



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:45 PM UTC

PDB ID : 2C2L / pdb\_00002c2l  
Title : Crystal structure of the CHIP U-box E3 ubiquitin ligase  
Authors : Zhang, M.; Roe, S.M.; Pearl, L.H.  
Deposited on : 2005-09-29  
Resolution : 3.30 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>.

---

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                                                             |

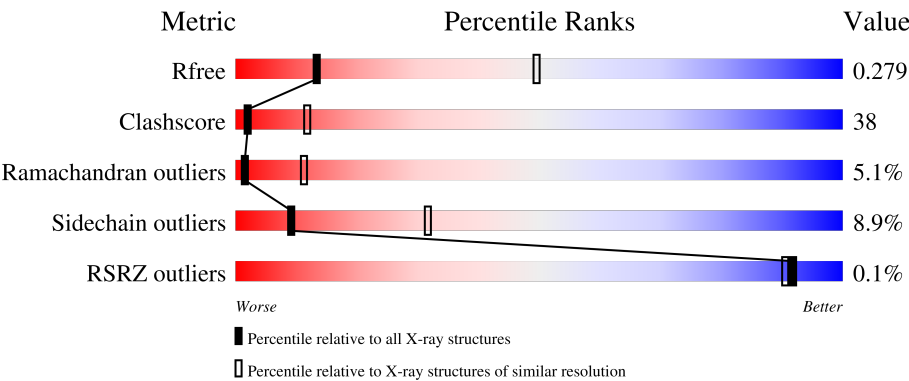
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



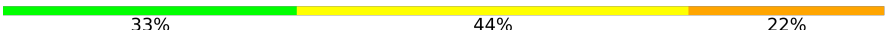
| Metric                | Whole archive<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-------------------------------------------------------|
| R <sub>free</sub>     | 180053                      | 1169 (3.32-3.28)                                      |
| Clashscore            | 190562                      | 1209 (3.32-3.28)                                      |
| Ramachandran outliers | 187476                      | 1188 (3.32-3.28)                                      |
| Sidechain outliers    | 187428                      | 1187 (3.32-3.28)                                      |
| RSRZ outliers         | 180081                      | 1169 (3.32-3.28)                                      |

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     | 281    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>42%50%8%</div>  |
| 1   | B     | 281    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>40%51%9%</div>  |
| 1   | C     | 281    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>42%49%8%</div>  |
| 1   | D     | 281    | <div><div></div><div></div><div></div><div></div><div></div></div> <div>40%49%9%</div>  |
| 2   | E     | 9      | <div><div></div><div></div><div></div><div></div><div></div></div> <div>33%44%22%</div> |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 2   | F     | 9      | <br>33% 44% 22% |
| 2   | G     | 9      | <br>33% 44% 22% |
| 2   | H     | 9      | <br>33% 44% 22% |

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 |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 3   | SO4  | A     | 1307 | -         | -        | X       | -                |

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9521 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 CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1   | A     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2294  | 1424 | 417 | 439 | 14 |         |         |       |
| 1   | B     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2294  | 1424 | 417 | 439 | 14 |         |         |       |
| 1   | C     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2294  | 1424 | 417 | 439 | 14 |         |         |       |
| 1   | D     | 281      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 2294  | 1424 | 417 | 439 | 14 |         |         |       |

- Molecule 2 is a protein called HSP90.

| Mol | Chain | Residues | Atoms |    |    |    |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|----|----|---|---------|---------|-------|
| 2   | E     | 9        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 74    | 41 | 12 | 20 | 1 |         |         |       |
| 2   | F     | 9        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 74    | 41 | 12 | 20 | 1 |         |         |       |
| 2   | G     | 9        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 74    | 41 | 12 | 20 | 1 |         |         |       |
| 2   | H     | 9        | Total | C  | N  | O  | S | 0       | 0       | 0     |
|     |       |          | 74    | 41 | 12 | 20 | 1 |         |         |       |

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



| Mol | Chain | Residues | Atoms |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | A     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | B     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | C     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |
| 3   | D     | 1        | Total | O | S | 0       | 0       |
|     |       |          | 5     | 4 | 1 |         |         |

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

| Mol | Chain | Residues | Atoms |    | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 4   | B     | 4        | Total | Ni | 0       | 0       |
|     |       |          | 4     | 4  |         |         |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 5   | A     | 4        | Total | O | 0       | 0       |
|     |       |          | 4     | 4 |         |         |

*Continued on next page...*

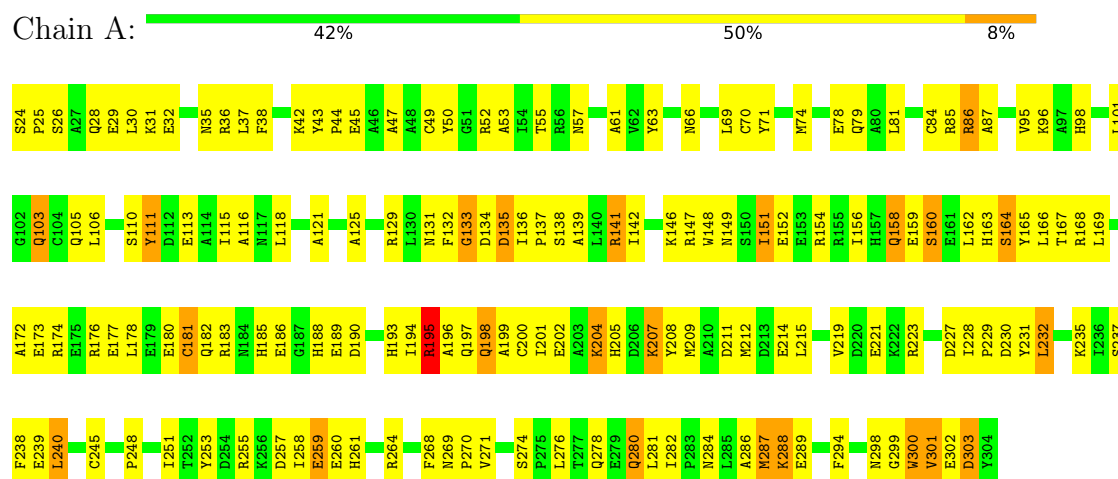
*Continued from previous page...*

| Mol | Chain | Residues | Atoms      |        | ZeroOcc | AltConf |
|-----|-------|----------|------------|--------|---------|---------|
| 5   | C     | 3        | Total<br>3 | O<br>3 | 0       | 0       |
| 5   | D     | 2        | Total<br>2 | O<br>2 | 0       | 0       |
| 5   | G     | 1        | Total<br>1 | O<br>1 | 0       | 0       |

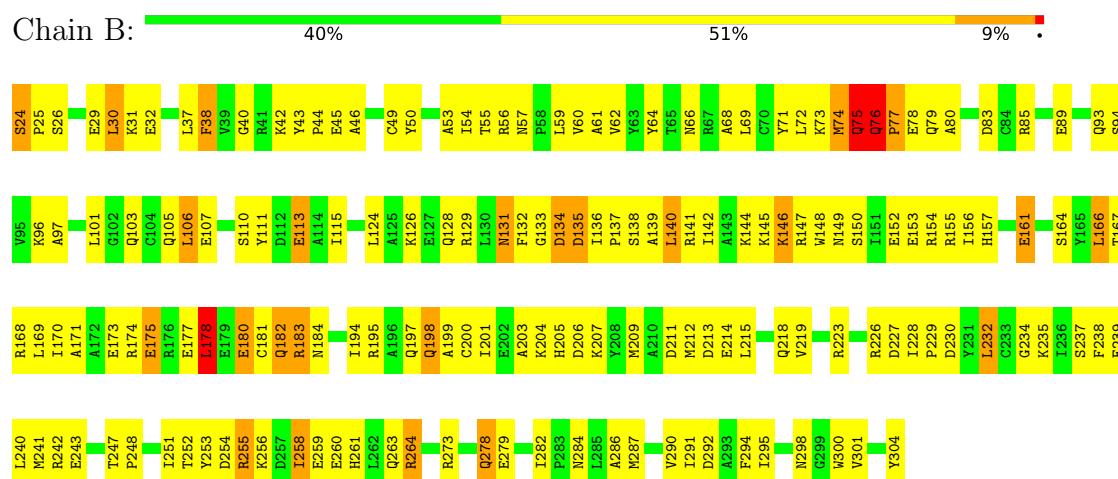
### 3 Residue-property plots

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

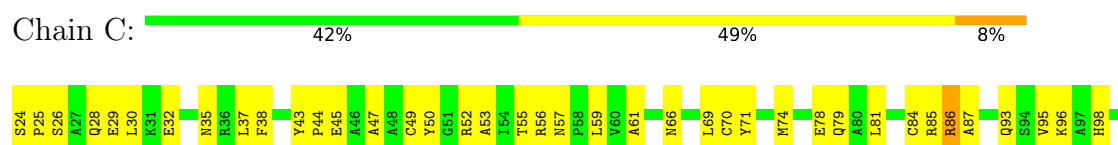
#### • Molecule 1: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN

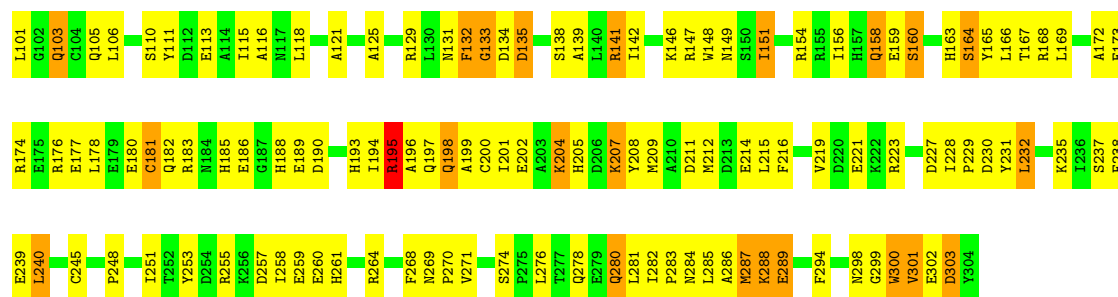


#### • Molecule 1: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN



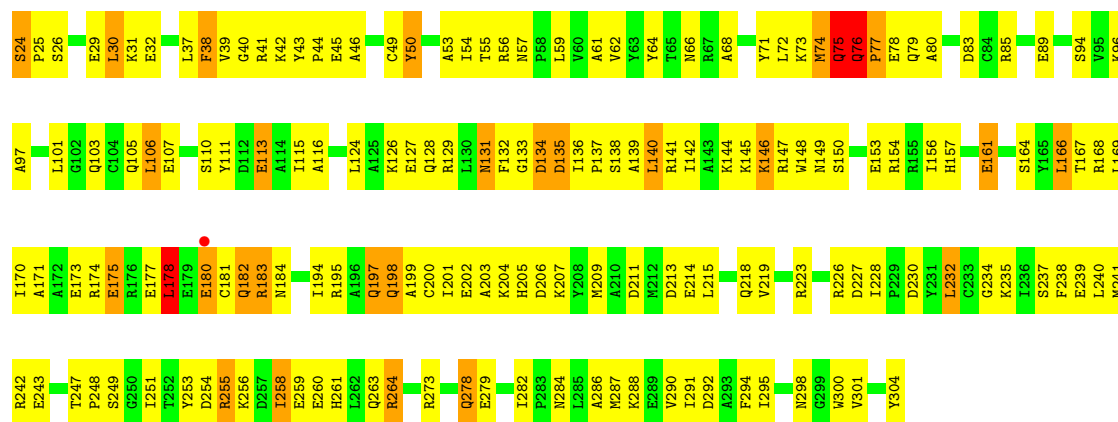
#### • Molecule 1: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN





• Molecule 1: CARBOXY TERMINUS OF HSP70-INTERACTING PROTEIN

Chain D: 40% 49% 9%



• Molecule 2: HSP90

Chain E: 33% 44% 22%



• Molecule 2: HSP90

Chain F: 33% 44% 22%



• Molecule 2: HSP90

Chain G: 33% 44% 22%



• Molecule 2: HSP90

Chain H: 33% 44% 22%

|      |
|------|
| DE01 |
| TS02 |
| RS03 |
| RE04 |
| MS05 |
| ES06 |
| ES07 |
| VS08 |
| DS09 |

## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | C 1 2 1                                                     | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 76.04Å 204.41Å 144.71Å<br>90.00° 90.75° 90.00°              | Depositor        |
| Resolution (Å)                                                          | 40.00 – 3.30<br>40.00 – 3.31                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 21.5 (40.00-3.30)<br>93.9 (40.00-3.31)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | 0.07                                                        | Depositor        |
| $R_{sym}$                                                               | (Not available)                                             | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.33 (at 3.31Å)                                             | Xtriage          |
| Refinement program                                                      | CNS 1.1                                                     | Depositor        |
| R, $R_{free}$                                                           | 0.247 , 0.286<br>0.242 , 0.279                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 1606 reflections (5.03%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 78.0                                                        | Xtriage          |
| Anisotropy                                                              | 0.815                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.30 , 76.1                                                 | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$ | Xtriage          |
| Estimated twinning fraction                                             | 0.327 for h,-k,-l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 9521                                                        | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 80.0                                                        | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: NI, SO4

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     | 0.59         | 0/2337  | 0.96        | 7/3144 (0.2%)   |
| 1   | B     | 0.63         | 0/2337  | 0.96        | 3/3144 (0.1%)   |
| 1   | C     | 0.60         | 0/2337  | 0.96        | 7/3144 (0.2%)   |
| 1   | D     | 0.64         | 0/2337  | 0.96        | 4/3144 (0.1%)   |
| 2   | E     | 0.69         | 0/73    | 0.77        | 0/95            |
| 2   | F     | 0.69         | 0/73    | 0.75        | 0/95            |
| 2   | G     | 0.68         | 0/73    | 0.77        | 0/95            |
| 2   | H     | 0.70         | 0/73    | 0.76        | 0/95            |
| All | All   | 0.62         | 0/9640  | 0.95        | 21/12956 (0.2%) |

There are no bond length outliers.

