HA3  | 2.01                     | 0.41              |
| 3:B:30:SER:O     | 3:B:31:SER:CB    | 2.69                     | 0.41              |
| 1:G:468:PHE:C    | 1:G:469:ARG:HG3  | 2.45                     | 0.41              |
| 2:A:100:GLN:CD   | 2:A:100:GLN:H    | 2.29                     | 0.41              |
| 3:B:77:GLN:HE21  | 3:B:77:GLN:HB3   | 1.68                     | 0.41              |
| 1:G:231:LYS:H    | 4:G:741:NAG:H83  | 1.85                     | 0.41              |
| 1:G:366:GLY:HA3  | 3:H:2:VAL:CG2    | 2.51                     | 0.41              |
| 3:H:5:GLN:NE2    | 3:H:5:GLN:HA     | 2.35                     | 0.41              |
| 3:H:78:PHE:CZ    | 3:H:92:CYS:HB2   | 2.55                     | 0.41              |
| 1:G:364:SER:H    | 1:G:470:PRO:HG2  | 1.86                     | 0.41              |
| 2:L:159:SER:HA   | 2:L:178:THR:O    | 2.21                     | 0.41              |
| 1:J:94:ASN:ND2   | 1:J:236:THR:HG22 | 2.33                     | 0.41              |
| 2:A:6:GLN:OE1    | 2:A:87:TYR:HA    | 2.20                     | 0.41              |
| 2:A:167:ASP:OD2  | 2:A:169:LYS:N    | 2.53                     | 0.41              |
| 3:B:125:ALA:HA   | 3:B:126:PRO:HD3  | 1.83                     | 0.41              |
| 2:A:182:SER:O    | 2:A:183:LYS:C    | 2.64                     | 0.41              |
| 3:H:38:ARG:HH21  | 3:H:46:GLN:HE22  | 1.68                     | 0.40              |
| 1:G:356:ASN:OD1  | 4:G:856:NAG:O5   | 2.34                     | 0.40              |
| 2:L:32:TYR:O     | 2:L:90:GLN:HA    | 2.22                     | 0.40              |
| 2:A:39:LYS:HE3   | 2:A:81:GLU:O     | 2.21                     | 0.40              |
| 2:A:143:GLU:CD   | 2:A:143:GLU:N    | 2.79                     | 0.40              |
| 3:B:127:SER:HB2  | 3:B:130:SER:H    | 1.86                     | 0.40              |
| 2:L:29:SER:HB3   | 2:L:32:TYR:CD1   | 2.55                     | 0.40              |
| 2:A:47:LEU:HD12  | 2:A:47:LEU:HA    | 1.93                     | 0.40              |
| 3:B:5:GLN:NE2    | 3:B:5:GLN:HA     | 2.35                     | 0.40              |
| 1:G:350:LYS:HG2  | 1:G:359:ILE:HD13 | 2.04                     | 0.40              |
| 3:H:66:ARG:NH2   | 3:H:86:ASP:OD2   | 2.46                     | 0.40              |
| 1:J:441:GLY:N    | 1:J:442:GLN:CA   | 2.72                     | 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   | G     | 283/321 (88%)   | 238 (84%)  | 41 (14%) | 4 (1%)   | 9           | 30 |
| 1   | J     | 283/321 (88%)   | 244 (86%)  | 32 (11%) | 7 (2%)   | 4           | 17 |
| 2   | A     | 213/215 (99%)   | 202 (95%)  | 9 (4%)   | 2 (1%)   | 14          | 41 |
| 2   | L     | 213/215 (99%)   | 204 (96%)  | 8 (4%)   | 1 (0%)   | 24          | 54 |
| 3   | B     | 223/225 (99%)   | 206 (92%)  | 16 (7%)  | 1 (0%)   | 30          | 59 |
| 3   | H     | 223/225 (99%)   | 206 (92%)  | 16 (7%)  | 1 (0%)   | 30          | 59 |
| All | All   | 1438/1522 (94%) | 1300 (90%) | 122 (8%) | 16 (1%)  | 11          | 36 |

All (16) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 438 | PRO  |
| 3   | B     | 102 | PRO  |
| 1   | G     | 464 | GLY  |
| 3   | H     | 102 | PRO  |
| 1   | J     | 435 | TYR  |
| 1   | J     | 464 | GLY  |
| 1   | J     | 438 | PRO  |
| 2   | L     | 8   | PRO  |
| 1   | J     | 428 | GLN  |
| 2   | A     | 8   | PRO  |
| 1   | G     | 99  | ASN  |
| 1   | J     | 99  | ASN  |
| 2   | A     | 7   | SER  |
| 1   | J     | 437 | PRO  |
| 1   | G     | 424 | ILE  |
| 1   | J     | 439 | ILE  |

