



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:31 AM UTC

PDB ID : 3PIQ / pdb\_00003piq  
Title : Crystal structure of human 2909 Fab, a quaternary structure-specific antibody against HIV-1  
Authors : Changela, A.; Gorny, M.K.; Zolla-Pazner, S.; Kwong, P.D.  
Deposited on : 2010-11-07  
Resolution : 3.33 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

|                                |   |                                                                  |
|--------------------------------|---|------------------------------------------------------------------|
| MolProbity                     | : | 4-5-2 with Phenix2.0                                             |
| 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                                                             |

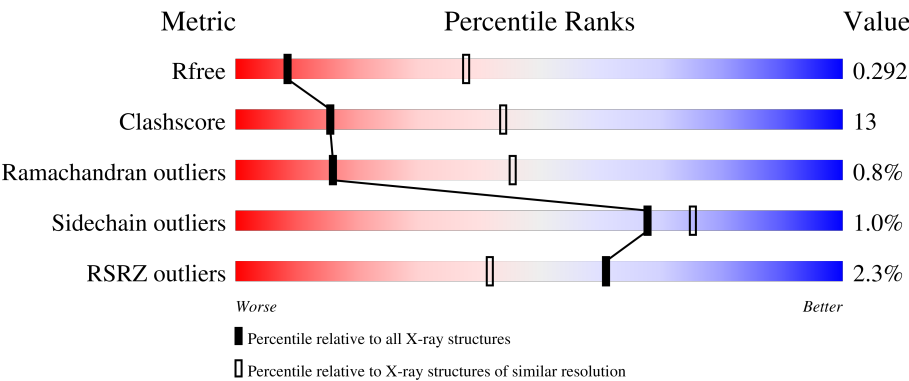
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.33 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                      | 1153 (3.34-3.30)                                      |
| Clashscore            | 190562                      | 1193 (3.34-3.30)                                      |
| Ramachandran outliers | 187476                      | 1172 (3.34-3.30)                                      |
| Sidechain outliers    | 187428                      | 1171 (3.34-3.30)                                      |
| RSRZ outliers         | 180081                      | 1153 (3.34-3.30)                                      |

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     | 231    | <div><div></div><div>65%27%7%</div></div>  |
| 1   | C     | 231    | <div><div>3%</div><div>69%26%.</div></div> |
| 1   | E     | 231    | <div><div></div><div>65%28%7%</div></div>  |
| 1   | G     | 231    | <div><div>3%</div><div>58%36%.</div></div> |
| 1   | H     | 231    | <div><div>3%</div><div>65%30%.</div></div> |

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| Mol | Chain | Length | Quality of chain                                                                      |
|-----|-------|--------|---------------------------------------------------------------------------------------|
| 1   | J     | 231    | <div><div></div><div>8%</div><div>62%</div><div>32%</div><div></div><div></div></div> |
| 2   | B     | 211    | <div><div></div><div>2%</div><div>82%</div><div>17%</div><div></div><div></div></div> |
| 2   | D     | 211    | <div><div></div><div></div><div>75%</div><div>23%</div><div></div><div></div></div>   |
| 2   | F     | 211    | <div><div></div><div>%</div><div>73%</div><div>25%</div><div></div><div></div></div>  |
| 2   | I     | 211    | <div><div></div><div>%</div><div>78%</div><div>19%</div><div></div><div></div></div>  |
| 2   | K     | 211    | <div><div></div><div>5%</div><div>72%</div><div>27%</div><div></div><div></div></div> |
| 2   | L     | 211    | <div><div></div><div></div><div>75%</div><div>23%</div><div></div><div></div></div>   |

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19449 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 Human monoclonal antibody 2909 Fab heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1   | H     | 224      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1709  | 1082 | 283 | 337 | 7 |         |         |       |
| 1   | A     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1622  | 1027 | 272 | 316 | 7 |         |         |       |
| 1   | C     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1071 | 280 | 333 | 7 |         |         |       |
| 1   | E     | 214      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1622  | 1027 | 272 | 316 | 7 |         |         |       |
| 1   | G     | 222      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1691  | 1071 | 280 | 333 | 7 |         |         |       |
| 1   | J     | 223      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1700  | 1077 | 282 | 334 | 7 |         |         |       |

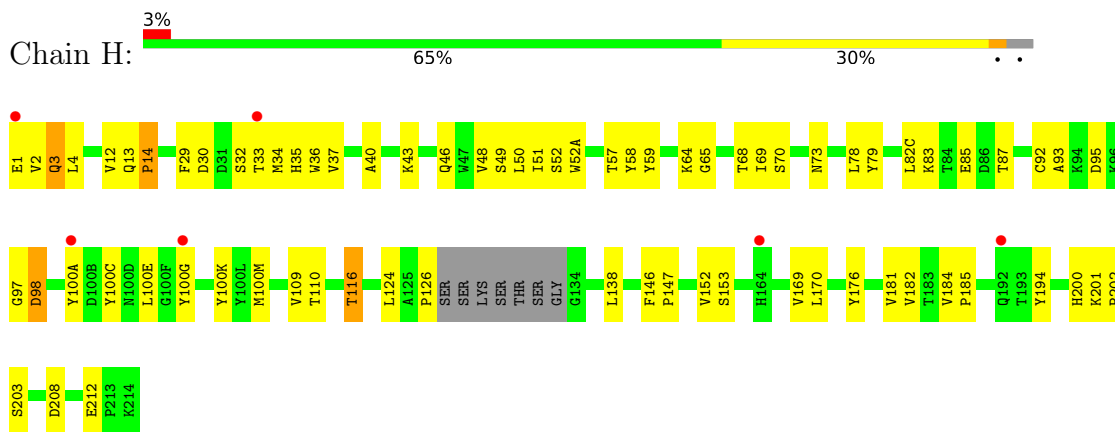
- Molecule 2 is a protein called Human monoclonal antibody 2909 Fab light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 2   | L     | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1577  | 987 | 268 | 318 | 4 |         |         |       |
| 2   | B     | 209      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1577  | 987 | 268 | 318 | 4 |         |         |       |
| 2   | D     | 208      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 978 | 267 | 316 | 4 |         |         |       |
| 2   | F     | 208      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 978 | 267 | 316 | 4 |         |         |       |
| 2   | I     | 208      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 978 | 267 | 316 | 4 |         |         |       |
| 2   | K     | 208      | Total | C   | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1565  | 978 | 267 | 316 | 4 |         |         |       |

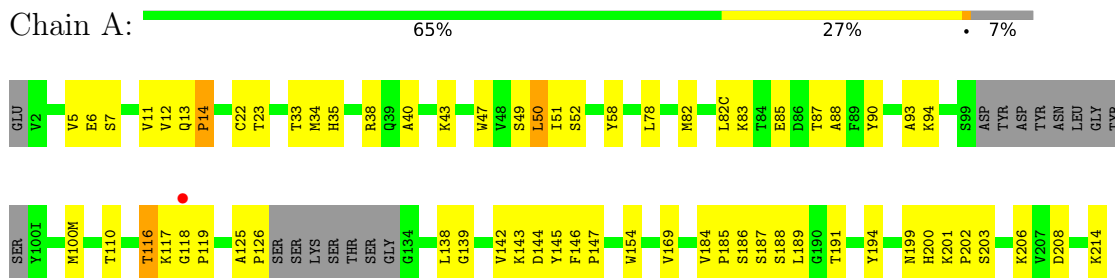
### 3 Residue-property plots [i](#)

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

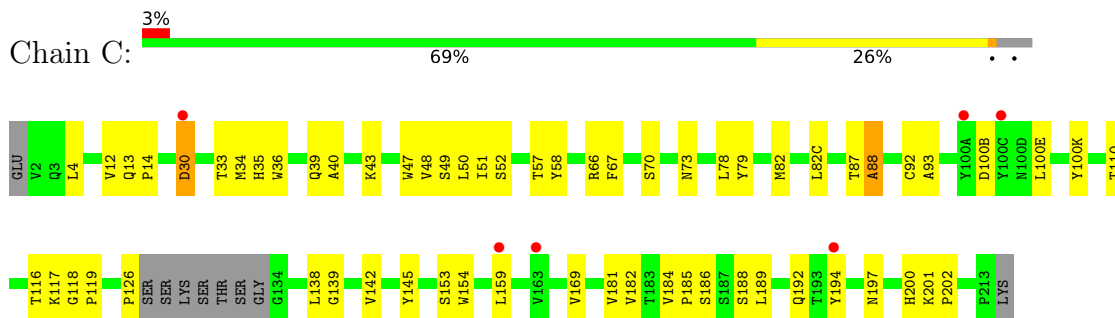
- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain



- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain

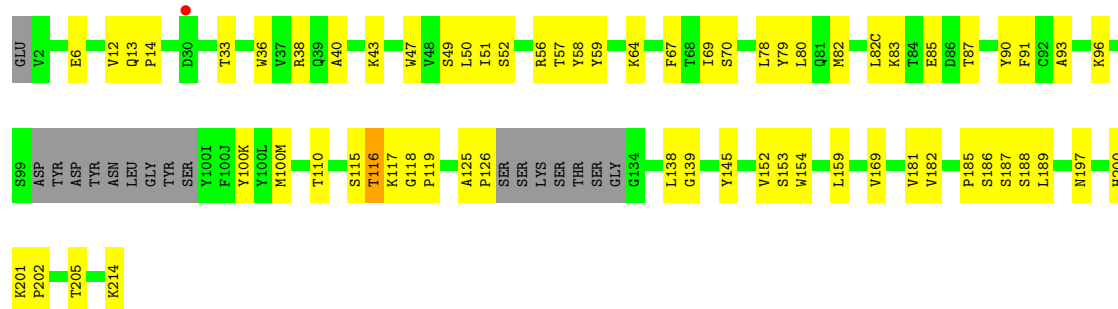


- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain



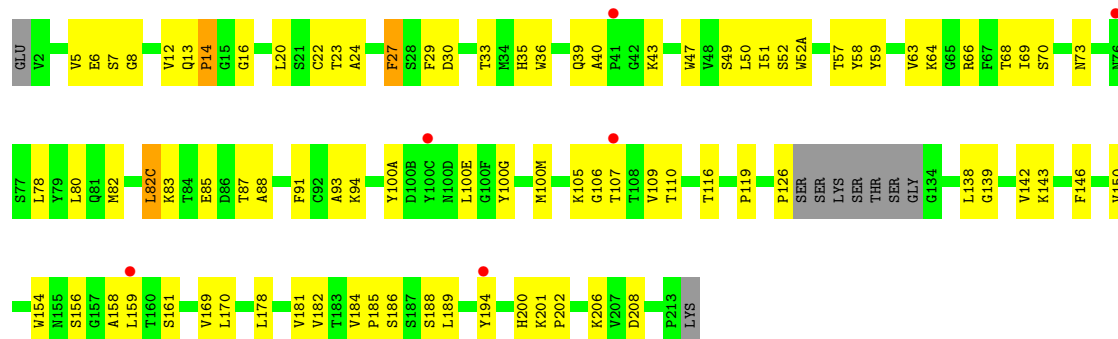
- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain

Chain E: 



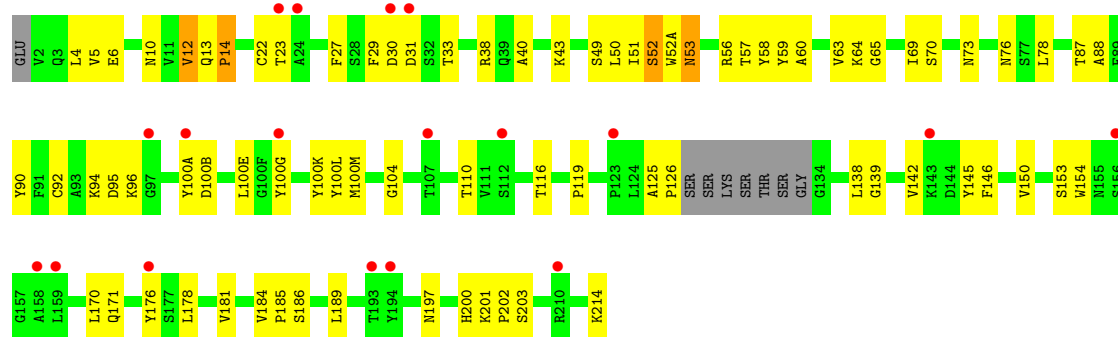
- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain

Chain G: 



- Molecule 1: Human monoclonal antibody 2909 Fab heavy chain

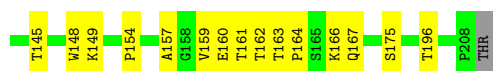
Chain J: 



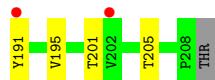
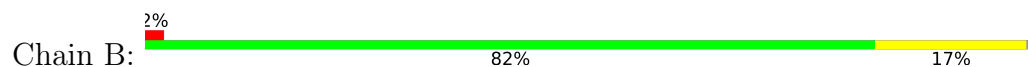
- Molecule 2: Human monoclonal antibody 2909 Fab light chain

Chain L: 

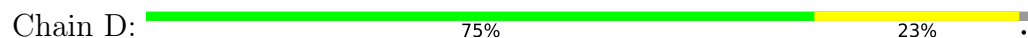




- Molecule 2: Human monoclonal antibody 2909 Fab light chain



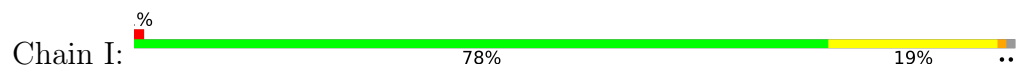
- Molecule 2: Human monoclonal antibody 2909 Fab light chain



- Molecule 2: Human monoclonal antibody 2909 Fab light chain

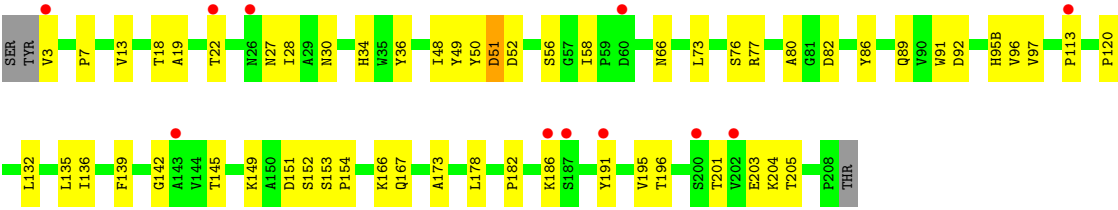


- Molecule 2: Human monoclonal antibody 2909 Fab light chain



- Molecule 2: Human monoclonal antibody 2909 Fab light chain





## 4 Data and refinement statistics

| Property                                                                | Value                                                       | Source           |
|-------------------------------------------------------------------------|-------------------------------------------------------------|------------------|
| Space group                                                             | P 32 2 1                                                    | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 180.37Å 180.37Å 222.53Å<br>90.00° 90.00° 120.00°            | Depositor        |
| Resolution (Å)                                                          | 22.38 – 3.33<br>22.38 – 3.33                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 77.6 (22.38-3.33)<br>80.6 (22.38-3.33)                      | Depositor<br>EDS |
| $R_{merge}$                                                             | (Not available)                                             | Depositor        |
| $R_{sym}$                                                               | 0.16                                                        | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 1.06 (at 3.30Å)                                             | Xtriage          |
| Refinement program                                                      | PHENIX (phenix.refine: 1.6.4_486)                           | Depositor        |
| R, $R_{free}$                                                           | 0.236 , 0.299<br>0.233 , 0.292                              | Depositor<br>DCC |
| $R_{free}$ test set                                                     | 2570 reflections (5.14%)                                    | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 67.8                                                        | Xtriage          |
| Anisotropy                                                              | 0.986                                                       | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.27 , 104.8                                                | EDS              |
| L-test for twinning <sup>2</sup>                                        | $\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$ | Xtriage          |
| Estimated twinning fraction                                             | 0.058 for -h,-k,l                                           | Xtriage          |
| $F_o, F_c$ correlation                                                  | 0.91                                                        | EDS              |
| Total number of atoms                                                   | 19449                                                       | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 115.0                                                       | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.10% 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 [i](#)

### 5.1 Standard geometry [i](#)

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     | 0.26         | 0/1662  | 0.68        | 0/2258         |
| 1   | C     | 0.26         | 0/1735  | 0.69        | 0/2361         |
| 1   | E     | 0.27         | 0/1662  | 0.72        | 0/2258         |
| 1   | G     | 0.28         | 0/1735  | 0.70        | 0/2361         |
| 1   | H     | 0.29         | 0/1753  | 0.72        | 2/2384 (0.1%)  |
| 1   | J     | 0.27         | 0/1744  | 0.71        | 0/2372         |
| 2   | B     | 0.28         | 0/1618  | 0.72        | 0/2216         |
| 2   | D     | 0.28         | 0/1605  | 0.72        | 0/2198         |
| 2   | F     | 0.29         | 0/1605  | 0.73        | 0/2198         |
| 2   | I     | 0.28         | 0/1605  | 0.71        | 0/2198         |
| 2   | K     | 0.30         | 0/1605  | 0.74        | 0/2198         |
| 2   | L     | 0.30         | 0/1618  | 0.76        | 2/2216 (0.1%)  |
| All | All   | 0.28         | 0/19947 | 0.72        | 4/27218 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2   | L     | 58  | ILE  | CA-C-N | 5.51 | 125.52      | 119.89   |
| 2   | L     | 58  | ILE  | C-N-CA | 5.51 | 125.52      | 119.89   |
| 1   | H     | 212 | GLU  | CA-C-N | 5.31 | 125.25      | 119.78   |
| 1   | H     | 212 | GLU  | C-N-CA | 5.31 | 125.25      | 119.78   |

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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     | 1622  | 0        | 1572     | 50      | 0            |
| 1   | C     | 1691  | 0        | 1620     | 42      | 0            |
| 1   | E     | 1622  | 0        | 1572     | 45      | 0            |
| 1   | G     | 1691  | 0        | 1620     | 71      | 0            |
| 1   | H     | 1709  | 0        | 1642     | 55      | 0            |
| 1   | J     | 1700  | 0        | 1633     | 64      | 0            |
| 2   | B     | 1577  | 0        | 1513     | 22      | 0            |
| 2   | D     | 1565  | 0        | 1504     | 39      | 0            |
| 2   | F     | 1565  | 0        | 1504     | 42      | 0            |
| 2   | I     | 1565  | 0        | 1504     | 36      | 0            |
| 2   | K     | 1565  | 0        | 1504     | 41      | 0            |
| 2   | L     | 1577  | 0        | 1513     | 40      | 0            |
| All | All   | 19449 | 0        | 18701    | 512     | 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 13.