All (21) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | B     | 106 | LEU  | N-CA-C | -7.05 | 104.75      | 113.15   |
| 1   | D     | 106 | LEU  | N-CA-C | -6.98 | 104.84      | 113.15   |
| 1   | A     | 118 | LEU  | N-CA-C | -6.75 | 103.85      | 111.14   |
| 1   | D     | 139 | ALA  | N-CA-C | -6.54 | 104.16      | 111.28   |
| 1   | B     | 139 | ALA  | N-CA-C | -6.31 | 104.41      | 111.28   |
| 1   | C     | 118 | LEU  | N-CA-C | -5.95 | 104.72      | 111.14   |
| 1   | C     | 195 | ARG  | N-CA-C | -5.94 | 105.52      | 112.89   |
| 1   | A     | 195 | ARG  | N-CA-C | -5.91 | 105.56      | 112.89   |
| 1   | D     | 59  | LEU  | N-CA-C | 5.87  | 120.06      | 113.01   |
| 1   | C     | 86  | ARG  | N-CA-C | -5.75 | 108.06      | 114.62   |
| 1   | A     | 303 | ASP  | N-CA-C | -5.66 | 106.53      | 113.50   |
| 1   | C     | 303 | ASP  | N-CA-C | -5.60 | 106.61      | 113.50   |
| 1   | A     | 61  | ALA  | N-CA-C | 5.60  | 117.38      | 111.28   |
| 1   | A     | 86  | ARG  | N-CA-C | -5.54 | 108.31      | 114.62   |
| 1   | C     | 87  | ALA  | N-CA-C | -5.42 | 105.45      | 111.36   |
| 1   | A     | 87  | ALA  | N-CA-C | -5.31 | 105.58      | 111.36   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | C     | 61  | ALA  | N-CA-C | 5.27  | 117.03      | 111.28   |
| 1   | B     | 59  | LEU  | N-CA-C | 5.25  | 119.32      | 113.01   |
| 1   | C     | 132 | PHE  | N-CA-C | -5.12 | 106.37      | 113.18   |
| 1   | D     | 50  | TYR  | N-CA-C | -5.10 | 105.80      | 111.36   |
| 1   | A     | 259 | GLU  | N-CA-C | -5.02 | 105.27      | 111.40   |

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     | 2294  | 0        | 2234     | 159     | 0            |
| 1   | B     | 2294  | 0        | 2234     | 215     | 0            |
| 1   | C     | 2294  | 0        | 2234     | 163     | 0            |
| 1   | D     | 2294  | 0        | 2234     | 207     | 0            |
| 2   | E     | 74    | 0        | 62       | 9       | 0            |
| 2   | F     | 74    | 0        | 62       | 18      | 0            |
| 2   | G     | 74    | 0        | 62       | 9       | 0            |
| 2   | H     | 74    | 0        | 62       | 16      | 0            |
| 3   | A     | 15    | 0        | 0        | 2       | 0            |
| 3   | B     | 10    | 0        | 0        | 0       | 0            |
| 3   | C     | 5     | 0        | 0        | 0       | 0            |
| 3   | D     | 5     | 0        | 0        | 0       | 0            |
| 4   | B     | 4     | 0        | 0        | 0       | 0            |
| 5   | A     | 4     | 0        | 0        | 0       | 0            |
| 5   | C     | 3     | 0        | 0        | 0       | 0            |
| 5   | D     | 2     | 0        | 0        | 0       | 0            |
| 5   | G     | 1     | 0        | 0        | 0       | 0            |
| All | All   | 9521  | 0        | 9184     | 717     | 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 38.

All (717) 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:74:MET:HG3   | 1:D:75:GLN:H     | 1.12                     | 1.05              |
| 1:B:74:MET:HG3   | 1:B:75:GLN:H     | 1.11                     | 1.05              |
| 1:D:71:TYR:HB3   | 1:D:76:GLN:HB3   | 1.42                     | 1.01              |
| 1:B:71:TYR:HB3   | 1:B:76:GLN:HB3   | 1.43                     | 0.99              |
| 1:C:194:ILE:HA   | 1:C:197:GLN:HB2  | 1.43                     | 0.96              |
| 1:D:138:SER:O    | 1:D:142:ILE:HD12 | 1.66                     | 0.96              |
| 1:A:194:ILE:HA   | 1:A:197:GLN:HB2  | 1.44                     | 0.95              |
| 1:B:138:SER:O    | 1:B:142:ILE:HD12 | 1.67                     | 0.95              |
| 1:A:182:GLN:HE21 | 1:A:198:GLN:HG3  | 1.36                     | 0.91              |
| 1:B:56:ARG:HH22  | 1:C:56:ARG:HH21  | 0.96                     | 0.90              |
| 1:A:151:ILE:HD13 | 1:A:151:ILE:H    | 1.36                     | 0.88              |
| 1:C:182:GLN:HE21 | 1:C:198:GLN:HG3  | 1.39                     | 0.88              |
| 1:B:258:ILE:HD12 | 1:B:259:GLU:H    | 1.37                     | 0.87              |
| 1:B:75:GLN:C     | 1:B:77:PRO:HD2   | 1.98                     | 0.87              |
| 1:A:221:GLU:HB3  | 1:A:223:ARG:HG2  | 1.57                     | 0.87              |
| 1:D:75:GLN:C     | 1:D:77:PRO:HD2   | 1.98                     | 0.86              |
| 1:C:151:ILE:H    | 1:C:151:ILE:HD13 | 1.37                     | 0.86              |
| 1:C:221:GLU:HB3  | 1:C:223:ARG:HG2  | 1.58                     | 0.86              |
| 1:D:258:ILE:HD12 | 1:D:259:GLU:H    | 1.38                     | 0.86              |
| 1:C:160:SER:HB3  | 1:C:163:HIS:HB2  | 1.57                     | 0.84              |
| 1:B:74:MET:HG3   | 1:B:75:GLN:N     | 1.91                     | 0.84              |
| 1:A:160:SER:HB3  | 1:A:163:HIS:HB2  | 1.58                     | 0.83              |
| 1:B:56:ARG:NH2   | 1:C:56:ARG:HH21  | 1.76                     | 0.83              |
| 1:C:164:SER:O    | 1:C:167:THR:HG22 | 1.79                     | 0.82              |
| 1:D:74:MET:HG3   | 1:D:75:GLN:N     | 1.92                     | 0.82              |
| 1:A:164:SER:O    | 1:A:167:THR:HG22 | 1.79                     | 0.82              |
| 1:D:26:SER:HA    | 1:D:56:ARG:HH12  | 1.45                     | 0.81              |
| 1:D:96:LYS:HG3   | 2:H:505:MET:HE2  | 1.62                     | 0.81              |
| 1:B:26:SER:HA    | 1:B:56:ARG:HH12  | 1.45                     | 0.81              |
| 1:B:131:ASN:HD22 | 1:B:131:ASN:H    | 1.28                     | 0.81              |
| 1:A:301:VAL:C    | 1:A:303:ASP:H    | 1.88                     | 0.81              |
| 1:C:301:VAL:C    | 1:C:303:ASP:H    | 1.87                     | 0.81              |
| 1:B:258:ILE:HD12 | 1:B:259:GLU:N    | 1.96                     | 0.80              |
| 1:D:258:ILE:HD12 | 1:D:259:GLU:N    | 1.96                     | 0.80              |
| 1:B:96:LYS:HG3   | 2:F:505:MET:HE2  | 1.64                     | 0.80              |
| 1:D:37:LEU:HB2   | 1:D:46:ALA:HB2   | 1.63                     | 0.79              |
| 1:D:71:TYR:HB3   | 1:D:76:GLN:CB    | 2.12                     | 0.79              |
| 1:D:131:ASN:H    | 1:D:131:ASN:HD22 | 1.29                     | 0.79              |
| 1:B:71:TYR:HB3   | 1:B:76:GLN:CB    | 2.12                     | 0.79              |
| 1:B:174:ARG:HG2  | 1:B:175:GLU:OE1  | 1.82                     | 0.78              |
| 1:D:174:ARG:HG2  | 1:D:175:GLU:OE1  | 1.82                     | 0.78              |
| 1:B:37:LEU:HB2   | 1:B:46:ALA:HB2   | 1.64                     | 0.78              |

Continued on next page...