### 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   | G     | 258/284 (91%)   | 248 (96%)  | 10 (4%)  | 28          | 63 |
| 1   | J     | 258/284 (91%)   | 248 (96%)  | 10 (4%)  | 28          | 63 |
| 2   | A     | 186/186 (100%)  | 179 (96%)  | 7 (4%)   | 29          | 64 |
| 2   | L     | 186/186 (100%)  | 180 (97%)  | 6 (3%)   | 34          | 68 |
| 3   | B     | 193/193 (100%)  | 187 (97%)  | 6 (3%)   | 35          | 69 |
| 3   | H     | 193/193 (100%)  | 187 (97%)  | 6 (3%)   | 35          | 69 |
| All | All   | 1274/1326 (96%) | 1229 (96%) | 45 (4%)  | 32          | 66 |

All (45) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 202 | THR  |
| 1   | G     | 298 | ARG  |
| 1   | G     | 392 | THR  |
| 1   | G     | 394 | ASN  |
| 1   | G     | 395 | ASP  |
| 1   | G     | 413 | ASN  |
| 1   | G     | 426 | MET  |
| 1   | G     | 446 | SER  |
| 1   | G     | 463 | ASN  |
| 1   | G     | 488 | VAL  |
| 2   | L     | 6   | GLN  |
| 2   | L     | 13  | LEU  |
| 2   | L     | 31  | ARG  |
| 2   | L     | 95  | VAL  |
| 2   | L     | 100 | GLN  |
| 2   | L     | 163 | VAL  |
| 3   | H     | 6   | GLU  |
| 3   | H     | 19  | SER  |
| 3   | H     | 30  | SER  |
| 3   | H     | 54  | SER  |
| 3   | H     | 178 | LEU  |
| 3   | H     | 209 | LYS  |
| 1   | J     | 202 | THR  |
| 1   | J     | 298 | ARG  |
| 1   | J     | 412 | ARG  |
| 1   | J     | 439 | ILE  |
| 1   | J     | 443 | ILE  |
| 1   | J     | 444 | ARG  |
| 1   | J     | 445 | CYS  |
| 1   | J     | 446 | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | J     | 463 | ASN  |
| 1   | J     | 488 | VAL  |
| 2   | A     | 6   | GLN  |
| 2   | A     | 13  | LEU  |
| 2   | A     | 21  | LEU  |
| 2   | A     | 31  | ARG  |
| 2   | A     | 95  | VAL  |
| 2   | A     | 100 | GLN  |
| 2   | A     | 163 | VAL  |
| 3   | B     | 6   | GLU  |
| 3   | B     | 19  | SER  |
| 3   | B     | 30  | SER  |
| 3   | B     | 54  | SER  |
| 3   | B     | 178 | LEU  |
| 3   | B     | 209 | LYS  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | G     | 94  | ASN  |
| 1   | G     | 103 | GLN  |
| 1   | G     | 216 | HIS  |
| 1   | G     | 330 | HIS  |
| 1   | G     | 337 | GLN  |
| 1   | G     | 352 | GLN  |
| 1   | G     | 442 | GLN  |
| 2   | L     | 100 | GLN  |
| 2   | L     | 147 | GLN  |
| 2   | L     | 199 | GLN  |
| 3   | H     | 32  | HIS  |
| 3   | H     | 46  | GLN  |
| 3   | H     | 77  | GLN  |
| 3   | H     | 164 | HIS  |
| 1   | J     | 94  | ASN  |
| 1   | J     | 103 | GLN  |
| 1   | J     | 300 | ASN  |
| 1   | J     | 352 | GLN  |
| 2   | A     | 100 | GLN  |
| 2   | A     | 147 | GLN  |
| 2   | A     | 199 | GLN  |
| 3   | B     | 32  | HIS  |
| 3   | B     | 46  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | B     | 77  | GLN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