All (512) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:F:27:ASN:H     | 2:F:69:ASN:HD22 | 1.23                     | 0.87              |
| 1:J:53:ASN:H     | 1:J:53:ASN:HD22 | 1.22                     | 0.87              |
| 1:G:33:THR:HG22  | 1:G:52:SER:HA   | 1.55                     | 0.87              |
| 1:E:169:VAL:HG21 | 2:F:160:GLU:HB3 | 1.58                     | 0.85              |
| 1:H:35:HIS:HB2   | 1:H:93:ALA:HB3  | 1.58                     | 0.85              |
| 2:B:149:LYS:HG2  | 2:B:154:PRO:HA  | 1.58                     | 0.84              |
| 1:C:169:VAL:HG21 | 2:D:160:GLU:HB3 | 1.63                     | 0.80              |
| 2:I:149:LYS:HG2  | 2:I:154:PRO:HA  | 1.64                     | 0.80              |
| 1:H:33:THR:HG22  | 1:H:52:SER:HA   | 1.65                     | 0.79              |
| 2:L:149:LYS:HG2  | 2:L:154:PRO:HA  | 1.64                     | 0.78              |
| 2:F:149:LYS:HG2  | 2:F:154:PRO:HA  | 1.66                     | 0.78              |
| 2:D:149:LYS:HG2  | 2:D:154:PRO:HA  | 1.64                     | 0.78              |
| 2:K:149:LYS:HG2  | 2:K:154:PRO:HA  | 1.66                     | 0.78              |
| 2:F:34:HIS:HD2   | 2:F:49:TYR:HB2  | 1.48                     | 0.77              |
| 1:J:12:VAL:HG12  | 1:J:13:GLN:H    | 1.50                     | 0.77              |
| 1:E:51:ILE:HG13  | 1:E:57:THR:HG22 | 1.66                     | 0.76              |
| 2:I:34:HIS:HD2   | 2:I:49:TYR:HB2  | 1.50                     | 0.75              |
| 1:C:35:HIS:HB2   | 1:C:93:ALA:HB3  | 1.68                     | 0.74              |
| 2:B:27:ASN:H     | 2:B:69:ASN:HD22 | 1.36                     | 0.73              |
| 1:H:169:VAL:HG21 | 2:L:160:GLU:HB3 | 1.69                     | 0.73              |
| 1:A:12:VAL:HG12  | 1:A:13:GLN:H    | 1.52                     | 0.73              |
| 1:E:126:PRO:HD3  | 1:E:138:LEU:HB3 | 1.70                     | 0.73              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:200:HIS:CD2    | 1:E:202:PRO:HD2    | 2.24                     | 0.72              |
| 1:A:191:THR:HA     | 1:J:76:ASN:HD21    | 1.54                     | 0.72              |
| 2:I:4:LEU:HD11     | 2:I:90:VAL:HG13    | 1.71                     | 0.71              |
| 1:G:169:VAL:HG21   | 2:I:160:GLU:HB3    | 1.72                     | 0.71              |
| 1:G:126:PRO:HD3    | 1:G:138:LEU:HB3    | 1.72                     | 0.71              |
| 1:E:33:THR:HG22    | 1:E:52:SER:HA      | 1.73                     | 0.71              |
| 1:G:200:HIS:CD2    | 1:G:202:PRO:HD2    | 2.26                     | 0.71              |
| 1:J:50:LEU:HD11    | 1:J:58:TYR:HD2     | 1.57                     | 0.69              |
| 2:K:132:LEU:HD12   | 2:K:178:LEU:HD23   | 1.75                     | 0.69              |
| 1:A:11:VAL:HG22    | 1:A:110:THR:HB     | 1.74                     | 0.68              |
| 1:H:49:SER:HB2     | 1:H:58:TYR:O       | 1.94                     | 0.68              |
| 1:A:47:TRP:HZ2     | 1:A:50:LEU:HD23    | 1.58                     | 0.68              |
| 1:A:22:CYS:HB3     | 1:A:78:LEU:HB3     | 1.76                     | 0.68              |
| 2:L:34:HIS:CD2     | 2:L:50:TYR:H       | 2.12                     | 0.67              |
| 1:H:200:HIS:CD2    | 1:H:202:PRO:HD2    | 2.30                     | 0.67              |
| 1:C:188:SER:HB2    | 1:C:192:GLN:NE2    | 2.10                     | 0.67              |
| 1:H:126:PRO:HD3    | 1:H:138:LEU:HB3    | 1.75                     | 0.67              |
| 1:J:100(A):TYR:HD1 | 1:J:100(G):TYR:HD1 | 1.42                     | 0.67              |
| 1:G:51:ILE:HA      | 1:G:57:THR:HG22    | 1.75                     | 0.67              |
| 2:F:132:LEU:HD12   | 2:F:178:LEU:HD23   | 1.78                     | 0.66              |
| 2:K:7:PRO:HD3      | 2:K:22:THR:HG23    | 1.78                     | 0.65              |
| 1:E:50:LEU:HD11    | 1:E:58:TYR:HD2     | 1.61                     | 0.65              |
| 2:B:34:HIS:HD2     | 2:B:49:TYR:HB2     | 1.60                     | 0.65              |
| 2:B:34:HIS:CD2     | 2:B:50:TYR:H       | 2.14                     | 0.65              |
| 1:G:181:VAL:HG21   | 2:I:135:LEU:HD13   | 1.79                     | 0.65              |
| 1:A:169:VAL:HG21   | 2:B:160:GLU:HB3    | 1.78                     | 0.65              |
| 1:C:47:TRP:CG      | 2:D:96:VAL:HB      | 2.32                     | 0.65              |
| 1:G:35:HIS:HB2     | 1:G:93:ALA:HB3     | 1.79                     | 0.65              |
| 1:J:29:PHE:CD2     | 1:J:76:ASN:HA      | 2.32                     | 0.65              |
| 2:F:27:ASN:H       | 2:F:69:ASN:ND2     | 1.92                     | 0.65              |
| 1:E:181:VAL:CG2    | 2:F:135:LEU:HD13   | 2.27                     | 0.64              |
| 1:J:22:CYS:HB3     | 1:J:78:LEU:HB3     | 1.78                     | 0.64              |
| 2:L:139:PHE:HE1    | 2:L:142:GLY:HA2    | 1.64                     | 0.63              |
| 1:H:87:THR:HG23    | 1:H:110:THR:HA     | 1.80                     | 0.63              |
| 1:C:13:GLN:HG3     | 1:C:14:PRO:HD2     | 1.78                     | 0.63              |
| 1:E:93:ALA:HB1     | 1:E:100(M):MET:HG2 | 1.81                     | 0.63              |
| 1:J:96:LYS:HD3     | 1:J:100(L):TYR:OH  | 1.99                     | 0.62              |
| 2:K:18:THR:HG22    | 2:K:76:SER:HA      | 1.81                     | 0.62              |
| 1:J:53:ASN:HD22    | 1:J:53:ASN:N       | 1.93                     | 0.62              |
| 1:C:82:MET:HB3     | 1:C:82(C):LEU:HD21 | 1.81                     | 0.62              |
| 2:L:139:PHE:CE1    | 2:L:142:GLY:HA2    | 2.34                     | 0.62              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:G:82:MET:HB3     | 1:G:82(C):LEU:HD21 | 1.81                     | 0.62              |
| 1:J:181:VAL:HG21   | 2:K:135:LEU:HD13   | 1.80                     | 0.62              |
| 2:I:167:GLN:OE1    | 2:I:173:ALA:HB2    | 2.00                     | 0.62              |
| 1:A:126:PRO:HD3    | 1:A:138:LEU:HB3    | 1.82                     | 0.62              |
| 1:J:100(A):TYR:HD1 | 1:J:100(G):TYR:CD1 | 2.18                     | 0.61              |
| 1:G:13:GLN:HG3     | 1:G:14:PRO:HD2     | 1.82                     | 0.61              |
| 2:B:27:ASN:H       | 2:B:69:ASN:ND2     | 1.98                     | 0.61              |
| 1:C:33:THR:HG22    | 1:C:52:SER:HA      | 1.83                     | 0.61              |
| 2:F:18:THR:HG22    | 2:F:76:SER:HA      | 1.83                     | 0.60              |
| 1:G:87:THR:HG23    | 1:G:110:THR:HA     | 1.82                     | 0.60              |
| 1:A:33:THR:HG22    | 1:A:52:SER:HA      | 1.83                     | 0.60              |
| 2:D:163:THR:HG23   | 2:D:164:PRO:HD2    | 1.84                     | 0.60              |
| 2:F:23:CYS:HB2     | 2:F:35:TRP:CH2     | 2.37                     | 0.60              |
| 1:A:82:MET:HB3     | 1:A:82(C):LEU:HD21 | 1.84                     | 0.60              |
| 1:J:139:GLY:HA2    | 1:J:154:TRP:HH2    | 1.66                     | 0.60              |
| 1:G:36:TRP:NE1     | 1:G:80:LEU:HB2     | 2.17                     | 0.60              |
| 1:J:33:THR:HG22    | 1:J:52:SER:HA      | 1.83                     | 0.59              |
| 1:C:100(B):ASP:HB2 | 1:C:100(E):LEU:HB3 | 1.83                     | 0.59              |
| 2:B:4:LEU:HD11     | 2:B:90:VAL:HG22    | 1.83                     | 0.59              |
| 1:G:181:VAL:CG2    | 2:I:135:LEU:HD13   | 2.32                     | 0.59              |
| 2:L:162:THR:HG23   | 2:L:175:SER:HB2    | 1.85                     | 0.59              |
| 2:I:18:THR:HG22    | 2:I:76:SER:HA      | 1.84                     | 0.59              |
| 2:D:120:PRO:HD3    | 2:D:132:LEU:HD23   | 1.84                     | 0.59              |
| 1:G:156:SER:HB3    | 2:K:56:SER:OG      | 2.03                     | 0.58              |
| 2:I:132:LEU:HD12   | 2:I:178:LEU:HD23   | 1.85                     | 0.58              |
| 2:K:27:ASN:HB3     | 2:K:30:ASN:ND2     | 2.18                     | 0.58              |
| 2:D:18:THR:HG22    | 2:D:76:SER:HA      | 1.84                     | 0.58              |
| 1:G:22:CYS:HB3     | 1:G:78:LEU:HB3     | 1.86                     | 0.58              |
| 2:D:36:TYR:HE1     | 2:D:89:GLN:HB3     | 1.66                     | 0.58              |
| 1:J:60:ALA:HB3     | 1:J:63:VAL:HG22    | 1.86                     | 0.58              |
| 1:G:30:ASP:O       | 1:G:52(A):TRP:HB2  | 2.04                     | 0.58              |
| 1:G:5:VAL:HB       | 1:G:23:THR:HB      | 1.86                     | 0.57              |
| 1:E:119:PRO:HB3    | 1:E:145:TYR:HB3    | 1.87                     | 0.57              |
| 1:E:153:SER:OG     | 1:E:197:ASN:HB2    | 2.04                     | 0.57              |
| 1:H:12:VAL:HG11    | 1:H:82(C):LEU:HD12 | 1.86                     | 0.57              |
| 1:G:47:TRP:HZ2     | 1:G:50:LEU:HG      | 1.69                     | 0.57              |
| 2:I:34:HIS:CD2     | 2:I:49:TYR:HB2     | 2.37                     | 0.57              |
| 1:C:200:HIS:CD2    | 1:C:202:PRO:HD2    | 2.40                     | 0.57              |
| 1:E:159:LEU:HD21   | 1:E:182:VAL:HG21   | 1.87                     | 0.57              |
| 2:F:27:ASN:HB3     | 2:F:30:ASN:ND2     | 2.20                     | 0.57              |
| 2:K:120:PRO:HD3    | 2:K:132:LEU:HD23   | 1.86                     | 0.57              |