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:181:CYS:HA   | 1:B:184:ASN:HD22 | 1.49                     | 0.78              |
| 1:D:181:CYS:HA   | 1:D:184:ASN:HD22 | 1.49                     | 0.78              |
| 1:D:66:ASN:CG    | 2:H:508:VAL:HG13 | 2.09                     | 0.78              |
| 1:D:149:ASN:O    | 1:D:153:GLU:HG3  | 1.84                     | 0.77              |
| 1:C:248:PRO:HA   | 1:D:282:ILE:HD13 | 1.66                     | 0.77              |
| 1:B:149:ASN:O    | 1:B:153:GLU:HG3  | 1.85                     | 0.77              |
| 1:B:93:GLN:HE21  | 1:C:93:GLN:HG3   | 1.50                     | 0.77              |
| 1:D:43:TYR:N     | 1:D:44:PRO:HD2   | 1.99                     | 0.77              |
| 1:B:43:TYR:N     | 1:B:44:PRO:HD2   | 1.99                     | 0.76              |
| 1:C:255:ARG:O    | 1:C:259:GLU:HB2  | 1.86                     | 0.76              |
| 1:A:287:MET:HE2  | 1:B:286:ALA:HB1  | 1.67                     | 0.75              |
| 1:A:284:ASN:HD21 | 1:B:284:ASN:HD21 | 1.32                     | 0.74              |
| 1:A:255:ARG:O    | 1:A:259:GLU:HB2  | 1.88                     | 0.74              |
| 1:C:66:ASN:CG    | 2:G:508:VAL:HG13 | 2.13                     | 0.73              |
| 1:C:287:MET:HE2  | 1:D:286:ALA:HB1  | 1.69                     | 0.73              |
| 1:B:72:LEU:HD23  | 1:B:76:GLN:HG2   | 1.71                     | 0.73              |
| 1:A:66:ASN:CG    | 2:E:508:VAL:HG13 | 2.13                     | 0.73              |
| 1:B:241:MET:HE1  | 1:B:253:TYR:C    | 2.14                     | 0.73              |
| 1:B:76:GLN:N     | 1:B:77:PRO:HD2   | 2.04                     | 0.73              |
| 1:D:241:MET:HE1  | 1:D:253:TYR:C    | 2.14                     | 0.73              |
| 1:B:56:ARG:HH22  | 1:C:56:ARG:NH2   | 1.80                     | 0.72              |
| 1:C:78:GLU:HB2   | 1:C:79:GLN:NE2   | 2.04                     | 0.72              |
| 1:D:72:LEU:HD23  | 1:D:76:GLN:HG2   | 1.71                     | 0.72              |
| 1:D:76:GLN:N     | 1:D:77:PRO:HD2   | 2.05                     | 0.72              |
| 1:A:78:GLU:HB2   | 1:A:79:GLN:NE2   | 2.05                     | 0.71              |
| 1:A:182:GLN:NE2  | 1:A:198:GLN:HG3  | 2.04                     | 0.71              |
| 1:B:194:ILE:HA   | 1:B:197:GLN:HB3  | 1.73                     | 0.70              |
| 1:A:248:PRO:HA   | 1:B:282:ILE:HD13 | 1.73                     | 0.70              |
| 1:D:194:ILE:HA   | 1:D:197:GLN:HB3  | 1.74                     | 0.70              |
| 1:D:194:ILE:O    | 1:D:198:GLN:HB2  | 1.91                     | 0.69              |
| 1:B:66:ASN:CG    | 2:F:508:VAL:HG13 | 2.18                     | 0.69              |
| 1:C:284:ASN:HD21 | 1:D:284:ASN:HD21 | 1.38                     | 0.68              |
| 1:D:50:TYR:OH    | 2:H:508:VAL:HG11 | 1.92                     | 0.68              |
| 1:B:182:GLN:HG3  | 1:B:198:GLN:NE2  | 2.09                     | 0.68              |
| 1:A:284:ASN:HD21 | 1:B:284:ASN:ND2  | 1.92                     | 0.68              |
| 1:B:110:SER:HB3  | 1:B:113:GLU:OE1  | 1.94                     | 0.68              |
| 1:B:194:ILE:O    | 1:B:198:GLN:HB2  | 1.92                     | 0.68              |
| 1:D:37:LEU:CB    | 1:D:46:ALA:HB2   | 2.24                     | 0.68              |
| 1:C:182:GLN:NE2  | 1:C:198:GLN:HG3  | 2.08                     | 0.68              |
| 1:C:212:MET:O    | 1:C:215:LEU:HB2  | 1.93                     | 0.68              |
| 1:B:264:ARG:O    | 1:B:264:ARG:HD3  | 1.94                     | 0.68              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:134:ASP:O    | 1:A:138:SER:HB3  | 1.94                     | 0.67              |
| 1:C:134:ASP:O    | 1:C:138:SER:HB3  | 1.94                     | 0.67              |
| 1:D:110:SER:HB3  | 1:D:113:GLU:OE1  | 1.94                     | 0.67              |
| 1:B:103:GLN:OE1  | 1:B:103:GLN:HA   | 1.93                     | 0.67              |
| 1:B:37:LEU:CB    | 1:B:46:ALA:HB2   | 2.25                     | 0.67              |
| 1:B:94:SER:HB3   | 1:B:97:ALA:HB3   | 1.76                     | 0.67              |
| 1:C:251:ILE:HD12 | 1:C:251:ILE:N    | 2.09                     | 0.67              |
| 1:D:145:LYS:HD3  | 1:D:304:TYR:CD2  | 2.29                     | 0.67              |
| 1:A:284:ASN:ND2  | 1:B:284:ASN:HD21 | 1.91                     | 0.67              |
| 1:B:145:LYS:HD3  | 1:B:304:TYR:CD2  | 2.30                     | 0.67              |
| 1:D:264:ARG:O    | 1:D:264:ARG:HD3  | 1.94                     | 0.67              |
| 1:A:212:MET:O    | 1:A:215:LEU:HB2  | 1.95                     | 0.67              |
| 1:D:94:SER:HB3   | 1:D:97:ALA:HB3   | 1.77                     | 0.66              |
| 1:A:251:ILE:N    | 1:A:251:ILE:HD12 | 2.10                     | 0.66              |
| 1:B:255:ARG:O    | 1:B:259:GLU:HB2  | 1.95                     | 0.66              |
| 1:D:182:GLN:HG3  | 1:D:198:GLN:NE2  | 2.11                     | 0.66              |
| 1:C:103:GLN:O    | 1:C:106:LEU:HB2  | 1.97                     | 0.65              |
| 1:D:103:GLN:OE1  | 1:D:103:GLN:HA   | 1.95                     | 0.65              |
| 1:A:103:GLN:O    | 1:A:106:LEU:HB2  | 1.97                     | 0.65              |
| 1:A:182:GLN:HG2  | 1:A:198:GLN:HE21 | 1.61                     | 0.65              |
| 1:D:255:ARG:O    | 1:D:259:GLU:HB2  | 1.96                     | 0.65              |
| 1:B:182:GLN:HG3  | 1:B:198:GLN:HE22 | 1.59                     | 0.64              |
| 1:B:50:TYR:OH    | 2:F:508:VAL:HG11 | 1.97                     | 0.64              |
| 2:F:508:VAL:HG12 | 2:F:508:VAL:O    | 1.97                     | 0.64              |
| 2:H:508:VAL:HG12 | 2:H:508:VAL:O    | 1.97                     | 0.64              |
| 2:E:508:VAL:HG12 | 2:E:508:VAL:O    | 1.96                     | 0.64              |
| 1:C:182:GLN:HG2  | 1:C:198:GLN:HE21 | 1.62                     | 0.63              |
| 2:G:508:VAL:HG12 | 2:G:508:VAL:O    | 1.96                     | 0.63              |
| 1:B:154:ARG:O    | 1:B:154:ARG:HD3  | 1.99                     | 0.63              |
| 1:A:148:TRP:HA   | 1:A:151:ILE:HD11 | 1.80                     | 0.63              |
| 1:B:284:ASN:OD1  | 1:B:287:MET:HB2  | 1.98                     | 0.63              |
| 1:A:201:ILE:HD12 | 1:A:204:LYS:HB3  | 1.80                     | 0.63              |
| 1:C:183:ARG:HG3  | 1:C:186:GLU:HG3  | 1.81                     | 0.63              |
| 1:D:154:ARG:O    | 1:D:154:ARG:HD3  | 1.99                     | 0.63              |
| 1:A:78:GLU:HB2   | 1:A:79:GLN:HE21  | 1.62                     | 0.63              |
| 1:C:78:GLU:HB2   | 1:C:79:GLN:HE21  | 1.62                     | 0.63              |
| 1:D:57:ASN:C     | 1:D:57:ASN:HD22  | 2.07                     | 0.62              |
| 1:A:183:ARG:HG3  | 1:A:186:GLU:HG3  | 1.81                     | 0.62              |
| 1:B:57:ASN:C     | 1:B:57:ASN:HD22  | 2.07                     | 0.62              |
| 1:D:131:ASN:HB2  | 2:H:502:THR:HG23 | 1.81                     | 0.62              |
| 1:A:85:ARG:HG3   | 1:A:85:ARG:HH11  | 1.64                     | 0.62              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:131:ASN:HD22 | 1:B:131:ASN:N    | 1.95                     | 0.62              |
| 1:C:284:ASN:ND2  | 1:D:284:ASN:HD21 | 1.96                     | 0.62              |
| 1:D:182:GLN:HG3  | 1:D:198:GLN:HE22 | 1.62                     | 0.62              |
| 1:C:148:TRP:HA   | 1:C:151:ILE:HD11 | 1.82                     | 0.62              |
| 1:D:85:ARG:HG3   | 1:D:85:ARG:HH11  | 1.64                     | 0.62              |
| 1:D:284:ASN:OD1  | 1:D:287:MET:HB2  | 2.00                     | 0.61              |
| 1:C:85:ARG:HG3   | 1:C:85:ARG:HH11  | 1.65                     | 0.61              |
| 1:C:185:HIS:HB3  | 1:C:188:HIS:HB2  | 1.82                     | 0.61              |
| 1:A:185:HIS:HB3  | 1:A:188:HIS:HB2  | 1.82                     | 0.61              |
| 1:A:189:GLU:HG2  | 1:A:193:HIS:ND1  | 2.16                     | 0.61              |
| 1:C:156:ILE:N    | 1:C:156:ILE:HD12 | 2.16                     | 0.61              |
| 1:D:131:ASN:CG   | 2:H:502:THR:HG23 | 2.26                     | 0.61              |
| 1:A:166:LEU:HD23 | 1:A:169:LEU:HD12 | 1.83                     | 0.61              |
| 1:B:85:ARG:HG3   | 1:B:85:ARG:HH11  | 1.65                     | 0.61              |
| 1:A:156:ILE:HD12 | 1:A:156:ILE:N    | 2.16                     | 0.60              |
| 1:B:291:ILE:O    | 1:B:295:ILE:HD12 | 2.00                     | 0.60              |
| 1:C:151:ILE:HD13 | 1:C:151:ILE:N    | 2.15                     | 0.60              |
| 1:C:201:ILE:HD12 | 1:C:204:LYS:HB3  | 1.83                     | 0.60              |
| 1:C:111:TYR:O    | 1:C:115:ILE:HG23 | 2.01                     | 0.60              |
| 1:C:142:ILE:O    | 1:C:146:LYS:HG3  | 2.02                     | 0.60              |
| 1:C:189:GLU:HG2  | 1:C:193:HIS:ND1  | 2.17                     | 0.60              |
| 1:B:71:TYR:CE2   | 1:B:79:GLN:HB3   | 2.37                     | 0.60              |
| 1:B:111:TYR:HE2  | 1:B:146:LYS:HB3  | 1.67                     | 0.60              |
| 1:D:71:TYR:CE2   | 1:D:79:GLN:HB3   | 2.37                     | 0.60              |
| 1:A:164:SER:C    | 1:A:167:THR:HG22 | 2.26                     | 0.60              |
| 1:C:166:LEU:HD23 | 1:C:169:LEU:HD12 | 1.84                     | 0.59              |
| 1:D:74:MET:CG    | 1:D:75:GLN:H     | 1.99                     | 0.59              |
| 1:C:131:ASN:ND2  | 2:G:502:THR:HG23 | 2.17                     | 0.59              |
| 1:C:164:SER:C    | 1:C:167:THR:HG22 | 2.27                     | 0.59              |
| 1:C:228:ILE:HD12 | 1:C:229:PRO:O    | 2.02                     | 0.59              |
| 1:C:284:ASN:HD21 | 1:D:284:ASN:ND2  | 2.00                     | 0.59              |
| 1:D:111:TYR:HE2  | 1:D:146:LYS:HB3  | 1.68                     | 0.59              |
| 1:A:142:ILE:O    | 1:A:146:LYS:HG3  | 2.03                     | 0.59              |
| 1:B:74:MET:CG    | 1:B:75:GLN:H     | 1.98                     | 0.59              |
| 1:A:165:TYR:O    | 1:A:168:ARG:HG2  | 2.02                     | 0.59              |
| 1:C:132:PHE:CZ   | 2:G:505:MET:HE3  | 2.37                     | 0.59              |
| 1:C:286:ALA:HB3  | 1:D:287:MET:HE3  | 1.84                     | 0.59              |
| 1:D:164:SER:O    | 1:D:167:THR:HG22 | 2.03                     | 0.59              |
| 1:A:228:ILE:HD12 | 1:A:229:PRO:O    | 2.02                     | 0.59              |
| 2:H:505:MET:C    | 2:H:507:GLU:H    | 2.11                     | 0.59              |
| 1:B:182:GLN:HE21 | 1:B:198:GLN:NE2  | 2.01                     | 0.58              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:E:505:MET:C    | 2:E:507:GLU:H    | 2.11                     | 0.58              |
| 1:D:42:LYS:C     | 1:D:44:PRO:HD2   | 2.28                     | 0.58              |
| 1:B:145:LYS:CE   | 1:B:304:TYR:HB3  | 2.33                     | 0.58              |
| 1:B:42:LYS:C     | 1:B:44:PRO:HD2   | 2.28                     | 0.58              |
| 1:B:54:ILE:HD13  | 1:B:64:TYR:CE1   | 2.38                     | 0.58              |
| 1:A:111:TYR:O    | 1:A:115:ILE:HG23 | 2.03                     | 0.58              |
| 1:B:26:SER:HB3   | 1:B:29:GLU:CD    | 2.28                     | 0.58              |
| 1:B:134:ASP:HA   | 1:B:137:PRO:HG2  | 1.86                     | 0.58              |
| 1:A:212:MET:HA   | 1:A:215:LEU:HD12 | 1.85                     | 0.58              |
| 1:B:164:SER:O    | 1:B:167:THR:HG22 | 2.04                     | 0.58              |
| 1:C:154:ARG:HH11 | 1:C:154:ARG:HG2  | 1.69                     | 0.58              |
| 1:C:212:MET:HA   | 1:C:215:LEU:HD12 | 1.85                     | 0.58              |
| 1:D:29:GLU:C     | 1:D:31:LYS:H     | 2.12                     | 0.58              |
| 1:D:211:ASP:O    | 1:D:214:GLU:HB3  | 2.03                     | 0.58              |
| 1:D:134:ASP:HA   | 1:D:137:PRO:HG2  | 1.86                     | 0.58              |
| 1:B:72:LEU:HA    | 1:B:76:GLN:HG3   | 1.85                     | 0.57              |
| 1:D:145:LYS:HD3  | 1:D:304:TYR:HD2  | 1.67                     | 0.57              |
| 2:G:505:MET:C    | 2:G:507:GLU:H    | 2.12                     | 0.57              |
| 1:B:132:PHE:HB3  | 1:B:135:ASP:HB2  | 1.86                     | 0.57              |
| 2:F:505:MET:C    | 2:F:507:GLU:H    | 2.12                     | 0.57              |
| 1:B:241:MET:HE1  | 1:B:254:ASP:N    | 2.19                     | 0.57              |
| 1:D:145:LYS:CE   | 1:D:304:TYR:HB3  | 2.34                     | 0.57              |
| 1:D:234:GLY:CA   | 1:D:241:MET:HE3  | 2.35                     | 0.57              |
| 1:C:98:HIS:HB3   | 1:C:121:ALA:HB2  | 1.87                     | 0.57              |
| 1:D:54:ILE:HD13  | 1:D:64:TYR:CE1   | 2.39                     | 0.57              |
| 1:C:165:TYR:O    | 1:C:168:ARG:HG2  | 2.04                     | 0.57              |
| 1:D:96:LYS:HG3   | 2:H:505:MET:CE   | 2.33                     | 0.57              |
| 1:A:154:ARG:HG2  | 1:A:154:ARG:HH11 | 1.70                     | 0.57              |
| 1:B:237:SER:O    | 1:B:238:PHE:HB2  | 2.04                     | 0.57              |
| 1:C:160:SER:HB3  | 1:C:163:HIS:CB   | 2.33                     | 0.57              |
| 1:C:174:ARG:HH21 | 1:C:205:HIS:CB   | 2.17                     | 0.57              |