27 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 4   | NAG  | G     | 741 | 1    | 14,14,15     | 0.48 | 0           | 17,19,21    | 1.07 | 1 (5%)      |
| 4   | NAG  | G     | 789 | 1    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.87 | 0           |
| 4   | NAG  | G     | 894 | 1    | 14,14,15     | 0.44 | 0           | 17,19,21    | 1.08 | 1 (5%)      |
| 4   | NAG  | G     | 776 | 1    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.74 | 0           |
| 4   | NAG  | G     | 762 | 1    | 14,14,15     | 0.63 | 0           | 17,19,21    | 0.94 | 1 (5%)      |
| 4   | NAG  | G     | 856 | 1    | 14,14,15     | 0.65 | 0           | 17,19,21    | 0.74 | 1 (5%)      |
| 4   | NAG  | J     | 741 | 1    | 14,14,15     | 0.60 | 0           | 17,19,21    | 1.23 | 2 (11%)     |
| 4   | NAG  | G     | 832 | 1    | 14,14,15     | 0.54 | 0           | 17,19,21    | 0.71 | 0           |
| 4   | NAG  | J     | 762 | 1    | 14,14,15     | 0.52 | 0           | 17,19,21    | 0.80 | 0           |
| 4   | NAG  | G     | 801 | 1    | 14,14,15     | 0.61 | 0           | 17,19,21    | 0.70 | 0           |
| 4   | NAG  | J     | 734 | 1    | 14,14,15     | 0.55 | 0           | 17,19,21    | 0.79 | 1 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | J     | 801 | 1    | 14,14,15     | 0.46 | 0        | 17,19,21    | 1.13 | 1 (5%)   |
| 4   | NAG  | J     | 886 | 1    | 14,14,15     | 0.29 | 0        | 17,19,21    | 1.08 | 2 (11%)  |
| 4   | NAG  | J     | 913 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 0.86 | 0        |
| 4   | NAG  | J     | 832 | 1    | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.80 | 0        |
| 4   | NAG  | G     | 795 | 1    | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.71 | 0        |
| 4   | NAG  | J     | 789 | 1    | 14,14,15     | 0.61 | 0        | 17,19,21    | 1.73 | 5 (29%)  |
| 4   | NAG  | J     | 894 | 1    | 14,14,15     | 0.51 | 0        | 17,19,21    | 0.73 | 1 (5%)   |
| 4   | NAG  | J     | 776 | 1    | 14,14,15     | 0.46 | 0        | 17,19,21    | 1.78 | 5 (29%)  |
| 4   | NAG  | G     | 963 | 1    | 14,14,15     | 1.58 | 2 (14%)  | 17,19,21    | 0.97 | 1 (5%)   |
| 4   | NAG  | J     | 856 | 1    | 14,14,15     | 0.64 | 0        | 17,19,21    | 0.87 | 0        |
| 4   | NAG  | G     | 886 | 1    | 14,14,15     | 0.58 | 0        | 17,19,21    | 1.01 | 1 (5%)   |
| 4   | NAG  | G     | 734 | 1    | 14,14,15     | 0.68 | 0        | 17,19,21    | 0.71 | 0        |
| 4   | NAG  | G     | 948 | 1    | 14,14,15     | 0.65 | 0        | 17,19,21    | 1.10 | 1 (5%)   |
| 4   | NAG  | J     | 963 | 1    | 14,14,15     | 0.61 | 0        | 17,19,21    | 1.12 | 1 (5%)   |
| 4   | NAG  | J     | 948 | 1    | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.71 | 0        |
| 4   | NAG  | J     | 795 | 1    | 14,14,15     | 0.53 | 0        | 17,19,21    | 0.84 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | G     | 741 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 789 | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 894 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 776 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 762 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 856 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 741 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 832 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 762 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 801 | 1    | 1/1/5/7 | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 801 | 1    | -       | 5/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 734 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 886 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 913 | 1    | 1/1/5/7 | 6/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | NAG  | J     | 832 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 795 | 1    | -       | 3/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 789 | 1    | -       | 6/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 894 | 1    | 1/1/5/7 | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 776 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 963 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 856 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 886 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 734 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | G     | 948 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 963 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 948 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | J     | 795 | 1    | -       | 3/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 4   | G     | 963 | NAG  | C1-C2 | 4.24 | 1.58        | 1.52     |
| 4   | G     | 963 | NAG  | C3-C2 | 2.16 | 1.57        | 1.52     |