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| Atom-1             | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|---------------------|--------------------------|-------------------|
| 1:C:126:PRO:HD3    | 1:C:138:LEU:HB3     | 1.86                     | 0.56              |
| 2:I:89:GLN:HG2     | 2:I:90:VAL:N        | 2.18                     | 0.56              |
| 2:D:191:TYR:O      | 2:D:205:THR:HG23    | 2.04                     | 0.56              |
| 1:G:50:LEU:HD11    | 1:G:58:TYR:HD2      | 1.70                     | 0.56              |
| 2:L:4:LEU:HD11     | 2:L:90:VAL:HG22     | 1.87                     | 0.56              |
| 1:H:4:LEU:HD22     | 1:H:92:CYS:SG       | 2.45                     | 0.56              |
| 1:E:59:TYR:HE1     | 1:E:69:ILE:HG22     | 1.69                     | 0.56              |
| 1:C:12:VAL:HG11    | 1:C:82(C):LEU:HD12  | 1.87                     | 0.56              |
| 2:I:49:TYR:CE2     | 2:I:55:PRO:HG3      | 2.41                     | 0.56              |
| 1:J:87:THR:HG23    | 1:J:110:THR:HA      | 1.86                     | 0.56              |
| 2:F:48:ILE:HD12    | 2:F:73:LEU:HD13     | 1.88                     | 0.56              |
| 1:H:13:GLN:HG3     | 1:H:14:PRO:HD2      | 1.88                     | 0.55              |
| 2:L:120:PRO:HD3    | 2:L:132:LEU:HD23    | 1.88                     | 0.55              |
| 2:B:191:TYR:O      | 2:B:205:THR:HG23    | 2.05                     | 0.55              |
| 2:K:36:TYR:HE1     | 2:K:89:GLN:HB3      | 1.69                     | 0.55              |
| 1:A:50:LEU:HD21    | 1:A:58:TYR:HD2      | 1.71                     | 0.55              |
| 1:G:35:HIS:CE1     | 1:G:100(M):MET:HE3  | 2.41                     | 0.55              |
| 1:A:13:GLN:HG3     | 1:A:14:PRO:HD2      | 1.88                     | 0.55              |
| 1:G:100(A):TYR:HD1 | 1:G:100(G):TYR:CD1  | 2.25                     | 0.55              |
| 2:D:33:VAL:HA      | 2:D:90:VAL:HG12     | 1.88                     | 0.55              |
| 2:D:89:GLN:HB2     | 2:D:98:PHE:CE1      | 2.42                     | 0.55              |
| 1:G:27:PHE:N       | 1:G:27:PHE:HD2      | 2.04                     | 0.55              |
| 1:E:181:VAL:HG21   | 2:F:135:LEU:HD13    | 1.87                     | 0.55              |
| 1:G:27:PHE:N       | 1:G:27:PHE:CD2      | 2.75                     | 0.55              |
| 1:G:70:SER:O       | 1:G:78:LEU:HD12     | 2.07                     | 0.55              |
| 1:A:186:SER:HA     | 1:A:189:LEU:HD13    | 1.89                     | 0.54              |
| 1:H:2:VAL:C        | 1:H:3:GLN:HG2       | 2.33                     | 0.54              |
| 1:G:100(E):LEU:O   | 1:G:100(E):LEU:HD23 | 2.07                     | 0.54              |
| 1:J:100(A):TYR:CD1 | 1:J:100(G):TYR:HD1  | 2.25                     | 0.54              |
| 1:G:30:ASP:HA      | 1:G:73:ASN:ND2      | 2.23                     | 0.54              |
| 2:F:191:TYR:O      | 2:F:205:THR:HG23    | 2.08                     | 0.54              |
| 1:C:34:MET:HB3     | 1:C:78:LEU:HD22     | 1.89                     | 0.54              |
| 1:C:139:GLY:HA2    | 1:C:154:TRP:CH2     | 2.42                     | 0.53              |
| 1:C:139:GLY:HA2    | 1:C:154:TRP:HH2     | 1.74                     | 0.53              |
| 1:J:139:GLY:HA2    | 1:J:154:TRP:CH2     | 2.43                     | 0.53              |
| 1:H:87:THR:HG23    | 1:H:109:VAL:O       | 2.08                     | 0.53              |
| 1:G:185:PRO:HG2    | 1:G:188:SER:OG      | 2.08                     | 0.53              |
| 1:J:13:GLN:HG3     | 1:J:14:PRO:HD2      | 1.91                     | 0.53              |
| 1:H:184:VAL:HB     | 1:H:185:PRO:HD2     | 1.91                     | 0.53              |
| 1:A:35:HIS:HB2     | 1:A:93:ALA:HB3      | 1.89                     | 0.53              |
| 1:A:208:ASP:HB2    | 1:G:206:LYS:HB2     | 1.91                     | 0.53              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:E:82:MET:HB3     | 1:E:82(C):LEU:HD21 | 1.91                     | 0.53              |
| 1:G:12:VAL:HG11    | 1:G:82(C):LEU:HD12 | 1.89                     | 0.53              |
| 1:H:100(K):TYR:HD2 | 2:L:91:TRP:CE3     | 2.27                     | 0.52              |
| 1:C:117:LYS:HG2    | 1:C:118:GLY:O      | 2.10                     | 0.52              |
| 1:H:184:VAL:HG11   | 1:H:194:TYR:CE1    | 2.44                     | 0.52              |
| 1:A:47:TRP:CZ2     | 1:A:50:LEU:HD23    | 2.42                     | 0.52              |
| 1:G:159:LEU:HD21   | 1:G:182:VAL:HG21   | 1.91                     | 0.52              |
| 2:K:167:GLN:OE1    | 2:K:173:ALA:HB2    | 2.09                     | 0.52              |
| 2:I:120:PRO:HD3    | 2:I:132:LEU:HD23   | 1.91                     | 0.52              |
| 1:H:59:TYR:HE1     | 1:H:69:ILE:HG22    | 1.75                     | 0.52              |
| 1:H:64:LYS:HD2     | 1:H:65:GLY:H       | 1.74                     | 0.52              |
| 2:L:49:TYR:CD2     | 2:L:49:TYR:N       | 2.78                     | 0.52              |
| 2:B:7:PRO:HD3      | 2:B:22:THR:HG23    | 1.92                     | 0.52              |
| 1:J:200:HIS:CD2    | 1:J:202:PRO:HD2    | 2.44                     | 0.52              |
| 2:I:48:ILE:HD12    | 2:I:73:LEU:HD13    | 1.91                     | 0.52              |
| 1:C:87:THR:O       | 1:C:88:ALA:HB2     | 2.09                     | 0.52              |
| 2:K:48:ILE:HD12    | 2:K:73:LEU:HD13    | 1.92                     | 0.52              |
| 1:J:52(A):TRP:CE3  | 1:J:53:ASN:HB3     | 2.45                     | 0.51              |
| 2:K:49:TYR:CD1     | 2:K:50:TYR:HD2     | 2.28                     | 0.51              |
| 1:H:50:LEU:HD12    | 1:H:50:LEU:C       | 2.35                     | 0.51              |
| 1:C:184:VAL:HG11   | 1:C:194:TYR:CE1    | 2.46                     | 0.51              |
| 1:G:35:HIS:CE1     | 1:G:50:LEU:HB3     | 2.45                     | 0.51              |
| 1:J:186:SER:HA     | 1:J:189:LEU:HD13   | 1.91                     | 0.51              |
| 2:K:49:TYR:HD1     | 2:K:50:TYR:CD2     | 2.28                     | 0.51              |
| 2:D:73:LEU:HD12    | 2:D:74:THR:N       | 2.25                     | 0.51              |
| 2:F:49:TYR:CE2     | 2:F:55:PRO:HG3     | 2.45                     | 0.51              |
| 2:B:167:GLN:OE1    | 2:B:173:ALA:HB2    | 2.10                     | 0.51              |
| 1:J:40:ALA:HB3     | 1:J:43:LYS:HB2     | 1.92                     | 0.51              |
| 1:J:64:LYS:HD2     | 1:J:65:GLY:H       | 1.76                     | 0.51              |
| 1:J:100(M):MET:HE1 | 2:K:96:VAL:HG11    | 1.92                     | 0.51              |
| 1:E:38:ARG:HB3     | 1:E:90:TYR:CE1     | 2.45                     | 0.51              |
| 1:C:30:ASP:HB3     | 1:C:73:ASN:HB3     | 1.93                     | 0.51              |
| 1:A:200:HIS:CD2    | 1:A:202:PRO:HD2    | 2.46                     | 0.51              |
| 2:F:36:TYR:HE1     | 2:F:89:GLN:HB3     | 1.75                     | 0.51              |
| 1:J:4:LEU:HD13     | 1:J:92:CYS:O       | 2.11                     | 0.51              |
| 2:D:23:CYS:HB2     | 2:D:35:TRP:CH2     | 2.45                     | 0.50              |
| 2:F:34:HIS:HD2     | 2:F:49:TYR:CB      | 2.22                     | 0.50              |
| 1:G:139:GLY:HA2    | 1:G:154:TRP:CH2    | 2.45                     | 0.50              |
| 2:B:18:THR:HG22    | 2:B:76:SER:HA      | 1.91                     | 0.50              |
| 2:D:50:TYR:O       | 2:D:51:ASP:HB2     | 2.11                     | 0.50              |
| 1:H:40:ALA:HB3     | 1:H:43:LYS:HB2     | 1.94                     | 0.50              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 1:H:100(A):TYR:HD1 | 1:H:100(G):TYR:CD1 | 2.29                     | 0.50              |
| 1:G:13:GLN:CG      | 1:G:14:PRO:HD2     | 2.41                     | 0.50              |
| 1:J:69:ILE:HD11    | 1:J:78:LEU:HD11    | 1.93                     | 0.50              |
| 1:H:59:TYR:CE1     | 1:H:69:ILE:HG22    | 2.47                     | 0.50              |
| 1:A:40:ALA:HB3     | 1:A:43:LYS:HB2     | 1.93                     | 0.50              |
| 1:C:87:THR:HG23    | 1:C:110:THR:HA     | 1.93                     | 0.50              |
| 2:F:92:ASP:HB3     | 2:F:95(B):HIS:H    | 1.76                     | 0.50              |
| 1:G:36:TRP:CD1     | 1:G:69:ILE:HD12    | 2.46                     | 0.50              |
| 1:G:40:ALA:HB3     | 1:G:43:LYS:HB2     | 1.94                     | 0.50              |
| 2:I:75:ILE:HG22    | 2:I:78:VAL:HG22    | 1.93                     | 0.50              |
| 2:L:33:VAL:HA      | 2:L:90:VAL:HG12    | 1.92                     | 0.50              |
| 1:J:126:PRO:HD3    | 1:J:138:LEU:HB3    | 1.92                     | 0.50              |
| 1:E:49:SER:HB2     | 1:E:58:TYR:O       | 2.12                     | 0.50              |
| 1:H:51:ILE:HG13    | 1:H:57:THR:HG22    | 1.92                     | 0.50              |
| 2:L:157:ALA:HB1    | 2:I:69:ASN:OD1     | 2.12                     | 0.50              |
| 1:C:50:LEU:HD12    | 1:C:50:LEU:C       | 2.36                     | 0.50              |
| 2:D:85:ASP:HA      | 2:D:102:THR:O      | 2.11                     | 0.50              |
| 1:E:185:PRO:HG2    | 1:E:188:SER:OG     | 2.12                     | 0.49              |
| 1:E:87:THR:HG23    | 1:E:110:THR:HA     | 1.94                     | 0.49              |
| 1:A:87:THR:HG23    | 1:A:110:THR:HA     | 1.94                     | 0.49              |
| 2:K:34:HIS:HD2     | 2:K:49:TYR:HB2     | 1.77                     | 0.49              |
| 1:A:83:LYS:HB3     | 1:A:85:GLU:OE1     | 2.11                     | 0.49              |
| 1:E:40:ALA:HB3     | 1:E:43:LYS:HB2     | 1.94                     | 0.49              |
| 1:G:30:ASP:HA      | 1:G:73:ASN:HD22    | 1.77                     | 0.49              |
| 1:A:94:LYS:O       | 1:A:100(M):MET:HA  | 2.13                     | 0.49              |
| 1:H:50:LEU:HD11    | 1:H:58:TYR:HD2     | 1.78                     | 0.49              |
| 1:A:125:ALA:HB3    | 1:A:214:LYS:HE2    | 1.93                     | 0.49              |
| 1:G:50:LEU:HD11    | 1:G:58:TYR:CD2     | 2.47                     | 0.49              |
| 1:J:30:ASP:HA      | 1:J:73:ASN:ND2     | 2.27                     | 0.49              |
| 2:L:120:PRO:HD3    | 2:L:132:LEU:CD2    | 2.42                     | 0.49              |
| 1:A:49:SER:HB2     | 1:A:58:TYR:O       | 2.13                     | 0.49              |
| 1:C:184:VAL:HG11   | 1:C:194:TYR:HE1    | 1.77                     | 0.49              |
| 1:C:186:SER:HA     | 1:C:189:LEU:HD13   | 1.94                     | 0.49              |
| 1:G:24:ALA:HB1     | 1:G:27:PHE:CE2     | 2.48                     | 0.49              |
| 2:I:49:TYR:HE2     | 2:I:55:PRO:HG3     | 1.77                     | 0.49              |
| 1:A:87:THR:O       | 1:A:88:ALA:HB2     | 2.13                     | 0.49              |
| 1:G:186:SER:HA     | 1:G:189:LEU:HD13   | 1.95                     | 0.48              |
| 2:D:89:GLN:HB2     | 2:D:98:PHE:CD1     | 2.48                     | 0.48              |
| 2:I:141:PRO:HD2    | 2:I:198:GLU:OE2    | 2.13                     | 0.48              |
| 1:J:100(K):TYR:HD2 | 2:K:91:TRP:CD2     | 2.31                     | 0.48              |
| 2:K:49:TYR:CD1     | 2:K:50:TYR:CD2     | 3.01                     | 0.48              |