| 1:A:160:SER:HB3  | 1:A:163:HIS:CB   | 2.33                     | 0.57              |
| 1:B:145:LYS:HD3  | 1:B:304:TYR:HD2  | 1.68                     | 0.57              |
| 1:B:211:ASP:O    | 1:B:214:GLU:HB3  | 2.04                     | 0.57              |
| 1:A:174:ARG:HH21 | 1:A:205:HIS:CB   | 2.18                     | 0.57              |
| 1:B:140:LEU:O    | 1:B:144:LYS:HG2  | 2.05                     | 0.57              |
| 1:D:140:LEU:O    | 1:D:144:LYS:HG2  | 2.05                     | 0.57              |
| 1:D:291:ILE:O    | 1:D:295:ILE:HD12 | 2.04                     | 0.57              |
| 1:A:98:HIS:HB3   | 1:A:121:ALA:HB2  | 1.87                     | 0.56              |
| 1:A:189:GLU:HG2  | 1:A:193:HIS:CE1  | 2.41                     | 0.56              |
| 1:B:241:MET:HE1  | 1:B:253:TYR:HA   | 1.86                     | 0.56              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:241:MET:HE1  | 1:D:253:TYR:CA   | 2.34                     | 0.56              |
| 1:A:196:ALA:O    | 1:A:200:CYS:HB2  | 2.05                     | 0.56              |
| 1:B:241:MET:HE1  | 1:B:253:TYR:CA   | 2.35                     | 0.56              |
| 1:C:299:GLY:O    | 1:C:300:TRP:O    | 2.23                     | 0.56              |
| 1:D:72:LEU:HA    | 1:D:76:GLN:HG3   | 1.86                     | 0.56              |
| 1:D:241:MET:HE1  | 1:D:253:TYR:HA   | 1.86                     | 0.56              |
| 1:A:132:PHE:CZ   | 2:E:505:MET:HE3  | 2.41                     | 0.56              |
| 1:C:28:GLN:O     | 1:C:32:GLU:HG3   | 2.04                     | 0.56              |
| 1:A:28:GLN:O     | 1:A:32:GLU:HG3   | 2.04                     | 0.56              |
| 1:A:151:ILE:H    | 1:A:151:ILE:CD1  | 2.12                     | 0.56              |
| 1:C:139:ALA:HA   | 1:C:142:ILE:HD12 | 1.88                     | 0.56              |
| 1:D:29:GLU:O     | 1:D:31:LYS:N     | 2.39                     | 0.56              |
| 1:D:132:PHE:HB3  | 1:D:135:ASP:HB2  | 1.87                     | 0.56              |
| 1:B:85:ARG:O     | 1:B:89:GLU:HG3   | 2.05                     | 0.56              |
| 1:A:139:ALA:HA   | 1:A:142:ILE:HD12 | 1.88                     | 0.56              |
| 1:D:66:ASN:OD1   | 2:H:508:VAL:HG13 | 2.06                     | 0.56              |
| 1:B:180:GLU:HG3  | 1:B:181:CYS:N    | 2.21                     | 0.56              |
| 1:D:180:GLU:HG3  | 1:D:181:CYS:N    | 2.21                     | 0.56              |
| 1:A:230:ASP:C    | 1:A:232:LEU:H    | 2.13                     | 0.55              |
| 1:B:29:GLU:C     | 1:B:31:LYS:H     | 2.14                     | 0.55              |
| 1:D:237:SER:O    | 1:D:238:PHE:HB2  | 2.05                     | 0.55              |
| 1:A:282:ILE:HD12 | 1:B:282:ILE:HD12 | 1.88                     | 0.55              |
| 1:B:298:ASN:O    | 1:B:301:VAL:HG23 | 2.06                     | 0.55              |
| 1:D:85:ARG:O     | 1:D:89:GLU:HG3   | 2.06                     | 0.55              |
| 1:D:241:MET:HE1  | 1:D:254:ASP:N    | 2.21                     | 0.55              |
| 1:A:131:ASN:ND2  | 2:E:502:THR:HG23 | 2.20                     | 0.55              |
| 1:A:174:ARG:HH21 | 1:A:205:HIS:HB2  | 1.71                     | 0.55              |
| 1:A:294:PHE:O    | 1:A:298:ASN:ND2  | 2.39                     | 0.55              |
| 1:A:36:ARG:HD2   | 3:A:1307:SO4:O1  | 2.06                     | 0.55              |
| 1:D:43:TYR:N     | 1:D:44:PRO:CD    | 2.67                     | 0.55              |
| 1:B:60:VAL:HG22  | 1:C:59:LEU:O     | 2.07                     | 0.55              |
| 1:B:96:LYS:HG3   | 2:F:505:MET:CE   | 2.35                     | 0.55              |
| 1:C:255:ARG:HA   | 1:C:258:ILE:HD11 | 1.89                     | 0.55              |
| 1:D:201:ILE:HD12 | 1:D:204:LYS:HZ2  | 1.72                     | 0.55              |
| 1:B:43:TYR:N     | 1:B:44:PRO:CD    | 2.67                     | 0.55              |
| 1:C:294:PHE:O    | 1:C:298:ASN:ND2  | 2.39                     | 0.55              |
| 1:A:255:ARG:HA   | 1:A:258:ILE:HD11 | 1.89                     | 0.55              |
| 1:C:189:GLU:HG2  | 1:C:193:HIS:CE1  | 2.42                     | 0.55              |
| 1:C:174:ARG:HH21 | 1:C:205:HIS:HB2  | 1.72                     | 0.55              |
| 1:D:26:SER:HB3   | 1:D:29:GLU:CD    | 2.32                     | 0.55              |
| 1:A:42:LYS:HE2   | 1:C:283:PRO:CD   | 2.37                     | 0.54              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:176:ARG:HH12 | 1:B:173:GLU:HG2  | 1.72                     | 0.54              |
| 1:C:44:PRO:HB3   | 1:C:74:MET:HE3   | 1.89                     | 0.54              |
| 1:C:301:VAL:O    | 1:C:302:GLU:HB3  | 2.06                     | 0.54              |
| 1:D:76:GLN:O     | 1:D:77:PRO:C     | 2.49                     | 0.54              |
| 1:A:219:VAL:O    | 1:A:219:VAL:HG13 | 2.07                     | 0.54              |
| 1:A:301:VAL:O    | 1:A:302:GLU:HB3  | 2.06                     | 0.54              |
| 1:B:131:ASN:HB2  | 2:F:502:THR:HG23 | 1.89                     | 0.54              |
| 1:D:29:GLU:C     | 1:D:31:LYS:N     | 2.65                     | 0.54              |
| 1:D:76:GLN:H     | 1:D:76:GLN:CD    | 2.10                     | 0.54              |
| 1:D:182:GLN:HE21 | 1:D:198:GLN:NE2  | 2.06                     | 0.54              |
| 1:C:196:ALA:O    | 1:C:200:CYS:HB2  | 2.08                     | 0.54              |
| 1:D:131:ASN:CB   | 2:H:502:THR:HG23 | 2.37                     | 0.54              |
| 1:A:151:ILE:HD13 | 1:A:151:ILE:N    | 2.14                     | 0.54              |
| 1:B:76:GLN:O     | 1:B:77:PRO:C     | 2.50                     | 0.54              |
| 1:C:230:ASP:C    | 1:C:232:LEU:H    | 2.15                     | 0.54              |
| 1:B:234:GLY:CA   | 1:B:241:MET:HE3  | 2.38                     | 0.54              |
| 1:C:219:VAL:HG22 | 1:C:219:VAL:O    | 2.07                     | 0.54              |
| 1:B:69:LEU:HD23  | 2:F:508:VAL:CG2  | 2.37                     | 0.54              |
| 1:B:93:GLN:NE2   | 1:C:93:GLN:HG3   | 2.21                     | 0.54              |
| 1:B:181:CYS:O    | 1:B:184:ASN:HB2  | 2.07                     | 0.54              |
| 1:D:298:ASN:O    | 1:D:301:VAL:HG23 | 2.07                     | 0.54              |
| 1:C:151:ILE:H    | 1:C:151:ILE:CD1  | 2.13                     | 0.54              |
| 1:A:189:GLU:HB3  | 1:A:194:ILE:HG23 | 1.89                     | 0.54              |
| 1:A:24:SER:N     | 1:A:25:PRO:HD2   | 2.23                     | 0.54              |
| 1:B:111:TYR:CE2  | 1:B:146:LYS:HB3  | 2.43                     | 0.54              |
| 1:D:181:CYS:O    | 1:D:184:ASN:HB2  | 2.08                     | 0.54              |
| 1:A:44:PRO:HB3   | 1:A:74:MET:HE3   | 1.89                     | 0.54              |
| 1:B:76:GLN:CD    | 1:B:76:GLN:H     | 2.11                     | 0.54              |
| 1:B:204:LYS:HZ3  | 1:B:205:HIS:CE1  | 2.26                     | 0.54              |
| 1:D:68:ALA:HB2   | 1:D:83:ASP:HB3   | 1.90                     | 0.54              |
| 1:B:273:ARG:HG2  | 1:B:273:ARG:HH11 | 1.73                     | 0.53              |
| 1:C:25:PRO:CG    | 1:C:30:LEU:HD21  | 2.38                     | 0.53              |
| 1:B:136:ILE:N    | 1:B:137:PRO:HD2  | 2.23                     | 0.53              |
| 1:C:219:VAL:O    | 1:C:219:VAL:HG13 | 2.09                     | 0.53              |
| 1:A:299:GLY:O    | 1:A:300:TRP:O    | 2.26                     | 0.53              |
| 1:C:212:MET:O    | 1:C:215:LEU:N    | 2.38                     | 0.53              |
| 1:A:25:PRO:CG    | 1:A:30:LEU:HD21  | 2.38                     | 0.53              |
| 1:A:84:CYS:C     | 1:A:86:ARG:H     | 2.17                     | 0.53              |
| 1:D:111:TYR:CE2  | 1:D:146:LYS:HB3  | 2.44                     | 0.53              |
| 1:C:24:SER:N     | 1:C:25:PRO:HD2   | 2.24                     | 0.53              |
| 1:C:301:VAL:C    | 1:C:303:ASP:N    | 2.56                     | 0.53              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:68:ALA:HB2   | 1:B:83:ASP:HB3   | 1.91                     | 0.53              |
| 1:A:176:ARG:NH1  | 1:B:173:GLU:HG2  | 2.24                     | 0.52              |
| 1:C:84:CYS:C     | 1:C:86:ARG:H     | 2.17                     | 0.52              |
| 1:B:24:SER:HB2   | 1:B:25:PRO:HD3   | 1.90                     | 0.52              |
| 1:B:29:GLU:O     | 1:B:31:LYS:N     | 2.42                     | 0.52              |
| 1:B:178:LEU:O    | 1:B:182:GLN:HB3  | 2.09                     | 0.52              |
| 1:C:167:THR:HG23 | 1:C:168:ARG:N    | 2.25                     | 0.52              |
| 1:D:136:ILE:N    | 1:D:137:PRO:HD2  | 2.24                     | 0.52              |
| 1:D:178:LEU:O    | 1:D:182:GLN:HB3  | 2.10                     | 0.52              |
| 1:B:29:GLU:C     | 1:B:31:LYS:N     | 2.68                     | 0.52              |
| 1:B:72:LEU:HD23  | 1:B:76:GLN:CG    | 2.40                     | 0.52              |
| 1:C:282:ILE:HD12 | 1:D:282:ILE:HD12 | 1.92                     | 0.52              |
| 1:A:286:ALA:HB3  | 1:B:287:MET:HE3  | 1.92                     | 0.52              |
| 1:A:212:MET:O    | 1:A:215:LEU:N    | 2.40                     | 0.52              |
| 1:A:284:ASN:ND2  | 1:B:284:ASN:ND2  | 2.55                     | 0.52              |
| 1:A:301:VAL:C    | 1:A:303:ASP:N    | 2.57                     | 0.52              |
| 1:B:201:ILE:O    | 1:B:201:ILE:HG23 | 2.10                     | 0.52              |
| 1:A:167:THR:HG23 | 1:A:168:ARG:N    | 2.25                     | 0.52              |
| 1:A:180:GLU:O    | 1:A:181:CYS:HB2  | 2.09                     | 0.52              |
| 1:B:66:ASN:OD1   | 2:F:508:VAL:HG13 | 2.10                     | 0.51              |
| 1:D:101:LEU:O    | 1:D:101:LEU:HD23 | 2.10                     | 0.51              |
| 1:D:105:GLN:C    | 1:D:107:GLU:H    | 2.17                     | 0.51              |
| 1:C:133:GLY:O    | 1:C:135:ASP:N    | 2.36                     | 0.51              |
| 1:C:286:ALA:CB   | 1:D:287:MET:HE3  | 2.40                     | 0.51              |
| 1:A:219:VAL:O    | 1:A:219:VAL:HG22 | 2.10                     | 0.51              |
| 1:B:105:GLN:C    | 1:B:107:GLU:H    | 2.18                     | 0.51              |
| 1:D:201:ILE:O    | 1:D:201:ILE:HG23 | 2.10                     | 0.51              |
| 1:B:251:ILE:N    | 1:B:251:ILE:HD12 | 2.25                     | 0.51              |
| 1:C:189:GLU:HB3  | 1:C:194:ILE:HG23 | 1.92                     | 0.51              |
| 1:B:93:GLN:HG3   | 1:C:93:GLN:HE21  | 1.76                     | 0.51              |
| 1:A:133:GLY:O    | 1:A:135:ASP:N    | 2.35                     | 0.51              |
| 1:B:76:GLN:N     | 1:B:77:PRO:CD    | 2.73                     | 0.51              |
| 1:C:101:LEU:HG   | 1:C:105:GLN:NE2  | 2.25                     | 0.51              |
| 1:A:257:ASP:C    | 1:A:259:GLU:H    | 2.19                     | 0.51              |
| 1:D:76:GLN:N     | 1:D:77:PRO:CD    | 2.73                     | 0.51              |
| 1:A:207:LYS:HB2  | 1:A:207:LYS:NZ   | 2.26                     | 0.51              |
| 1:D:72:LEU:HD23  | 1:D:76:GLN:CG    | 2.41                     | 0.51              |
| 1:A:209:MET:O    | 1:A:212:MET:HB3  | 2.11                     | 0.51              |
| 1:C:180:GLU:O    | 1:C:181:CYS:HB2  | 2.10                     | 0.51              |
| 1:A:37:LEU:HD23  | 1:C:285:LEU:HD11 | 1.94                     | 0.50              |
| 1:C:44:PRO:HG2   | 1:C:45:GLU:OE1   | 2.11                     | 0.50              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:235:LYS:N    | 1:D:235:LYS:HE2  | 2.26                     | 0.50              |
| 1:A:24:SER:N     | 1:A:25:PRO:CD    | 2.74                     | 0.50              |
| 1:C:173:GLU:O    | 1:C:177:GLU:HG2  | 2.11                     | 0.50              |
| 1:C:257:ASP:C    | 1:C:259:GLU:H    | 2.19                     | 0.50              |
| 1:D:24:SER:HB2   | 1:D:25:PRO:HD3   | 1.92                     | 0.50              |
| 1:D:251:ILE:N    | 1:D:251:ILE:HD12 | 2.26                     | 0.50              |
| 1:D:273:ARG:HG2  | 1:D:273:ARG:HH11 | 1.76                     | 0.50              |
| 1:B:56:ARG:HG2   | 1:B:56:ARG:HH11  | 1.77                     | 0.50              |
| 1:A:173:GLU:O    | 1:A:177:GLU:HG2  | 2.11                     | 0.50              |
| 1:B:37:LEU:HD23  | 1:B:42:LYS:HE2   | 1.94                     | 0.50              |
| 1:A:30:LEU:HD13  | 1:A:52:ARG:HB2   | 1.94                     | 0.50              |
| 1:A:42:LYS:HE3   | 1:D:249:SER:O    | 2.11                     | 0.50              |
| 1:A:162:LEU:HD21 | 1:B:212:MET:HA   | 1.93                     | 0.50              |
| 1:C:209:MET:O    | 1:C:212:MET:HB3  | 2.12                     | 0.50              |
| 1:C:253:TYR:CD1  | 1:C:258:ILE:HG21 | 2.47                     | 0.49              |
| 1:D:131:ASN:HD22 | 1:D:131:ASN:N    | 1.97                     | 0.49              |
| 1:B:101:LEU:O    | 1:B:101:LEU:HD23 | 2.12                     | 0.49              |
| 1:C:207:LYS:HB2  | 1:C:207:LYS:NZ   | 2.27                     | 0.49              |
| 1:C:301:VAL:O    | 1:C:303:ASP:N    | 2.44                     | 0.49              |
| 1:D:37:LEU:HD13  | 1:D:45:GLU:HB3   | 1.93                     | 0.49              |