All (26) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | J     | 776 | NAG  | O5-C1-C2 | -4.17 | 104.84      | 111.29   |
| 4   | J     | 963 | NAG  | C1-O5-C5 | 3.96  | 117.49      | 112.19   |
| 4   | J     | 789 | NAG  | O5-C1-C2 | -3.90 | 105.26      | 111.29   |
| 4   | G     | 894 | NAG  | C1-O5-C5 | 3.57  | 116.97      | 112.19   |
| 4   | G     | 948 | NAG  | C4-C3-C2 | 3.44  | 116.05      | 111.02   |
| 4   | J     | 741 | NAG  | C1-O5-C5 | 3.41  | 116.76      | 112.19   |
| 4   | J     | 789 | NAG  | C1-C2-N2 | 3.23  | 115.53      | 110.43   |
| 4   | G     | 886 | NAG  | C1-O5-C5 | 2.97  | 116.17      | 112.19   |
| 4   | J     | 801 | NAG  | O5-C1-C2 | -2.95 | 106.73      | 111.29   |
| 4   | J     | 776 | NAG  | C1-C2-N2 | 2.76  | 114.78      | 110.43   |
| 4   | J     | 789 | NAG  | C1-O5-C5 | 2.63  | 115.71      | 112.19   |
| 4   | J     | 776 | NAG  | C1-O5-C5 | 2.56  | 115.62      | 112.19   |
| 4   | J     | 741 | NAG  | O5-C1-C2 | 2.51  | 115.17      | 111.29   |
| 4   | J     | 776 | NAG  | C4-C3-C2 | -2.50 | 107.35      | 111.02   |
| 4   | G     | 741 | NAG  | O5-C1-C2 | -2.49 | 107.44      | 111.29   |
| 4   | J     | 776 | NAG  | C2-N2-C7 | -2.38 | 119.71      | 122.90   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | J     | 789 | NAG  | C4-C3-C2 | -2.36 | 107.56      | 111.02   |
| 4   | G     | 963 | NAG  | O5-C1-C2 | -2.32 | 107.70      | 111.29   |
| 4   | J     | 886 | NAG  | C1-O5-C5 | -2.24 | 109.18      | 112.19   |
| 4   | J     | 886 | NAG  | C1-C2-N2 | -2.20 | 106.97      | 110.43   |
| 4   | J     | 734 | NAG  | C1-O5-C5 | 2.12  | 115.03      | 112.19   |
| 4   | J     | 789 | NAG  | C2-N2-C7 | 2.08  | 125.69      | 122.90   |
| 4   | G     | 856 | NAG  | C4-C3-C2 | 2.04  | 114.02      | 111.02   |
| 4   | G     | 762 | NAG  | C1-O5-C5 | 2.02  | 114.90      | 112.19   |
| 4   | J     | 894 | NAG  | O5-C5-C6 | 2.02  | 111.60      | 107.66   |
| 4   | J     | 795 | NAG  | C1-O5-C5 | 2.01  | 114.88      | 112.19   |

All (3) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 4   | J     | 801 | NAG  | C1   |
| 4   | J     | 894 | NAG  | C1   |
| 4   | J     | 913 | NAG  | C1   |

All (93) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | G     | 741 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 741 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 741 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 789 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 789 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 795 | NAG  | C1-C2-N2-C7 |
| 4   | G     | 801 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 801 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 832 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 832 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 832 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 856 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 856 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 886 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 963 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 963 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 963 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 734 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 734 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 776 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 776 | NAG  | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | J     | 789 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 789 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 795 | NAG  | C3-C2-N2-C7 |
| 4   | J     | 795 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 795 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 801 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 801 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 832 | NAG  | C3-C2-N2-C7 |
| 4   | J     | 832 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 832 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 894 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 894 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 913 | NAG  | C1-C2-N2-C7 |
| 4   | J     | 913 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 913 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 948 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 948 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 963 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 963 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 886 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 762 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 762 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 886 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 856 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 734 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 948 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 801 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 801 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 734 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 801 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 856 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 948 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 894 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 894 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 886 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 886 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 856 | NAG  | O7-C7-N2-C2 |
| 4   | J     | 789 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 776 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 963 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 856 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 801 | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 4   | G     | 832 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 894 | NAG  | O5-C5-C6-O6 |
| 4   | J     | 776 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 776 | NAG  | C8-C7-N2-C2 |
| 4   | G     | 776 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 948 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 963 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 948 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 789 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 832 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 886 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 789 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 795 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 856 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 734 | NAG  | C8-C7-N2-C2 |
| 4   | J     | 913 | NAG  | C4-C5-C6-O6 |
| 4   | J     | 913 | NAG  | C3-C2-N2-C7 |
| 4   | J     | 789 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 856 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 795 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 734 | NAG  | O7-C7-N2-C2 |
| 4   | G     | 894 | NAG  | C4-C5-C6-O6 |
| 4   | G     | 963 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 789 | NAG  | C3-C2-N2-C7 |
| 4   | J     | 789 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 789 | NAG  | C1-C2-N2-C7 |
| 4   | J     | 789 | NAG  | C1-C2-N2-C7 |
| 4   | J     | 913 | NAG  | O5-C5-C6-O6 |
| 4   | G     | 801 | NAG  | C3-C2-N2-C7 |
| 4   | G     | 856 | NAG  | C3-C2-N2-C7 |

There are no ring outliers.