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| Atom-1              | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|---------------------|---------------------|--------------------------|-------------------|
| 1:H:100(E):LEU:HD23 | 1:H:100(E):LEU:O    | 2.13                     | 0.48              |
| 1:A:191:THR:HA      | 1:J:76:ASN:ND2      | 2.26                     | 0.48              |
| 1:E:50:LEU:C        | 1:E:50:LEU:HD12     | 2.38                     | 0.48              |
| 2:I:145:THR:HB      | 2:I:196:THR:HB      | 1.96                     | 0.48              |
| 1:H:100(K):TYR:HD2  | 2:L:91:TRP:CD2      | 2.31                     | 0.48              |
| 1:E:181:VAL:HG22    | 2:F:135:LEU:HD13    | 1.94                     | 0.48              |
| 2:F:49:TYR:HE2      | 2:F:55:PRO:HG3      | 1.78                     | 0.48              |
| 1:A:47:TRP:CG       | 2:B:96:VAL:HB       | 2.49                     | 0.48              |
| 1:E:70:SER:O        | 1:E:78:LEU:HD12     | 2.14                     | 0.48              |
| 1:E:70:SER:OG       | 1:E:79:TYR:HB2      | 2.12                     | 0.48              |
| 2:F:7:PRO:HD3       | 2:F:22:THR:HG23     | 1.95                     | 0.48              |
| 1:H:83:LYS:HB3      | 1:H:85:GLU:OE1      | 2.14                     | 0.48              |
| 2:F:27:ASN:HB3      | 2:F:30:ASN:HD21     | 1.78                     | 0.48              |
| 2:K:120:PRO:HD3     | 2:K:132:LEU:CD2     | 2.44                     | 0.48              |
| 1:A:12:VAL:HG12     | 1:A:13:GLN:N        | 2.24                     | 0.48              |
| 2:L:34:HIS:HD2      | 2:L:50:TYR:H        | 1.59                     | 0.48              |
| 2:D:54:ARG:HD2      | 2:D:58:ILE:O        | 2.14                     | 0.48              |
| 2:D:167:GLN:OE1     | 2:D:173:ALA:HB2     | 2.14                     | 0.48              |
| 1:J:52(A):TRP:CZ3   | 1:J:53:ASN:HB3      | 2.49                     | 0.48              |
| 1:J:27:PHE:CE2      | 1:J:94:LYS:HD2      | 2.49                     | 0.48              |
| 2:F:34:HIS:CD2      | 2:F:49:TYR:HB2      | 2.39                     | 0.47              |
| 1:G:83:LYS:HB3      | 1:G:85:GLU:OE1      | 2.13                     | 0.47              |
| 2:D:34:HIS:CD2      | 2:D:50:TYR:H        | 2.32                     | 0.47              |
| 1:G:24:ALA:HB1      | 1:G:27:PHE:CZ       | 2.48                     | 0.47              |
| 1:G:169:VAL:HG22    | 1:G:170:LEU:H       | 1.78                     | 0.47              |
| 2:K:3:VAL:HG22      | 2:K:3:VAL:O         | 2.15                     | 0.47              |
| 1:E:201:LYS:N       | 1:E:202:PRO:CD      | 2.78                     | 0.47              |
| 1:A:201:LYS:C       | 1:A:203:SER:H       | 2.23                     | 0.47              |
| 1:C:39:GLN:C        | 1:C:88:ALA:HB1      | 2.40                     | 0.47              |
| 2:D:89:GLN:HE21     | 2:D:96:VAL:HG13     | 1.80                     | 0.47              |
| 2:L:36:TYR:HE1      | 2:L:89:GLN:HB3      | 1.80                     | 0.47              |
| 1:C:82:MET:HE2      | 1:C:82(C):LEU:HD21  | 1.97                     | 0.47              |
| 1:E:13:GLN:HG3      | 1:E:14:PRO:HD2      | 1.97                     | 0.47              |
| 1:E:125:ALA:HB3     | 1:E:214:LYS:HE2     | 1.96                     | 0.47              |
| 1:J:100(E):LEU:O    | 1:J:100(E):LEU:HD23 | 2.15                     | 0.47              |
| 2:B:132:LEU:HD12    | 2:B:178:LEU:HD23    | 1.96                     | 0.47              |
| 2:D:120:PRO:HD3     | 2:D:132:LEU:CD2     | 2.45                     | 0.47              |
| 1:G:184:VAL:HB      | 1:G:185:PRO:HD2     | 1.97                     | 0.47              |
| 1:J:6:GLU:OE1       | 1:J:104:GLY:HA3     | 2.14                     | 0.47              |
| 1:J:29:PHE:CE2      | 1:J:76:ASN:HA       | 2.49                     | 0.47              |
| 1:J:60:ALA:HA       | 2:K:95(B):HIS:CE1   | 2.49                     | 0.47              |