| 1:C:245:CYS:HA   | 1:C:284:ASN:H    | 1.77                     | 0.49              |
| 1:A:169:LEU:HD22 | 1:B:173:GLU:CD   | 2.37                     | 0.49              |
| 1:A:215:LEU:CD2  | 1:B:219:VAL:HG21 | 2.42                     | 0.49              |
| 1:B:235:LYS:HE2  | 1:B:235:LYS:N    | 2.28                     | 0.49              |
| 1:D:145:LYS:HD3  | 1:D:304:TYR:HB3  | 1.94                     | 0.49              |
| 1:B:129:ARG:HG2  | 1:B:129:ARG:HH11 | 1.78                     | 0.49              |
| 1:D:37:LEU:HD23  | 1:D:42:LYS:HE2   | 1.95                     | 0.49              |
| 1:A:259:GLU:HA   | 1:A:259:GLU:OE2  | 2.13                     | 0.49              |
| 1:A:301:VAL:O    | 1:A:303:ASP:N    | 2.45                     | 0.49              |
| 1:C:24:SER:N     | 1:C:25:PRO:CD    | 2.76                     | 0.49              |
| 1:B:164:SER:O    | 1:B:168:ARG:HG3  | 2.13                     | 0.49              |
| 1:B:255:ARG:HA   | 1:B:258:ILE:HD11 | 1.95                     | 0.49              |
| 1:C:235:LYS:HB2  | 1:C:253:TYR:CD2  | 2.48                     | 0.49              |
| 1:D:56:ARG:HG2   | 1:D:56:ARG:HH11  | 1.78                     | 0.49              |
| 1:D:164:SER:O    | 1:D:168:ARG:HG3  | 2.13                     | 0.48              |
| 1:A:253:TYR:CD1  | 1:A:258:ILE:HG21 | 2.48                     | 0.48              |
| 1:C:260:GLU:HG3  | 1:C:261:HIS:N    | 2.27                     | 0.48              |
| 1:D:182:GLN:C    | 1:D:184:ASN:H    | 2.20                     | 0.48              |
| 1:A:36:ARG:NH1   | 3:A:1307:SO4:S   | 2.86                     | 0.48              |
| 1:A:294:PHE:CD1  | 1:A:298:ASN:ND2  | 2.81                     | 0.48              |
| 1:B:37:LEU:HD13  | 1:B:45:GLU:HB3   | 1.94                     | 0.48              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:182:GLN:CG   | 1:A:198:GLN:HE21 | 2.27                     | 0.48              |
| 1:A:287:MET:O    | 1:A:288:LYS:C    | 2.56                     | 0.48              |
| 1:B:76:GLN:HB2   | 1:B:80:ALA:HB2   | 1.95                     | 0.48              |
| 1:C:50:TYR:OH    | 2:G:508:VAL:HG11 | 2.14                     | 0.48              |
| 1:D:26:SER:HA    | 1:D:56:ARG:NH1   | 2.22                     | 0.48              |
| 1:D:76:GLN:HB2   | 1:D:80:ALA:HB2   | 1.95                     | 0.48              |
| 1:A:245:CYS:HA   | 1:A:284:ASN:H    | 1.77                     | 0.48              |
| 1:D:286:ALA:O    | 1:D:290:VAL:HG23 | 2.13                     | 0.48              |
| 1:B:57:ASN:C     | 1:B:57:ASN:ND2   | 2.69                     | 0.48              |
| 1:B:131:ASN:H    | 1:B:131:ASN:ND2  | 2.04                     | 0.48              |
| 1:B:131:ASN:CG   | 2:F:502:THR:HG23 | 2.39                     | 0.48              |
| 1:B:182:GLN:CG   | 1:B:198:GLN:HE22 | 2.26                     | 0.48              |
| 1:C:30:LEU:HD13  | 1:C:52:ARG:HB2   | 1.96                     | 0.48              |
| 1:D:148:TRP:CE2  | 1:D:300:TRP:HA   | 2.49                     | 0.48              |
| 1:D:164:SER:HA   | 1:D:167:THR:HG22 | 1.96                     | 0.48              |
| 1:D:242:ARG:HG2  | 1:D:242:ARG:HH11 | 1.79                     | 0.48              |
| 1:D:255:ARG:HA   | 1:D:258:ILE:HD11 | 1.95                     | 0.48              |
| 1:B:76:GLN:N     | 1:B:76:GLN:CD    | 2.70                     | 0.48              |
| 1:B:145:LYS:HD3  | 1:B:304:TYR:HB3  | 1.94                     | 0.48              |
| 1:B:239:GLU:O    | 1:B:240:LEU:C    | 2.57                     | 0.48              |
| 1:B:286:ALA:O    | 1:B:290:VAL:HG23 | 2.13                     | 0.48              |
| 1:D:30:LEU:HB2   | 1:D:53:ALA:HB2   | 1.96                     | 0.48              |
| 1:A:235:LYS:HB2  | 1:A:253:TYR:CD2  | 2.49                     | 0.48              |
| 1:D:94:SER:HB3   | 1:D:97:ALA:CB    | 2.43                     | 0.48              |
| 1:D:254:ASP:C    | 1:D:256:LYS:H    | 2.22                     | 0.48              |
| 1:A:101:LEU:HG   | 1:A:105:GLN:NE2  | 2.29                     | 0.48              |
| 1:B:94:SER:HB3   | 1:B:97:ALA:CB    | 2.43                     | 0.48              |
| 1:B:182:GLN:HG3  | 1:B:198:GLN:CD   | 2.38                     | 0.48              |
| 1:D:76:GLN:N     | 1:D:76:GLN:CD    | 2.70                     | 0.48              |
| 1:B:242:ARG:HG2  | 1:B:242:ARG:HH11 | 1.79                     | 0.48              |
| 1:B:263:GLN:O    | 1:B:264:ARG:HB2  | 2.13                     | 0.48              |
| 1:C:248:PRO:HA   | 1:D:282:ILE:CD1  | 2.40                     | 0.48              |
| 1:D:96:LYS:HA    | 2:H:505:MET:HE1  | 1.96                     | 0.48              |
| 1:B:182:GLN:C    | 1:B:184:ASN:H    | 2.21                     | 0.47              |
| 1:C:258:ILE:HD13 | 1:C:281:LEU:HD11 | 1.96                     | 0.47              |
| 1:D:57:ASN:C     | 1:D:57:ASN:ND2   | 2.70                     | 0.47              |
| 1:A:212:MET:HE2  | 1:B:166:LEU:HD21 | 1.96                     | 0.47              |
| 1:B:278:GLN:HG3  | 1:B:279:GLU:N    | 2.29                     | 0.47              |
| 1:C:57:ASN:C     | 1:C:57:ASN:HD22  | 2.21                     | 0.47              |
| 1:D:129:ARG:HG2  | 1:D:129:ARG:HH11 | 1.79                     | 0.47              |
| 1:D:132:PHE:CE1  | 2:H:505:MET:HG2  | 2.49                     | 0.47              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:182:GLN:HG3  | 1:D:198:GLN:CD   | 2.38                     | 0.47              |
| 1:B:61:ALA:O     | 1:B:62:VAL:C     | 2.58                     | 0.47              |
| 1:C:259:GLU:OE2  | 1:C:259:GLU:HA   | 2.14                     | 0.47              |
| 1:C:287:MET:O    | 1:C:288:LYS:C    | 2.57                     | 0.47              |
| 1:B:254:ASP:C    | 1:B:256:LYS:H    | 2.22                     | 0.47              |
| 1:A:138:SER:HA   | 1:A:238:PHE:CD1  | 2.50                     | 0.47              |
| 1:C:38:PHE:CZ    | 1:C:69:LEU:HG    | 2.50                     | 0.47              |
| 1:D:239:GLU:O    | 1:D:240:LEU:C    | 2.57                     | 0.47              |
| 1:D:263:GLN:O    | 1:D:264:ARG:HB2  | 2.13                     | 0.47              |
| 1:A:260:GLU:HG3  | 1:A:261:HIS:N    | 2.28                     | 0.47              |
| 1:B:26:SER:HA    | 1:B:56:ARG:NH1   | 2.23                     | 0.47              |
| 1:D:131:ASN:H    | 1:D:131:ASN:ND2  | 2.05                     | 0.47              |
| 1:A:44:PRO:HG2   | 1:A:45:GLU:OE1   | 2.14                     | 0.47              |
| 1:A:230:ASP:C    | 1:A:232:LEU:N    | 2.73                     | 0.47              |
| 1:B:148:TRP:CE2  | 1:B:300:TRP:HA   | 2.50                     | 0.47              |
| 1:C:129:ARG:NH2  | 1:C:264:ARG:HH21 | 2.12                     | 0.47              |
| 1:C:229:PRO:HB3  | 1:C:231:TYR:CE2  | 2.49                     | 0.47              |
| 1:C:294:PHE:CD1  | 1:C:298:ASN:ND2  | 2.83                     | 0.47              |
| 1:D:223:ARG:NH1  | 1:D:223:ARG:HG2  | 2.30                     | 0.47              |
| 1:A:239:GLU:HG2  | 1:A:240:LEU:N    | 2.30                     | 0.47              |
| 1:D:133:GLY:O    | 1:D:135:ASP:N    | 2.47                     | 0.47              |
| 1:D:223:ARG:HG2  | 1:D:223:ARG:HH11 | 1.80                     | 0.47              |
| 1:D:278:GLN:HG3  | 1:D:279:GLU:N    | 2.29                     | 0.47              |
| 1:B:201:ILE:HD12 | 1:B:204:LYS:HZ2  | 1.80                     | 0.47              |
| 1:B:204:LYS:HZ3  | 1:B:205:HIS:HE1  | 1.62                     | 0.47              |
| 1:C:176:ARG:HH12 | 1:D:173:GLU:HG2  | 1.80                     | 0.47              |
| 1:A:138:SER:O    | 1:A:142:ILE:HG13 | 2.15                     | 0.47              |
| 1:A:199:ALA:HA   | 1:A:202:GLU:HB2  | 1.97                     | 0.47              |
| 1:A:286:ALA:CB   | 1:B:287:MET:HE3  | 2.45                     | 0.47              |
| 1:C:163:HIS:O    | 1:C:164:SER:C    | 2.57                     | 0.47              |
| 1:A:43:TYR:N     | 1:A:44:PRO:HD2   | 2.30                     | 0.46              |
| 1:A:229:PRO:HB3  | 1:A:231:TYR:CE2  | 2.50                     | 0.46              |
| 1:C:71:TYR:CD2   | 1:C:79:GLN:HB2   | 2.51                     | 0.46              |
| 1:C:111:TYR:HB3  | 1:C:147:ARG:HG3  | 1.96                     | 0.46              |
| 1:C:138:SER:O    | 1:C:142:ILE:HG13 | 2.15                     | 0.46              |
| 1:C:169:LEU:HD22 | 1:D:173:GLU:CD   | 2.41                     | 0.46              |
| 1:C:182:GLN:CG   | 1:C:198:GLN:HE21 | 2.28                     | 0.46              |
| 1:B:223:ARG:NH1  | 1:B:223:ARG:HG2  | 2.30                     | 0.46              |
| 1:A:38:PHE:CE1   | 2:E:508:VAL:HG23 | 2.50                     | 0.46              |
| 1:C:167:THR:CG2  | 1:C:168:ARG:N    | 2.78                     | 0.46              |
| 1:D:61:ALA:O     | 1:D:62:VAL:C     | 2.59                     | 0.46              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:154:ARG:HG3  | 1:D:154:ARG:HH11 | 1.80                     | 0.46              |
| 1:A:163:HIS:O    | 1:A:164:SER:C    | 2.58                     | 0.46              |
| 1:C:81:LEU:HD13  | 1:C:81:LEU:O     | 2.16                     | 0.46              |
| 1:C:172:ALA:O    | 1:C:176:ARG:HG3  | 2.16                     | 0.46              |
| 1:A:211:ASP:HA   | 1:A:214:GLU:OE1  | 2.16                     | 0.46              |
| 1:B:164:SER:HA   | 1:B:167:THR:HG22 | 1.98                     | 0.46              |
| 1:B:223:ARG:HG2  | 1:B:223:ARG:HH11 | 1.81                     | 0.46              |
| 1:C:66:ASN:OD1   | 2:G:508:VAL:HG13 | 2.15                     | 0.46              |
| 1:C:239:GLU:HG2  | 1:C:240:LEU:N    | 2.31                     | 0.46              |
| 1:D:76:GLN:N     | 1:D:76:GLN:OE1   | 2.45                     | 0.46              |
| 1:A:26:SER:OG    | 1:A:29:GLU:HG3   | 2.15                     | 0.46              |
| 1:B:96:LYS:HA    | 2:F:505:MET:HE1  | 1.97                     | 0.46              |
| 1:B:273:ARG:HG2  | 1:B:273:ARG:NH1  | 2.29                     | 0.46              |
| 1:A:38:PHE:CZ    | 1:A:69:LEU:HG    | 2.51                     | 0.46              |
| 1:B:294:PHE:CE1  | 1:B:298:ASN:ND2  | 2.84                     | 0.46              |
| 1:C:158:GLN:C    | 1:C:158:GLN:CD   | 2.83                     | 0.46              |
| 1:C:211:ASP:HA   | 1:C:214:GLU:OE1  | 2.16                     | 0.46              |
| 1:D:148:TRP:C    | 1:D:150:SER:N    | 2.73                     | 0.46              |
| 1:D:157:HIS:O    | 1:D:161:GLU:HB2  | 2.15                     | 0.46              |
| 1:D:169:LEU:O    | 1:D:173:GLU:HG3  | 2.15                     | 0.45              |
| 1:A:47:ALA:HB2   | 1:A:70:CYS:HB3   | 1.98                     | 0.45              |
| 1:A:129:ARG:NH2  | 1:A:264:ARG:HH21 | 2.14                     | 0.45              |
| 1:B:182:GLN:NE2  | 1:B:198:GLN:NE2  | 2.63                     | 0.45              |
| 1:D:38:PHE:O     | 1:D:41:ARG:N     | 2.50                     | 0.45              |
| 1:D:182:GLN:CG   | 1:D:198:GLN:HE22 | 2.29                     | 0.45              |
| 1:A:156:ILE:C    | 1:A:158:GLN:H    | 2.25                     | 0.45              |
| 1:A:167:THR:CG2  | 1:A:168:ARG:N    | 2.79                     | 0.45              |
| 1:B:154:ARG:HH11 | 1:B:154:ARG:HG3  | 1.80                     | 0.45              |
| 1:C:138:SER:HA   | 1:C:238:PHE:CD1  | 2.51                     | 0.45              |
| 1:C:230:ASP:C    | 1:C:232:LEU:N    | 2.75                     | 0.45              |
| 1:D:254:ASP:O    | 1:D:256:LYS:N    | 2.48                     | 0.45              |
| 1:A:158:GLN:C    | 1:A:158:GLN:CD   | 2.83                     | 0.45              |
| 1:B:76:GLN:N     | 1:B:76:GLN:OE1   | 2.46                     | 0.45              |
| 1:B:148:TRP:C    | 1:B:150:SER:N    | 2.74                     | 0.45              |
| 1:D:258:ILE:CD1  | 1:D:259:GLU:N    | 2.74                     | 0.45              |
| 1:A:258:ILE:HD13 | 1:A:281:LEU:HD11 | 1.99                     | 0.45              |
| 1:B:73:LYS:O     | 1:B:74:MET:HB3   | 2.17                     | 0.45              |
| 1:B:258:ILE:CD1  | 1:B:259:GLU:N    | 2.74                     | 0.45              |
| 1:C:156:ILE:C    | 1:C:158:GLN:H    | 2.25                     | 0.45              |
| 1:A:42:LYS:HD3   | 1:C:283:PRO:HG3  | 1.97                     | 0.45              |
| 1:A:110:SER:HB3  | 1:A:113:GLU:OE1  | 2.16                     | 0.45              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:A:172:ALA:O    | 1:A:176:ARG:HG3  | 2.17                     | 0.45              |
| 1:B:133:GLY:O    | 1:B:135:ASP:N    | 2.49                     | 0.45              |
| 1:C:32:GLU:O     | 1:C:35:ASN:HB2   | 2.17                     | 0.45              |
| 2:H:502:THR:HG22 | 2:H:503:SER:N    | 2.32                     | 0.45              |
| 1:B:46:ALA:HA    | 1:B:49:CYS:HB3   | 1.99                     | 0.45              |
| 1:B:254:ASP:O    | 1:B:256:LYS:N    | 2.49                     | 0.45              |
| 1:C:176:ARG:NH1  | 1:D:173:GLU:HG2  | 2.32                     | 0.45              |
| 1:C:199:ALA:HA   | 1:C:202:GLU:HB2  | 1.99                     | 0.45              |
| 1:D:226:ARG:HD3  | 1:D:300:TRP:CZ3  | 2.52                     | 0.45              |
| 1:B:169:LEU:O    | 1:B:173:GLU:HG3  | 2.16                     | 0.45              |