13 monomers are involved in 19 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | G     | 741 | NAG  | 1       | 0            |
| 4   | G     | 789 | NAG  | 2       | 0            |
| 4   | G     | 762 | NAG  | 1       | 0            |
| 4   | G     | 856 | NAG  | 2       | 0            |
| 4   | J     | 734 | NAG  | 3       | 0            |
| 4   | J     | 886 | NAG  | 1       | 0            |
| 4   | J     | 913 | NAG  | 3       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4   | J     | 789 | NAG  | 1       | 0            |
| 4   | J     | 776 | NAG  | 1       | 0            |
| 4   | G     | 963 | NAG  | 2       | 0            |
| 4   | J     | 856 | NAG  | 1       | 0            |
| 4   | G     | 734 | NAG  | 1       | 0            |
| 4   | J     | 795 | NAG  | 2       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ > 2 |       | OWAB(Å <sup>2</sup> ) | Q < 0.9 |
|-----|-------|-----------------|--------|-----------|-------|-----------------------|---------|
| 1   | G     | 289/321 (90%)   | 0.39   | 17 (5%)   | 28 22 | 55, 106, 187, 231     | 0       |
| 1   | J     | 289/321 (90%)   | 0.45   | 18 (6%)   | 26 21 | 87, 137, 199, 252     | 0       |
| 2   | A     | 215/215 (100%)  | 0.06   | 2 (0%)    | 81 75 | 83, 124, 165, 206     | 0       |
| 2   | L     | 215/215 (100%)  | -0.36  | 1 (0%)    | 87 83 | 48, 78, 105, 164      | 0       |
| 3   | B     | 225/225 (100%)  | 0.21   | 5 (2%)    | 62 53 | 78, 115, 168, 213     | 0       |
| 3   | H     | 225/225 (100%)  | -0.23  | 4 (1%)    | 67 59 | 42, 60, 108, 178      | 0       |
| All | All   | 1458/1522 (95%) | 0.12   | 47 (3%)   | 50 41 | 42, 106, 179, 252     | 0       |