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| Atom-1            | Atom-2              | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|---------------------|--------------------------|-------------------|
| 1:A:199:ASN:HD21  | 1:A:206:LYS:HE2     | 1.79                     | 0.47              |
| 2:L:119:PRO:HA    | 2:L:132:LEU:HD23    | 1.96                     | 0.47              |
| 1:G:119:PRO:HB2   | 1:G:142:VAL:HG13    | 1.96                     | 0.47              |
| 1:J:100(B):ASP:CB | 1:J:100(E):LEU:HB3  | 2.45                     | 0.47              |
| 1:H:78:LEU:HD12   | 1:H:79:TYR:H        | 1.80                     | 0.47              |
| 2:L:18:THR:HG22   | 2:L:76:SER:HA       | 1.95                     | 0.47              |
| 1:A:119:PRO:HB3   | 1:A:145:TYR:HB3     | 1.96                     | 0.47              |
| 1:G:12:VAL:HG12   | 1:G:13:GLN:N        | 2.30                     | 0.47              |
| 1:H:170:LEU:HD13  | 1:H:176:TYR:CE2     | 2.50                     | 0.46              |
| 1:C:159:LEU:HD21  | 1:C:182:VAL:HG21    | 1.97                     | 0.46              |
| 2:D:54:ARG:CG     | 2:D:58:ILE:HB       | 2.45                     | 0.46              |
| 2:F:89:GLN:HE21   | 2:F:96:VAL:HG13     | 1.80                     | 0.46              |
| 1:G:184:VAL:HG11  | 1:G:194:TYR:HE1     | 1.80                     | 0.46              |
| 1:J:12:VAL:HG12   | 1:J:13:GLN:N        | 2.25                     | 0.46              |
| 1:C:47:TRP:CZ3    | 2:D:95(B):HIS:HA    | 2.51                     | 0.46              |
| 2:D:24:GLY:HA2    | 2:D:70:THR:HA       | 1.97                     | 0.46              |
| 2:D:73:LEU:HD12   | 2:D:74:THR:H        | 1.80                     | 0.46              |
| 2:D:132:LEU:HD12  | 2:D:178:LEU:HD23    | 1.97                     | 0.46              |
| 2:F:120:PRO:HD3   | 2:F:132:LEU:HD23    | 1.96                     | 0.46              |
| 1:G:139:GLY:HA2   | 1:G:154:TRP:HH2     | 1.80                     | 0.46              |
| 2:I:162:THR:HG23  | 2:I:175:SER:HB2     | 1.96                     | 0.46              |
| 2:K:195:VAL:O     | 2:K:201:THR:HA      | 2.16                     | 0.46              |
| 2:F:23:CYS:HB2    | 2:F:35:TRP:HH2      | 1.81                     | 0.46              |
| 1:H:29:PHE:CE2    | 1:H:73:ASN:HA       | 2.50                     | 0.46              |
| 2:B:120:PRO:HD3   | 2:B:132:LEU:HD23    | 1.98                     | 0.46              |
| 1:C:185:PRO:HG2   | 1:C:188:SER:OG      | 2.16                     | 0.46              |
| 1:G:50:LEU:C      | 1:G:50:LEU:HD12     | 2.41                     | 0.46              |
| 1:G:201:LYS:N     | 1:G:202:PRO:CD      | 2.77                     | 0.46              |
| 1:A:199:ASN:ND2   | 1:A:206:LYS:HE2     | 2.31                     | 0.46              |
| 1:C:100(E):LEU:C  | 1:C:100(E):LEU:HD23 | 2.41                     | 0.46              |
| 1:C:119:PRO:HB2   | 1:C:142:VAL:HG13    | 1.98                     | 0.46              |
| 1:J:59:TYR:HE1    | 1:J:69:ILE:HG22     | 1.81                     | 0.46              |
| 2:D:145:THR:HB    | 2:D:196:THR:HB      | 1.98                     | 0.46              |
| 1:E:67:PHE:CE2    | 1:E:82:MET:HE3      | 2.50                     | 0.46              |
| 2:F:141:PRO:HD2   | 2:F:198:GLU:OE2     | 2.16                     | 0.46              |
| 2:F:149:LYS:HD2   | 2:F:152:SER:O       | 2.16                     | 0.46              |
| 2:F:167:GLN:OE1   | 2:F:173:ALA:HB2     | 2.16                     | 0.46              |
| 1:H:37:VAL:HG13   | 1:H:46:GLN:O        | 2.16                     | 0.45              |
| 2:L:89:GLN:HE21   | 2:L:96:VAL:HG13     | 1.81                     | 0.45              |
| 2:L:163:THR:HG23  | 2:L:164:PRO:HD2     | 1.98                     | 0.45              |
| 1:A:139:GLY:HA2   | 1:A:154:TRP:CH2     | 2.51                     | 0.45              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 2:B:50:TYR:O       | 2:B:51:ASP:HB2    | 2.16                     | 0.45              |
| 1:E:12:VAL:HG12    | 1:E:13:GLN:N      | 2.31                     | 0.45              |
| 1:H:50:LEU:HD11    | 1:H:58:TYR:CD2    | 2.52                     | 0.45              |
| 2:F:195:VAL:O      | 2:F:201:THR:HA    | 2.17                     | 0.45              |
| 1:H:1:GLU:HG3      | 1:H:2:VAL:H       | 1.80                     | 0.45              |
| 2:L:13:VAL:HG11    | 2:L:19:ALA:HB2    | 1.99                     | 0.45              |
| 2:B:65:SER:OG      | 2:B:72:THR:HB     | 2.16                     | 0.45              |
| 2:F:46:LEU:HD21    | 2:F:49:TYR:CD2    | 2.51                     | 0.45              |
| 1:G:68:THR:O       | 1:G:80:LEU:HD12   | 2.16                     | 0.45              |
| 2:B:91:TRP:HE3     | 2:B:96:VAL:HG22   | 1.81                     | 0.45              |
| 1:G:161:SER:HB3    | 2:K:77:ARG:HH12   | 1.81                     | 0.45              |
| 1:J:119:PRO:HB2    | 1:J:142:VAL:HG13  | 1.99                     | 0.45              |
| 1:C:51:ILE:HG13    | 1:C:57:THR:HG22   | 1.99                     | 0.45              |
| 1:C:49:SER:HB2     | 1:C:58:TYR:O      | 2.16                     | 0.45              |
| 1:J:153:SER:OG     | 1:J:197:ASN:HB2   | 2.16                     | 0.45              |
| 2:K:191:TYR:O      | 2:K:205:THR:HG23  | 2.16                     | 0.45              |
| 2:D:55:PRO:HD2     | 2:D:58:ILE:HG13   | 1.97                     | 0.45              |
| 2:F:163:THR:HG23   | 2:F:164:PRO:HD2   | 1.98                     | 0.45              |
| 1:J:150:VAL:HG13   | 1:J:178:LEU:HD21  | 1.99                     | 0.45              |
| 1:A:206:LYS:HB2    | 1:G:208:ASP:HB2   | 1.99                     | 0.45              |
| 1:C:188:SER:HB2    | 1:C:192:GLN:HE21  | 1.81                     | 0.45              |
| 1:G:36:TRP:CE2     | 1:G:80:LEU:HB2    | 2.50                     | 0.45              |
| 1:J:49:SER:HB2     | 1:J:58:TYR:O      | 2.17                     | 0.45              |
| 1:H:181:VAL:HG21   | 2:L:135:LEU:HD13  | 1.98                     | 0.45              |
| 1:G:184:VAL:HG11   | 1:G:194:TYR:CE1   | 2.52                     | 0.45              |
| 1:C:119:PRO:HB3    | 1:C:145:TYR:HB3   | 1.99                     | 0.45              |
| 1:E:52:SER:HB3     | 1:E:56:ARG:HG2    | 1.99                     | 0.45              |
| 1:G:116:THR:HA     | 1:G:146:PHE:O     | 2.17                     | 0.45              |
| 1:H:201:LYS:N      | 1:H:202:PRO:CD    | 2.80                     | 0.44              |
| 2:I:13:VAL:HG11    | 2:I:19:ALA:HB2    | 1.98                     | 0.44              |
| 2:L:161:THR:HG23   | 2:L:175:SER:O     | 2.17                     | 0.44              |
| 1:C:100(K):TYR:HD2 | 2:D:91:TRP:CD2    | 2.35                     | 0.44              |
| 2:K:80:ALA:C       | 2:K:82:ASP:H      | 2.26                     | 0.44              |
| 1:E:185:PRO:C      | 1:E:187:SER:H     | 2.25                     | 0.44              |
| 1:C:4:LEU:HD22     | 1:C:92:CYS:SG     | 2.58                     | 0.44              |
| 1:G:5:VAL:HG13     | 1:G:105:LYS:HD2   | 1.98                     | 0.44              |
| 1:G:39:GLN:C       | 1:G:88:ALA:HB1    | 2.43                     | 0.44              |
| 1:G:63:VAL:HG12    | 1:G:66:ARG:NH2    | 2.32                     | 0.44              |
| 1:G:94:LYS:O       | 1:G:100(M):MET:HA | 2.17                     | 0.44              |
| 1:E:47:TRP:CG      | 2:F:96:VAL:HB     | 2.52                     | 0.44              |
| 1:J:116:THR:HA     | 1:J:146:PHE:O     | 2.18                     | 0.44              |