| 1:B:260:GLU:O    | 1:B:261:HIS:C    | 2.58                     | 0.45              |
| 1:D:156:ILE:HD12 | 1:D:156:ILE:N    | 2.32                     | 0.45              |
| 1:D:294:PHE:CE1  | 1:D:298:ASN:ND2  | 2.85                     | 0.45              |
| 1:A:141:ARG:NH1  | 1:A:141:ARG:HG3  | 2.31                     | 0.45              |
| 1:B:69:LEU:HD12  | 1:B:69:LEU:O     | 2.17                     | 0.45              |
| 1:B:175:GLU:C    | 1:B:177:GLU:H    | 2.25                     | 0.45              |
| 1:D:175:GLU:C    | 1:D:177:GLU:H    | 2.24                     | 0.45              |
| 2:E:502:THR:HG22 | 2:E:503:SER:N    | 2.31                     | 0.45              |
| 1:A:81:LEU:HD13  | 1:A:81:LEU:O     | 2.17                     | 0.45              |
| 1:A:85:ARG:HH11  | 1:A:85:ARG:CG    | 2.29                     | 0.45              |
| 1:A:134:ASP:O    | 1:A:135:ASP:C    | 2.57                     | 0.45              |
| 1:D:46:ALA:HA    | 1:D:49:CYS:HB3   | 1.99                     | 0.45              |
| 1:D:178:LEU:C    | 1:D:180:GLU:H    | 2.23                     | 0.45              |
| 1:D:182:GLN:O    | 1:D:184:ASN:N    | 2.50                     | 0.45              |
| 1:D:242:ARG:HH11 | 1:D:242:ARG:CG   | 2.30                     | 0.45              |
| 1:A:32:GLU:O     | 1:A:35:ASN:HB2   | 2.17                     | 0.44              |
| 1:B:26:SER:HB3   | 1:B:29:GLU:CG    | 2.48                     | 0.44              |
| 1:B:69:LEU:HD23  | 2:F:508:VAL:HG22 | 1.97                     | 0.44              |
| 1:B:115:ILE:HD13 | 1:B:144:LYS:HD3  | 1.99                     | 0.44              |
| 1:B:132:PHE:O    | 1:B:135:ASP:HB2  | 2.17                     | 0.44              |
| 1:B:156:ILE:N    | 1:B:156:ILE:HD12 | 2.32                     | 0.44              |
| 1:B:253:TYR:HB2  | 1:B:258:ILE:HG12 | 1.99                     | 0.44              |
| 1:C:110:SER:HB3  | 1:C:113:GLU:OE1  | 2.17                     | 0.44              |
| 1:C:141:ARG:NH1  | 1:C:141:ARG:HG3  | 2.31                     | 0.44              |
| 1:D:253:TYR:HB2  | 1:D:258:ILE:HG12 | 1.99                     | 0.44              |
| 1:D:204:LYS:NZ   | 1:D:205:HIS:HE1  | 2.15                     | 0.44              |
| 1:A:30:LEU:HB2   | 1:A:53:ALA:HB2   | 1.99                     | 0.44              |
| 1:B:134:ASP:O    | 1:B:138:SER:CB   | 2.66                     | 0.44              |
| 1:B:178:LEU:C    | 1:B:180:GLU:H    | 2.24                     | 0.44              |
| 1:D:132:PHE:O    | 1:D:135:ASP:HB2  | 2.17                     | 0.44              |
| 1:D:134:ASP:O    | 1:D:138:SER:CB   | 2.65                     | 0.44              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:F:502:THR:HG22 | 2:F:503:SER:N    | 2.33                     | 0.44              |
| 1:C:269:ASN:C    | 1:C:271:VAL:H    | 2.24                     | 0.44              |
| 1:D:115:ILE:HD13 | 1:D:144:LYS:HD3  | 1.99                     | 0.44              |
| 1:D:226:ARG:HD3  | 1:D:300:TRP:CE3  | 2.52                     | 0.44              |
| 1:A:269:ASN:C    | 1:A:271:VAL:H    | 2.24                     | 0.44              |
| 1:B:131:ASN:CB   | 2:F:502:THR:HG23 | 2.48                     | 0.44              |
| 1:B:132:PHE:CE1  | 2:F:505:MET:HG2  | 2.52                     | 0.44              |
| 1:B:242:ARG:HH11 | 1:B:242:ARG:CG   | 2.30                     | 0.44              |
| 1:D:260:GLU:O    | 1:D:261:HIS:C    | 2.59                     | 0.44              |
| 1:C:47:ALA:HB2   | 1:C:70:CYS:HB3   | 1.99                     | 0.44              |
| 1:D:96:LYS:NZ    | 2:H:505:MET:HE2  | 2.33                     | 0.44              |
| 1:D:182:GLN:OE1  | 1:D:183:ARG:HB2  | 2.17                     | 0.44              |
| 1:D:230:ASP:C    | 1:D:232:LEU:H    | 2.26                     | 0.44              |
| 1:A:174:ARG:O    | 1:A:178:LEU:HD13 | 2.18                     | 0.44              |
| 1:B:79:GLN:O     | 1:B:80:ALA:C     | 2.61                     | 0.44              |
| 1:C:105:GLN:OE1  | 1:C:113:GLU:HB3  | 2.17                     | 0.44              |
| 1:B:148:TRP:O    | 1:B:149:ASN:C    | 2.60                     | 0.44              |
| 1:B:157:HIS:O    | 1:B:161:GLU:HB2  | 2.17                     | 0.44              |
| 1:C:85:ARG:HH11  | 1:C:85:ARG:CG    | 2.30                     | 0.44              |
| 1:C:95:VAL:HG11  | 1:C:125:ALA:HB2  | 2.00                     | 0.44              |
| 1:D:79:GLN:O     | 1:D:80:ALA:C     | 2.61                     | 0.44              |
| 1:D:273:ARG:HG2  | 1:D:273:ARG:NH1  | 2.31                     | 0.44              |
| 1:D:148:TRP:O    | 1:D:149:ASN:C    | 2.60                     | 0.44              |
| 1:D:207:LYS:C    | 1:D:209:MET:N    | 2.74                     | 0.44              |
| 2:G:502:THR:HG22 | 2:G:503:SER:N    | 2.32                     | 0.44              |
| 1:B:198:GLN:O    | 1:B:199:ALA:C    | 2.61                     | 0.43              |
| 1:C:237:SER:O    | 1:C:238:PHE:HB2  | 2.18                     | 0.43              |
| 1:D:78:GLU:H     | 1:D:78:GLU:CD    | 2.25                     | 0.43              |
| 1:D:247:THR:HB   | 1:D:248:PRO:CD   | 2.48                     | 0.43              |
| 1:A:36:ARG:HD3   | 1:C:289:GLU:CD   | 2.43                     | 0.43              |
| 1:A:71:TYR:CD2   | 1:A:79:GLN:HB2   | 2.53                     | 0.43              |
| 1:A:300:TRP:C    | 1:A:301:VAL:O    | 2.60                     | 0.43              |
| 1:B:204:LYS:NZ   | 1:B:205:HIS:HE1  | 2.16                     | 0.43              |
| 1:B:226:ARG:HD3  | 1:B:300:TRP:CE3  | 2.53                     | 0.43              |
| 1:C:163:HIS:O    | 1:C:165:TYR:N    | 2.52                     | 0.43              |
| 1:D:73:LYS:O     | 1:D:74:MET:HB3   | 2.17                     | 0.43              |
| 1:B:198:GLN:C    | 1:B:200:CYS:N    | 2.75                     | 0.43              |
| 1:C:37:LEU:HD23  | 1:C:37:LEU:HA    | 1.82                     | 0.43              |
| 1:B:140:LEU:O    | 1:B:141:ARG:C    | 2.58                     | 0.43              |
| 1:B:182:GLN:O    | 1:B:184:ASN:N    | 2.52                     | 0.43              |
| 1:B:226:ARG:HD3  | 1:B:300:TRP:CZ3  | 2.53                     | 0.43              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:C:26:SER:OG    | 1:C:29:GLU:HG3   | 2.17                     | 0.43              |
| 1:C:134:ASP:O    | 1:C:135:ASP:C    | 2.59                     | 0.43              |
| 1:C:195:ARG:HG3  | 1:C:195:ARG:HH11 | 1.83                     | 0.43              |
| 1:C:212:MET:HE2  | 1:D:166:LEU:HD21 | 2.00                     | 0.43              |
| 1:A:57:ASN:C     | 1:A:57:ASN:HD22  | 2.25                     | 0.43              |
| 1:C:30:LEU:HB2   | 1:C:53:ALA:HB2   | 2.01                     | 0.43              |
| 1:C:174:ARG:O    | 1:C:178:LEU:HD13 | 2.19                     | 0.43              |
| 1:C:215:LEU:CD2  | 1:D:219:VAL:HG21 | 2.48                     | 0.43              |
| 2:H:507:GLU:O    | 2:H:507:GLU:HG3  | 2.19                     | 0.43              |
| 1:A:111:TYR:HB3  | 1:A:147:ARG:HG3  | 2.00                     | 0.43              |
| 1:B:38:PHE:C     | 1:B:40:GLY:N     | 2.75                     | 0.43              |
| 1:B:77:PRO:HB2   | 1:B:78:GLU:H     | 1.63                     | 0.43              |
| 1:B:243:GLU:HB3  | 1:B:255:ARG:HB2  | 1.99                     | 0.43              |
| 1:C:278:GLN:C    | 1:C:280:GLN:H    | 2.26                     | 0.43              |
| 1:D:38:PHE:C     | 1:D:40:GLY:N     | 2.75                     | 0.43              |
| 2:F:507:GLU:O    | 2:F:507:GLU:HG3  | 2.19                     | 0.43              |
| 1:A:278:GLN:C    | 1:A:280:GLN:H    | 2.26                     | 0.43              |
| 1:B:30:LEU:HB2   | 1:B:53:ALA:HB2   | 2.01                     | 0.43              |
| 1:C:284:ASN:ND2  | 1:D:284:ASN:ND2  | 2.62                     | 0.43              |
| 1:C:300:TRP:C    | 1:C:301:VAL:O    | 2.61                     | 0.43              |
| 1:D:77:PRO:HB2   | 1:D:78:GLU:H     | 1.63                     | 0.43              |
| 1:A:81:LEU:HD22  | 1:A:101:LEU:HD12 | 2.00                     | 0.43              |
| 1:B:110:SER:HB3  | 1:B:113:GLU:CD   | 2.43                     | 0.43              |
| 1:B:134:ASP:O    | 1:B:138:SER:HB2  | 2.19                     | 0.43              |
| 1:B:182:GLN:OE1  | 1:B:183:ARG:HB2  | 2.19                     | 0.43              |
| 1:B:247:THR:HB   | 1:B:248:PRO:CD   | 2.49                     | 0.43              |
| 1:C:235:LYS:HD3  | 1:C:235:LYS:HA   | 1.85                     | 0.43              |
| 1:A:235:LYS:HA   | 1:A:235:LYS:HD3  | 1.82                     | 0.43              |
| 1:B:78:GLU:H     | 1:B:78:GLU:CD    | 2.26                     | 0.43              |
| 1:C:81:LEU:HD22  | 1:C:101:LEU:HD12 | 2.01                     | 0.43              |
| 1:D:110:SER:HB3  | 1:D:113:GLU:CD   | 2.44                     | 0.43              |
| 1:B:228:ILE:HD12 | 1:B:294:PHE:HE2  | 1.84                     | 0.43              |
| 1:C:258:ILE:HD13 | 1:C:281:LEU:CD1  | 2.49                     | 0.43              |
| 1:D:170:ILE:HG22 | 1:D:171:ALA:N    | 2.33                     | 0.43              |
| 1:C:43:TYR:N     | 1:C:44:PRO:HD2   | 2.34                     | 0.42              |
| 1:D:294:PHE:O    | 1:D:298:ASN:ND2  | 2.52                     | 0.42              |
| 1:A:50:TYR:OH    | 2:E:508:VAL:HG11 | 2.19                     | 0.42              |
| 1:A:195:ARG:HG3  | 1:A:195:ARG:HH11 | 1.84                     | 0.42              |
| 1:B:215:LEU:O    | 1:B:218:GLN:HB2  | 2.20                     | 0.42              |
| 1:C:178:LEU:HD12 | 1:C:178:LEU:N    | 2.35                     | 0.42              |
| 1:D:133:GLY:C    | 1:D:135:ASP:H    | 2.27                     | 0.42              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:B:203:ALA:HA   | 1:B:206:ASP:OD2  | 2.19                     | 0.42              |
| 1:B:241:MET:CE   | 1:B:254:ASP:N    | 2.82                     | 0.42              |
| 1:A:257:ASP:C    | 1:A:259:GLU:N    | 2.77                     | 0.42              |
| 1:B:145:LYS:NZ   | 1:B:304:TYR:HB3  | 2.35                     | 0.42              |
| 1:C:176:ARG:HA   | 1:C:180:GLU:HB2  | 2.01                     | 0.42              |
| 1:C:284:ASN:OD1  | 1:C:287:MET:HB2  | 2.18                     | 0.42              |
| 1:A:178:LEU:N    | 1:A:178:LEU:HD12 | 2.35                     | 0.42              |
| 1:B:145:LYS:CD   | 1:B:304:TYR:HB3  | 2.50                     | 0.42              |
| 1:D:247:THR:HB   | 1:D:248:PRO:HD2  | 2.00                     | 0.42              |
| 1:D:254:ASP:C    | 1:D:256:LYS:N    | 2.78                     | 0.42              |
| 1:A:37:LEU:HD23  | 1:A:37:LEU:HA    | 1.82                     | 0.42              |
| 1:A:154:ARG:O    | 1:A:154:ARG:HG3  | 2.19                     | 0.42              |
| 1:B:69:LEU:HD23  | 2:F:508:VAL:HG23 | 2.01                     | 0.42              |
| 1:B:170:ILE:HG22 | 1:B:171:ALA:N    | 2.33                     | 0.42              |
| 1:D:113:GLU:O    | 1:D:116:ALA:HB3  | 2.19                     | 0.42              |
| 1:D:132:PHE:O    | 1:D:133:GLY:C    | 2.62                     | 0.42              |
| 1:D:182:GLN:NE2  | 1:D:198:GLN:NE2  | 2.67                     | 0.42              |
| 1:A:176:ARG:HA   | 1:A:180:GLU:HB2  | 2.01                     | 0.42              |
| 1:C:154:ARG:HG3  | 1:C:154:ARG:O    | 2.20                     | 0.42              |
| 1:C:257:ASP:C    | 1:C:259:GLU:N    | 2.77                     | 0.42              |
| 1:D:140:LEU:O    | 1:D:141:ARG:C    | 2.59                     | 0.42              |
| 1:D:228:ILE:HD12 | 1:D:294:PHE:HE2  | 1.85                     | 0.42              |
| 1:D:243:GLU:HB3  | 1:D:255:ARG:HB2  | 2.00                     | 0.42              |
| 2:F:505:MET:C    | 2:F:507:GLU:N    | 2.77                     | 0.42              |
| 1:B:128:GLN:O    | 1:B:129:ARG:C    | 2.62                     | 0.42              |
| 1:B:254:ASP:C    | 1:B:256:LYS:N    | 2.78                     | 0.42              |
| 1:D:85:ARG:HH11  | 1:D:85:ARG:CG    | 2.32                     | 0.42              |
| 1:D:128:GLN:O    | 1:D:129:ARG:C    | 2.62                     | 0.42              |
| 1:A:31:LYS:HB3   | 1:A:31:LYS:HE2   | 1.86                     | 0.42              |
| 1:A:237:SER:O    | 1:A:238:PHE:HB2  | 2.20                     | 0.42              |
| 1:B:207:LYS:C    | 1:B:209:MET:N    | 2.75                     | 0.42              |
| 2:H:505:MET:C    | 2:H:507:GLU:N    | 2.76                     | 0.42              |
| 1:C:113:GLU:O    | 1:C:116:ALA:HB3  | 2.19                     | 0.41              |
| 1:D:38:PHE:O     | 1:D:40:GLY:N     | 2.53                     | 0.41              |
| 1:D:107:GLU:OE1  | 1:D:107:GLU:HA   | 2.20                     | 0.41              |
| 1:A:31:LYS:HD3   | 1:A:63:TYR:HE1   | 1.85                     | 0.41              |
| 1:A:105:GLN:OE1  | 1:A:113:GLU:HB3  | 2.19                     | 0.41              |
| 1:B:85:ARG:HH11  | 1:B:85:ARG:CG    | 2.32                     | 0.41              |
| 1:B:124:LEU:C    | 1:B:126:LYS:N    | 2.76                     | 0.41              |
| 1:B:254:ASP:O    | 1:B:258:ILE:HD11 | 2.20                     | 0.41              |
| 1:C:38:PHE:CE1   | 2:G:508:VAL:HG23 | 2.54                     | 0.41              |