All (47) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 472 | GLY  | 8.3  |
| 1   | J     | 433 | ALA  | 6.5  |
| 1   | J     | 439 | ILE  | 5.2  |
| 1   | G     | 439 | ILE  | 4.6  |
| 3   | H     | 130 | SER  | 4.1  |
| 1   | J     | 90  | THR  | 4.1  |
| 1   | G     | 427 | TRP  | 4.0  |
| 1   | J     | 430 | VAL  | 3.9  |
| 1   | J     | 427 | TRP  | 3.8  |
| 1   | G     | 470 | PRO  | 3.7  |
| 1   | G     | 471 | GLY  | 3.6  |
| 1   | G     | 438 | PRO  | 3.5  |
| 1   | G     | 430 | VAL  | 3.4  |
| 1   | G     | 473 | GLY  | 3.2  |
| 3   | B     | 130 | SER  | 3.2  |
| 1   | J     | 471 | GLY  | 3.1  |
| 1   | J     | 424 | ILE  | 3.1  |
| 1   | G     | 423 | ILE  | 2.9  |
| 1   | J     | 395 | ASP  | 2.9  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | G     | 90  | THR  | 2.8  |
| 1   | G     | 424 | ILE  | 2.8  |
| 1   | J     | 426 | MET  | 2.8  |
| 3   | B     | 10  | GLY  | 2.8  |
| 1   | J     | 472 | GLY  | 2.7  |
| 1   | J     | 473 | GLY  | 2.7  |
| 1   | J     | 436 | ALA  | 2.6  |
| 1   | G     | 426 | MET  | 2.6  |
| 1   | J     | 437 | PRO  | 2.5  |
| 1   | G     | 297 | THR  | 2.5  |
| 1   | G     | 458 | GLY  | 2.4  |
| 1   | G     | 202 | THR  | 2.4  |
| 3   | B     | 9   | PRO  | 2.3  |
| 2   | L     | 214 | CYS  | 2.3  |
| 2   | A     | 110 | VAL  | 2.3  |
| 3   | H     | 131 | THR  | 2.2  |
| 2   | A     | 154 | LEU  | 2.2  |
| 3   | H     | 1   | GLN  | 2.2  |
| 1   | G     | 92  | ASN  | 2.1  |
| 3   | B     | 84  | ALA  | 2.1  |
| 1   | J     | 445 | CYS  | 2.1  |
| 1   | J     | 441 | GLY  | 2.1  |
| 3   | H     | 133 | GLY  | 2.1  |
| 1   | J     | 297 | THR  | 2.1  |
| 3   | B     | 131 | THR  | 2.1  |
| 1   | J     | 434 | MET  | 2.0  |
| 1   | G     | 91  | GLU  | 2.0  |
| 1   | J     | 435 | TYR  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR  | B-factors(Å <sup>2</sup> ) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 4   | NAG  | J     | 913 | 14/15 | 0.08 | 0.16 | 143,144,144,144            | 0     |
| 4   | NAG  | G     | 801 | 14/15 | 0.15 | 0.17 | 159,159,159,159            | 0     |
| 4   | NAG  | J     | 963 | 14/15 | 0.16 | 0.19 | 169,170,170,170            | 0     |
| 4   | NAG  | J     | 801 | 14/15 | 0.22 | 0.14 | 155,155,155,155            | 0     |
| 4   | NAG  | G     | 963 | 14/15 | 0.34 | 0.16 | 168,168,168,168            | 0     |
| 4   | NAG  | J     | 741 | 14/15 | 0.38 | 0.15 | 166,167,167,167            | 0     |
| 4   | NAG  | J     | 856 | 14/15 | 0.44 | 0.15 | 179,180,180,180            | 0     |
| 4   | NAG  | J     | 886 | 14/15 | 0.51 | 0.17 | 42,53,62,65                | 0     |
| 4   | NAG  | G     | 894 | 14/15 | 0.54 | 0.14 | 151,152,152,152            | 0     |
| 4   | NAG  | G     | 856 | 14/15 | 0.58 | 0.14 | 180,180,180,180            | 0     |
| 4   | NAG  | G     | 734 | 14/15 | 0.59 | 0.19 | 164,165,165,165            | 0     |
| 4   | NAG  | J     | 776 | 14/15 | 0.62 | 0.12 | 114,115,115,115            | 0     |
| 4   | NAG  | J     | 789 | 14/15 | 0.69 | 0.11 | 129,130,130,131            | 0     |
| 4   | NAG  | J     | 894 | 14/15 | 0.69 | 0.13 | 144,144,144,144            | 0     |
| 4   | NAG  | J     | 734 | 14/15 | 0.71 | 0.12 | 166,166,166,166            | 0     |
| 4   | NAG  | J     | 795 | 14/15 | 0.71 | 0.12 | 138,139,139,139            | 0     |
| 4   | NAG  | G     | 789 | 14/15 | 0.71 | 0.13 | 130,130,131,131            | 0     |
| 4   | NAG  | G     | 886 | 14/15 | 0.71 | 0.14 | 110,110,111,111            | 0     |
| 4   | NAG  | G     | 741 | 14/15 | 0.73 | 0.12 | 166,166,166,166            | 0     |
| 4   | NAG  | J     | 832 | 14/15 | 0.74 | 0.11 | 142,142,142,142            | 0     |
| 4   | NAG  | J     | 948 | 14/15 | 0.74 | 0.13 | 129,129,130,130            | 0     |
| 4   | NAG  | G     | 776 | 14/15 | 0.74 | 0.10 | 118,118,118,118            | 0     |
| 4   | NAG  | G     | 795 | 14/15 | 0.77 | 0.11 | 134,135,135,135            | 0     |
| 4   | NAG  | G     | 832 | 14/15 | 0.83 | 0.11 | 139,140,140,140            | 0     |
| 4   | NAG  | J     | 762 | 14/15 | 0.92 | 0.09 | 99,99,100,100              | 0     |
| 4   | NAG  | G     | 948 | 14/15 | 0.92 | 0.11 | 124,124,124,124            | 0     |
| 4   | NAG  | G     | 762 | 14/15 | 0.96 | 0.08 | 96,96,97,97                | 0     |

## 6.5 Other polymers ⓘ

There are no such residues in this entry.