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| Atom-1             | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|--------------------|--------------------------|-------------------|
| 2:L:49:TYR:N       | 2:L:49:TYR:HD2     | 2.16                     | 0.44              |
| 1:G:82:MET:CB      | 1:G:82(C):LEU:HD21 | 2.46                     | 0.44              |
| 2:L:80:ALA:C       | 2:L:82:ASP:H       | 2.26                     | 0.44              |
| 2:K:113:PRO:HA     | 2:K:139:PHE:HB3    | 1.98                     | 0.44              |
| 1:H:30:ASP:O       | 1:H:52(A):TRP:HB2  | 2.17                     | 0.44              |
| 1:A:38:ARG:HB3     | 1:A:90:TYR:CE1     | 2.52                     | 0.44              |
| 1:E:50:LEU:HD11    | 1:E:58:TYR:CD2     | 2.46                     | 0.44              |
| 1:J:49:SER:HB2     | 1:J:59:TYR:HD1     | 1.82                     | 0.44              |
| 2:L:145:THR:HB     | 2:L:196:THR:HB     | 2.00                     | 0.44              |
| 2:K:153:SER:HA     | 2:K:154:PRO:HD3    | 1.85                     | 0.44              |
| 1:C:153:SER:OG     | 1:C:197:ASN:HB2    | 2.17                     | 0.43              |
| 2:F:203:GLU:O      | 2:F:204:LYS:HD3    | 2.17                     | 0.43              |
| 1:G:6:GLU:OE1      | 1:G:91:PHE:HA      | 2.18                     | 0.43              |
| 1:G:8:GLY:O        | 1:G:20:LEU:HD23    | 2.18                     | 0.43              |
| 2:K:56:SER:C       | 2:K:58:ILE:H       | 2.25                     | 0.43              |
| 2:K:166:LYS:HE3    | 2:K:166:LYS:HB2    | 1.86                     | 0.43              |
| 1:H:201:LYS:C      | 1:H:203:SER:H      | 2.26                     | 0.43              |
| 2:L:83:GLU:O       | 2:L:84:ALA:HB2     | 2.18                     | 0.43              |
| 2:L:134:CYS:HB2    | 2:L:148:TRP:CH2    | 2.53                     | 0.43              |
| 1:A:146:PHE:HA     | 1:A:147:PRO:HA     | 1.79                     | 0.43              |
| 1:J:94:LYS:HG2     | 1:J:95:ASP:N       | 2.32                     | 0.43              |
| 1:A:184:VAL:HG11   | 1:A:194:TYR:CE1    | 2.52                     | 0.43              |
| 1:H:51:ILE:HA      | 1:H:57:THR:HG22    | 2.01                     | 0.43              |
| 2:L:159:VAL:HG12   | 2:L:160:GLU:N      | 2.33                     | 0.43              |
| 2:D:34:HIS:HD2     | 2:D:49:TYR:HA      | 1.83                     | 0.43              |
| 1:G:7:SER:HA       | 1:G:107:THR:HG21   | 1.99                     | 0.43              |
| 2:B:47:VAL:O       | 2:B:55:PRO:HD2     | 2.19                     | 0.43              |
| 1:C:40:ALA:HB3     | 1:C:43:LYS:HB2     | 2.00                     | 0.43              |
| 1:C:70:SER:OG      | 1:C:79:TYR:HB2     | 2.18                     | 0.43              |
| 1:H:93:ALA:HB1     | 1:H:100(M):MET:HB3 | 2.01                     | 0.43              |
| 1:C:181:VAL:HG21   | 2:D:135:LEU:HD13   | 2.01                     | 0.43              |
| 1:G:156:SER:C      | 1:G:158:ALA:H      | 2.27                     | 0.43              |
| 1:J:125:ALA:HB3    | 1:J:214:LYS:HE2    | 2.00                     | 0.43              |
| 1:H:146:PHE:HA     | 1:H:147:PRO:HA     | 1.79                     | 0.43              |
| 1:E:36:TRP:NE1     | 1:E:80:LEU:HB2     | 2.34                     | 0.43              |
| 1:E:100(K):TYR:HD2 | 2:F:91:TRP:CE3     | 2.37                     | 0.43              |
| 2:I:130:ALA:HB3    | 2:I:180:LEU:O      | 2.19                     | 0.43              |
| 1:H:70:SER:O       | 1:H:78:LEU:HD12    | 2.18                     | 0.43              |
| 2:B:201:THR:O      | 2:B:201:THR:HG22   | 2.18                     | 0.43              |
| 1:J:30:ASP:HA      | 1:J:73:ASN:HD22    | 1.83                     | 0.43              |
| 1:J:119:PRO:HB3    | 1:J:145:TYR:HB3    | 2.00                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:K:13:VAL:HG11  | 2:K:19:ALA:HB2   | 2.00                     | 0.43              |
| 2:K:182:PRO:O    | 2:K:186:LYS:HG3  | 2.19                     | 0.43              |
| 1:H:51:ILE:HG13  | 1:H:57:THR:CG2   | 2.49                     | 0.43              |
| 1:A:5:VAL:HB     | 1:A:23:THR:HB    | 2.01                     | 0.43              |
| 1:E:117:LYS:HG2  | 1:E:118:GLY:O    | 2.19                     | 0.43              |
| 2:F:54:ARG:HA    | 2:F:55:PRO:HD3   | 1.78                     | 0.43              |
| 2:I:4:LEU:HD11   | 2:I:90:VAL:CG1   | 2.45                     | 0.43              |
| 2:D:51:ASP:O     | 2:D:64:GLY:HA3   | 2.18                     | 0.42              |
| 1:G:105:LYS:HG3  | 1:G:106:GLY:H    | 1.82                     | 0.42              |
| 2:K:139:PHE:HE1  | 2:K:142:GLY:HA2  | 1.83                     | 0.42              |
| 1:H:97:GLY:O     | 1:H:98:ASP:C     | 2.63                     | 0.42              |
| 2:L:7:PRO:HD3    | 2:L:22:THR:HG23  | 2.02                     | 0.42              |
| 2:L:59:PRO:C     | 2:L:61:ARG:H     | 2.27                     | 0.42              |
| 2:D:7:PRO:HD3    | 2:D:22:THR:HG23  | 2.02                     | 0.42              |
| 1:G:143:LYS:HB2  | 1:G:143:LYS:HE3  | 1.83                     | 0.42              |
| 2:I:132:LEU:HD21 | 2:I:185:TRP:CZ3  | 2.54                     | 0.42              |
| 1:J:5:VAL:HB     | 1:J:23:THR:HB    | 2.00                     | 0.42              |
| 1:H:34:MET:HB3   | 1:H:78:LEU:HD22  | 2.02                     | 0.42              |
| 2:L:162:THR:CG2  | 2:L:175:SER:HB2  | 2.49                     | 0.42              |
| 2:F:107:GLY:O    | 2:F:108:GLN:HG3  | 2.19                     | 0.42              |
| 1:H:33:THR:OG1   | 1:H:95:ASP:HB3   | 2.19                     | 0.42              |
| 1:E:64:LYS:HD2   | 1:E:64:LYS:HA    | 1.78                     | 0.42              |
| 1:E:152:VAL:HG12 | 1:E:153:SER:N    | 2.33                     | 0.42              |
| 1:E:13:GLN:HE21  | 1:E:13:GLN:HB2   | 1.63                     | 0.42              |
| 1:J:33:THR:OG1   | 1:J:95:ASP:HB3   | 2.19                     | 0.42              |
| 1:J:171:GLN:OE1  | 1:J:171:GLN:HA   | 2.19                     | 0.42              |
| 2:L:34:HIS:HD2   | 2:L:49:TYR:HB2   | 1.84                     | 0.42              |
| 2:F:50:TYR:O     | 2:F:51:ASP:HB2   | 2.19                     | 0.42              |
| 2:I:159:VAL:HG22 | 2:I:178:LEU:HD13 | 2.02                     | 0.42              |
| 2:I:163:THR:HG23 | 2:I:164:PRO:HD2  | 2.02                     | 0.42              |
| 1:H:124:LEU:HB3  | 2:L:118:PHE:CE1  | 2.55                     | 0.42              |
| 2:L:166:LYS:HB2  | 2:L:166:LYS:HE3  | 1.89                     | 0.42              |
| 1:A:50:LEU:HD12  | 1:A:51:ILE:N     | 2.34                     | 0.42              |
| 1:E:96:LYS:HE2   | 1:E:96:LYS:HB3   | 1.83                     | 0.42              |
| 2:I:48:ILE:HD12  | 2:I:73:LEU:CD1   | 2.50                     | 0.42              |
| 2:I:166:LYS:HB2  | 2:I:166:LYS:HE3  | 1.85                     | 0.42              |
| 1:H:208:ASP:O    | 1:E:205:THR:HA   | 2.19                     | 0.42              |
| 1:J:87:THR:O     | 1:J:88:ALA:HB2   | 2.19                     | 0.42              |
| 2:D:151:ASP:O    | 2:D:152:SER:HB2  | 2.20                     | 0.42              |
| 1:G:150:VAL:HG13 | 1:G:178:LEU:HD21 | 2.00                     | 0.42              |
| 2:K:51:ASP:CG    | 2:K:66:ASN:HD22  | 2.27                     | 0.42              |