*Continued on next page...*

*Continued from previous page...*

| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:D:148:TRP:O    | 1:D:150:SER:N    | 2.53                     | 0.41              |
| 1:A:95:VAL:HG11  | 1:A:125:ALA:HB2  | 2.02                     | 0.41              |
| 1:A:113:GLU:O    | 1:A:116:ALA:HB3  | 2.20                     | 0.41              |
| 1:A:258:ILE:HD13 | 1:A:281:LEU:CD1  | 2.50                     | 0.41              |
| 1:B:133:GLY:C    | 1:B:135:ASP:H    | 2.28                     | 0.41              |
| 1:D:148:TRP:CZ2  | 1:D:300:TRP:HB3  | 2.55                     | 0.41              |
| 1:A:163:HIS:O    | 1:A:165:TYR:N    | 2.54                     | 0.41              |
| 1:B:178:LEU:C    | 1:B:180:GLU:N    | 2.76                     | 0.41              |
| 1:C:268:PHE:HA   | 1:C:274:SER:O    | 2.21                     | 0.41              |
| 1:D:26:SER:HB3   | 1:D:29:GLU:CG    | 2.51                     | 0.41              |
| 1:D:182:GLN:C    | 1:D:184:ASN:N    | 2.76                     | 0.41              |
| 1:B:166:LEU:O    | 1:B:169:LEU:N    | 2.53                     | 0.41              |
| 1:B:182:GLN:C    | 1:B:184:ASN:N    | 2.77                     | 0.41              |
| 1:C:235:LYS:HB2  | 1:C:253:TYR:CE2  | 2.56                     | 0.41              |
| 1:D:198:GLN:C    | 1:D:200:CYS:N    | 2.78                     | 0.41              |
| 1:D:200:CYS:C    | 1:D:202:GLU:H    | 2.29                     | 0.41              |
| 1:A:248:PRO:HA   | 1:B:282:ILE:CD1  | 2.46                     | 0.41              |
| 1:A:268:PHE:HA   | 1:A:274:SER:O    | 2.21                     | 0.41              |
| 1:B:132:PHE:O    | 1:B:133:GLY:C    | 2.63                     | 0.41              |
| 1:B:230:ASP:C    | 1:B:232:LEU:H    | 2.28                     | 0.41              |
| 1:C:163:HIS:C    | 1:C:165:TYR:N    | 2.76                     | 0.41              |
| 1:D:127:GLU:C    | 1:D:129:ARG:H    | 2.28                     | 0.41              |
| 1:B:105:GLN:C    | 1:B:107:GLU:N    | 2.77                     | 0.41              |
| 1:B:107:GLU:OE1  | 1:B:107:GLU:HA   | 2.21                     | 0.41              |
| 1:C:216:PHE:C    | 1:C:219:VAL:HG12 | 2.46                     | 0.41              |
| 1:C:248:PRO:HD2  | 1:C:276:LEU:HD13 | 2.03                     | 0.41              |
| 1:D:105:GLN:C    | 1:D:107:GLU:N    | 2.77                     | 0.41              |
| 1:D:134:ASP:O    | 1:D:138:SER:HB2  | 2.21                     | 0.41              |
| 1:D:145:LYS:CD   | 1:D:304:TYR:HB3  | 2.50                     | 0.41              |
| 1:D:254:ASP:O    | 1:D:258:ILE:HD11 | 2.21                     | 0.41              |
| 1:D:288:LYS:HE3  | 1:D:288:LYS:HB2  | 1.87                     | 0.41              |
| 1:A:37:LEU:HD13  | 1:A:45:GLU:HB3   | 2.03                     | 0.41              |
| 1:A:248:PRO:HD2  | 1:A:276:LEU:HD13 | 2.03                     | 0.41              |
| 1:B:146:LYS:O    | 1:B:147:ARG:C    | 2.64                     | 0.41              |
| 1:B:247:THR:HB   | 1:B:248:PRO:HD2  | 2.02                     | 0.41              |
| 1:D:124:LEU:C    | 1:D:126:LYS:N    | 2.77                     | 0.41              |
| 1:D:198:GLN:O    | 1:D:199:ALA:C    | 2.64                     | 0.41              |
| 1:D:215:LEU:O    | 1:D:218:GLN:HB2  | 2.21                     | 0.41              |
| 1:D:255:ARG:O    | 1:D:255:ARG:HG3  | 2.21                     | 0.41              |
| 2:E:507:GLU:O    | 2:E:507:GLU:HG3  | 2.21                     | 0.41              |
| 1:B:152:GLU:CD   | 1:B:155:ARG:HH21 | 2.28                     | 0.41              |

*Continued on next page...*

Continued from previous page...

| Atom-1          | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-----------------|------------------|--------------------------|-------------------|
| 1:C:251:ILE:N   | 1:C:251:ILE:CD1  | 2.78                     | 0.41              |
| 1:D:131:ASN:ND2 | 1:D:131:ASN:O    | 2.54                     | 0.41              |
| 1:B:38:PHE:O    | 1:B:40:GLY:N     | 2.54                     | 0.40              |
| 1:D:146:LYS:O   | 1:D:147:ARG:C    | 2.65                     | 0.40              |
| 1:D:178:LEU:C   | 1:D:180:GLU:N    | 2.77                     | 0.40              |
| 1:D:241:MET:CE  | 1:D:254:ASP:N    | 2.84                     | 0.40              |
| 1:A:287:MET:HA  | 1:B:287:MET:HE1  | 2.02                     | 0.40              |
| 1:B:37:LEU:HD12 | 1:B:46:ALA:HA    | 2.03                     | 0.40              |
| 1:D:203:ALA:HA  | 1:D:206:ASP:OD2  | 2.21                     | 0.40              |
| 1:A:136:ILE:N   | 1:A:137:PRO:HD2  | 2.36                     | 0.40              |
| 1:C:71:TYR:CG   | 1:C:79:GLN:HB2   | 2.57                     | 0.40              |
| 1:D:85:ARG:HG3  | 1:D:85:ARG:NH1   | 2.35                     | 0.40              |
| 1:A:141:ARG:HG3 | 1:A:141:ARG:HH11 | 1.86                     | 0.40              |
| 1:A:152:GLU:C   | 1:A:154:ARG:H    | 2.28                     | 0.40              |
| 1:A:194:ILE:O   | 1:A:198:GLN:HB2  | 2.22                     | 0.40              |
| 1:B:154:ARG:HD3 | 1:B:154:ARG:C    | 2.46                     | 0.40              |
| 1:C:302:GLU:HA  | 1:C:302:GLU:OE2  | 2.22                     | 0.40              |
| 1:B:241:MET:SD  | 1:B:252:THR:HG22 | 2.61                     | 0.40              |
| 1:C:299:GLY:C   | 1:C:300:TRP:O    | 2.64                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

| Mol | Chain | Analysed      | Favoured  | Allowed  | Outliers | Percentiles |    |
|-----|-------|---------------|-----------|----------|----------|-------------|----|
| 1   | A     | 279/281 (99%) | 223 (80%) | 45 (16%) | 11 (4%)  | 2           | 16 |
| 1   | B     | 279/281 (99%) | 214 (77%) | 51 (18%) | 14 (5%)  | 1           | 11 |
| 1   | C     | 279/281 (99%) | 223 (80%) | 46 (16%) | 10 (4%)  | 2           | 17 |
| 1   | D     | 279/281 (99%) | 216 (77%) | 48 (17%) | 15 (5%)  | 1           | 10 |
| 2   | E     | 7/9 (78%)     | 3 (43%)   | 2 (29%)  | 2 (29%)  | 0           | 0  |

Continued on next page...

*Continued from previous page...*

| Mol | Chain | Analysed        | Favoured  | Allowed   | Outliers | Percentiles |    |
|-----|-------|-----------------|-----------|-----------|----------|-------------|----|
| 2   | F     | 7/9 (78%)       | 3 (43%)   | 2 (29%)   | 2 (29%)  | 0           | 0  |
| 2   | G     | 7/9 (78%)       | 3 (43%)   | 2 (29%)   | 2 (29%)  | 0           | 0  |
| 2   | H     | 7/9 (78%)       | 3 (43%)   | 2 (29%)   | 2 (29%)  | 0           | 0  |
| All | All   | 1144/1160 (99%) | 888 (78%) | 198 (17%) | 58 (5%)  | 1           | 11 |

All (58) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 159 | GLU  |
| 1   | A     | 181 | CYS  |
| 1   | A     | 300 | TRP  |
| 1   | A     | 301 | VAL  |
| 1   | B     | 38  | PHE  |
| 1   | B     | 77  | PRO  |
| 1   | B     | 134 | ASP  |
| 1   | B     | 182 | GLN  |
| 1   | B     | 264 | ARG  |
| 1   | C     | 159 | GLU  |
| 1   | C     | 181 | CYS  |
| 1   | C     | 300 | TRP  |
| 1   | C     | 301 | VAL  |
| 1   | D     | 38  | PHE  |
| 1   | D     | 77  | PRO  |
| 1   | D     | 134 | ASP  |
| 1   | D     | 182 | GLN  |
| 1   | D     | 264 | ARG  |
| 2   | E     | 502 | THR  |
| 2   | F     | 502 | THR  |
| 2   | G     | 502 | THR  |
| 2   | H     | 502 | THR  |
| 1   | B     | 74  | MET  |
| 1   | B     | 75  | GLN  |
| 1   | B     | 180 | GLU  |
| 1   | D     | 74  | MET  |
| 1   | D     | 75  | GLN  |
| 1   | D     | 180 | GLU  |
| 2   | E     | 503 | SER  |
| 2   | F     | 503 | SER  |
| 2   | G     | 503 | SER  |
| 2   | H     | 503 | SER  |
| 1   | A     | 133 | GLY  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 158 | GLN  |
| 1   | A     | 160 | SER  |
| 1   | B     | 30  | LEU  |
| 1   | B     | 227 | ASP  |
| 1   | B     | 255 | ARG  |
| 1   | C     | 158 | GLN  |
| 1   | C     | 160 | SER  |
| 1   | D     | 30  | LEU  |
| 1   | D     | 183 | ARG  |
| 1   | D     | 227 | ASP  |
| 1   | D     | 255 | ARG  |
| 1   | B     | 183 | ARG  |
| 1   | C     | 133 | GLY  |
| 1   | A     | 190 | ASP  |
| 1   | B     | 178 | LEU  |
| 1   | C     | 164 | SER  |
| 1   | C     | 190 | ASP  |
| 1   | A     | 111 | TYR  |
| 1   | A     | 164 | SER  |
| 1   | D     | 178 | LEU  |
| 1   | A     | 270 | PRO  |
| 1   | C     | 270 | PRO  |
| 1   | B     | 76  | GLN  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 39  | VAL  |

### 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     | 244/244 (100%) | 224 (92%) | 20 (8%)  | 10          | 35 |
| 1   | B     | 244/244 (100%) | 221 (91%) | 23 (9%)  | 8           | 30 |
| 1   | C     | 244/244 (100%) | 224 (92%) | 20 (8%)  | 10          | 35 |
| 1   | D     | 244/244 (100%) | 221 (91%) | 23 (9%)  | 8           | 30 |
| 2   | E     | 9/9 (100%)     | 8 (89%)   | 1 (11%)  | 6           | 22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed         | Rotameric | Outliers | Percentiles |    |
|-----|-------|------------------|-----------|----------|-------------|----|
| 2   | F     | 9/9 (100%)       | 8 (89%)   | 1 (11%)  | 6           | 22 |
| 2   | G     | 9/9 (100%)       | 8 (89%)   | 1 (11%)  | 6           | 22 |
| 2   | H     | 9/9 (100%)       | 8 (89%)   | 1 (11%)  | 6           | 22 |
| All | All   | 1012/1012 (100%) | 922 (91%) | 90 (9%)  | 9           | 32 |

All (90) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 49  | CYS  |
| 1   | A     | 55  | THR  |
| 1   | A     | 96  | LYS  |
| 1   | A     | 103 | GLN  |
| 1   | A     | 135 | ASP  |
| 1   | A     | 141 | ARG  |
| 1   | A     | 149 | ASN  |
| 1   | A     | 151 | ILE  |
| 1   | A     | 195 | ARG  |
| 1   | A     | 198 | GLN  |
| 1   | A     | 204 | LYS  |
| 1   | A     | 207 | LYS  |
| 1   | A     | 208 | TYR  |
| 1   | A     | 227 | ASP  |
| 1   | A     | 232 | LEU  |
| 1   | A     | 240 | LEU  |
| 1   | A     | 280 | GLN  |
| 1   | A     | 287 | MET  |
| 1   | A     | 288 | LYS  |
| 1   | A     | 289 | GLU  |
| 1   | B     | 24  | SER  |
| 1   | B     | 32  | GLU  |
| 1   | B     | 55  | THR  |
| 1   | B     | 75  | GLN  |
| 1   | B     | 76  | GLN  |
| 1   | B     | 106 | LEU  |
| 1   | B     | 113 | GLU  |
| 1   | B     | 131 | ASN  |
| 1   | B     | 135 | ASP  |
| 1   | B     | 140 | LEU  |
| 1   | B     | 146 | LYS  |
| 1   | B     | 161 | GLU  |
| 1   | B     | 166 | LEU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 175 | GLU  |
| 1   | B     | 178 | LEU  |
| 1   | B     | 195 | ARG  |
| 1   | B     | 198 | GLN  |
| 1   | B     | 213 | ASP  |
| 1   | B     | 229 | PRO  |
| 1   | B     | 232 | LEU  |
| 1   | B     | 258 | ILE  |
| 1   | B     | 278 | GLN  |
| 1   | B     | 292 | ASP  |
| 1   | C     | 49  | CYS  |
| 1   | C     | 55  | THR  |
| 1   | C     | 96  | LYS  |
| 1   | C     | 103 | GLN  |
| 1   | C     | 135 | ASP  |
| 1   | C     | 141 | ARG  |
| 1   | C     | 149 | ASN  |
| 1   | C     | 151 | ILE  |
| 1   | C     | 195 | ARG  |
| 1   | C     | 198 | GLN  |
| 1   | C     | 204 | LYS  |
| 1   | C     | 207 | LYS  |
| 1   | C     | 208 | TYR  |
| 1   | C     | 227 | ASP  |
| 1   | C     | 232 | LEU  |
| 1   | C     | 240 | LEU  |
| 1   | C     | 280 | GLN  |
| 1   | C     | 287 | MET  |
| 1   | C     | 288 | LYS  |
| 1   | C     | 289 | GLU  |
| 1   | D     | 24  | SER  |
| 1   | D     | 32  | GLU  |
| 1   | D     | 55  | THR  |
| 1   | D     | 75  | GLN  |
| 1   | D     | 76  | GLN  |
| 1   | D     | 106 | LEU  |
| 1   | D     | 113 | GLU  |
| 1   | D     | 131 | ASN  |
| 1   | D     | 135 | ASP  |
| 1   | D     | 140 | LEU  |
| 1   | D     | 146 | LYS  |
| 1   | D     | 161 | GLU  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | D     | 166 | LEU  |
| 1   | D     | 175 | GLU  |
| 1   | D     | 178 | LEU  |
| 1   | D     | 195 | ARG  |
| 1   | D     | 197 | GLN  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 213 | ASP  |
| 1   | D     | 232 | LEU  |
| 1   | D     | 258 | ILE  |
| 1   | D     | 278 | GLN  |
| 1   | D     | 292 | ASP  |
| 2   | E     | 509 | ASP  |
| 2   | F     | 509 | ASP  |
| 2   | G     | 509 | ASP  |
| 2   | H     | 509 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 57  | ASN  |
| 1   | A     | 66  | ASN  |
| 1   | A     | 79  | GLN  |
| 1   | A     | 117 | ASN  |
| 1   | A     | 131 | ASN  |
| 1   | A     | 182 | GLN  |
| 1   | A     | 198 | GLN  |
| 1   | A     | 205 | HIS  |
| 1   | A     | 261 | HIS  |
| 1   | A     | 280 | GLN  |
| 1   | A     | 298 | ASN  |
| 1   | B     | 57  | ASN  |
| 1   | B     | 93  | GLN  |
| 1   | B     | 131 | ASN  |
| 1   | B     | 149 | ASN  |
| 1   | B     | 184 | ASN  |
| 1   | B     | 193 | HIS  |
| 1   | B     | 198 | GLN  |
| 1   | B     | 205 | HIS  |
| 1   | B     | 263 | GLN  |
| 1   | B     | 267 | HIS  |
| 1   | B     | 278 | GLN  |
| 1   | B     | 280 | GLN  |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 284 | ASN  |
| 1   | C     | 66  | ASN  |
| 1   | C     | 79  | GLN  |
| 1   | C     | 93  | GLN  |
| 1   | C     | 117 | ASN  |
| 1   | C     | 131 | ASN  |
| 1   | C     | 182 | GLN  |
| 1   | C     | 198 | GLN  |
| 1   | C     | 205 | HIS  |
| 1   | C     | 261 | HIS  |
| 1   | C     | 280 | GLN  |
| 1   | C     | 298 | ASN  |
| 1   | D     | 57  | ASN  |
| 1   | D     | 131 | ASN  |
| 1   | D     | 149 | ASN  |
| 1   | D     | 184 | ASN  |
| 1   | D     | 193 | HIS  |
| 1   | D     | 198 | GLN  |
| 1   | D     | 205 | HIS  |
| 1   | D     | 263 | GLN  |
| 1   | D     | 267 | HIS  |
| 1   | D     | 278 | GLN  |
| 1   | D     | 280 | GLN  |
| 1   | D     | 284 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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   | SO4  | A     | 1306 | -    | 4,4,4        | 0.40 | 0           | 6,6,6       | 0.08 | 0           |
| 3   | SO4  | A     | 1307 | -    | 4,4,4        | 0.60 | 0           | 6,6,6       | 0.16 | 0           |
| 3   | SO4  | A     | 1305 | -    | 4,4,4        | 0.34 | 0           | 6,6,6       | 0.06 | 0           |
| 3   | SO4  | B     | 1305 | -    | 4,4,4        | 0.39 | 0           | 6,6,6       | 0.16 | 0           |
| 3   | SO4  | B     | 1306 | -    | 4,4,4        | 0.38 | 0           | 6,6,6       | 0.16 | 0           |
| 3   | SO4  | D     | 1305 | -    | 4,4,4        | 0.43 | 0           | 6,6,6       | 0.17 | 0           |
| 3   | SO4  | C     | 1305 | -    | 4,4,4        | 0.38 | 0           | 6,6,6       | 0.08 | 0           |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

| Mol | Chain | Res  | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 3   | A     | 1307 | SO4  | 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 [i](#)

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

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

| Mol | Chain | Analysed         | <RSRZ> | #RSRZ>2      | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|------------------|--------|--------------|-----------------------|-------|
| 1   | A     | 281/281 (100%)   | -0.83  | 0 100 100    | 36, 74, 120, 136      | 0     |
| 1   | B     | 281/281 (100%)   | -0.80  | 0 100 100    | 36, 78, 117, 136      | 0     |
| 1   | C     | 281/281 (100%)   | -0.83  | 0 100 100    | 36, 74, 120, 135      | 0     |
| 1   | D     | 281/281 (100%)   | -0.78  | 1 (0%) 88 79 | 36, 78, 117, 136      | 0     |
| 2   | E     | 9/9 (100%)       | -0.58  | 0 100 100    | 95, 103, 114, 120     | 0     |
| 2   | F     | 9/9 (100%)       | -0.44  | 0 100 100    | 95, 103, 115, 120     | 0     |
| 2   | G     | 9/9 (100%)       | -0.61  | 0 100 100    | 96, 102, 115, 120     | 0     |
| 2   | H     | 9/9 (100%)       | -0.45  | 0 100 100    | 95, 103, 116, 121     | 0     |
| All | All   | 1160/1160 (100%) | -0.80  | 1 (0%) 92 90 | 36, 78, 120, 136      | 0     |

All (1) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | D     | 180 | GLU  | 2.2  |

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

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

| Mol | Type | Chain | Res  | Atoms | RSCC | RSR  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|------|-------|------|------|-----------------------------|-------|
| 4   | NI   | B     | 1309 | 1/1   | 0.89 | 0.20 | 200,200,200,200             | 0     |
| 4   | NI   | B     | 1307 | 1/1   | 0.94 | 0.13 | 200,200,200,200             | 0     |
| 4   | NI   | B     | 1310 | 1/1   | 0.94 | 0.14 | 200,200,200,200             | 0     |
| 4   | NI   | B     | 1308 | 1/1   | 0.97 | 0.16 | 200,200,200,200             | 0     |
| 3   | SO4  | B     | 1306 | 5/5   | 0.99 | 0.04 | 89,89,91,91                 | 0     |
| 3   | SO4  | C     | 1305 | 5/5   | 0.99 | 0.04 | 88,89,90,91                 | 0     |
| 3   | SO4  | D     | 1305 | 5/5   | 0.99 | 0.04 | 105,106,107,107             | 0     |
| 3   | SO4  | A     | 1305 | 5/5   | 0.99 | 0.06 | 89,90,90,91                 | 0     |
| 3   | SO4  | A     | 1306 | 5/5   | 0.99 | 0.07 | 78,79,80,80                 | 0     |
| 3   | SO4  | A     | 1307 | 5/5   | 0.99 | 0.07 | 108,109,111,112             | 0     |
| 3   | SO4  | B     | 1305 | 5/5   | 0.99 | 0.06 | 82,83,85,86                 | 0     |

## 6.5 Other polymers [i](#)

There are no such residues in this entry.