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| Atom-1            | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|--------------------|--------------------------|-------------------|
| 2:K:89:GLN:HA     | 2:K:97:VAL:O       | 2.20                     | 0.42              |
| 2:K:91:TRP:CE2    | 2:K:92:ASP:O       | 2.73                     | 0.42              |
| 2:K:203:GLU:O     | 2:K:204:LYS:HD3    | 2.20                     | 0.42              |
| 1:H:184:VAL:HG11  | 1:H:194:TYR:HE1    | 1.83                     | 0.42              |
| 2:L:94:ASN:OD1    | 2:I:153:SER:HB3    | 2.20                     | 0.42              |
| 1:J:51:ILE:HG13   | 1:J:57:THR:HG22    | 2.01                     | 0.42              |
| 1:H:152:VAL:HG12  | 1:H:153:SER:N      | 2.35                     | 0.41              |
| 1:E:83:LYS:HB3    | 1:E:85:GLU:OE1     | 2.20                     | 0.41              |
| 2:F:77:ARG:O      | 2:F:78:VAL:C       | 2.63                     | 0.41              |
| 1:H:116:THR:HA    | 1:H:146:PHE:O      | 2.20                     | 0.41              |
| 1:G:29:PHE:HD2    | 1:G:73:ASN:HA      | 1.85                     | 0.41              |
| 2:I:54:ARG:HA     | 2:I:55:PRO:HD3     | 1.83                     | 0.41              |
| 2:I:120:PRO:HD3   | 2:I:132:LEU:CD2    | 2.50                     | 0.41              |
| 2:I:151:ASP:O     | 2:I:152:SER:HB2    | 2.19                     | 0.41              |
| 1:A:82:MET:CB     | 1:A:82(C):LEU:HD21 | 2.50                     | 0.41              |
| 1:A:117:LYS:HG2   | 1:A:118:GLY:O      | 2.20                     | 0.41              |
| 1:E:115:SER:O     | 1:E:116:THR:C      | 2.63                     | 0.41              |
| 2:F:80:ALA:C      | 2:F:82:ASP:H       | 2.27                     | 0.41              |
| 2:I:61:ARG:HD2    | 2:I:76:SER:O       | 2.20                     | 0.41              |
| 2:K:28:ILE:O      | 2:K:28:ILE:HG12    | 2.20                     | 0.41              |
| 1:A:184:VAL:HG11  | 1:A:194:TYR:HE1    | 1.86                     | 0.41              |
| 2:B:134:CYS:HB2   | 2:B:148:TRP:CH2    | 2.55                     | 0.41              |
| 1:C:201:LYS:N     | 1:C:202:PRO:CD     | 2.82                     | 0.41              |
| 1:E:6:GLU:OE1     | 1:E:91:PHE:HA      | 2.19                     | 0.41              |
| 1:G:87:THR:O      | 1:G:88:ALA:HB2     | 2.20                     | 0.41              |
| 2:F:89:GLN:HE21   | 2:F:96:VAL:CG1     | 2.34                     | 0.41              |
| 2:K:151:ASP:O     | 2:K:152:SER:HB2    | 2.20                     | 0.41              |
| 1:A:34:MET:HB3    | 1:A:78:LEU:HD22    | 2.02                     | 0.41              |
| 2:B:151:ASP:O     | 2:B:152:SER:HB2    | 2.20                     | 0.41              |
| 1:C:36:TRP:O      | 1:C:48:VAL:HB      | 2.20                     | 0.41              |
| 2:D:34:HIS:HD2    | 2:D:49:TYR:CB      | 2.34                     | 0.41              |
| 1:J:51:ILE:HA     | 1:J:57:THR:HG22    | 2.03                     | 0.41              |
| 1:J:100(M):MET:SD | 1:J:100(M):MET:N   | 2.94                     | 0.41              |
| 1:J:201:LYS:C     | 1:J:203:SER:H      | 2.28                     | 0.41              |
| 1:H:36:TRP:O      | 1:H:48:VAL:HB      | 2.21                     | 0.41              |
| 1:H:64:LYS:HD2    | 1:H:65:GLY:N       | 2.36                     | 0.41              |
| 2:D:139:PHE:CE1   | 2:D:142:GLY:HA2    | 2.55                     | 0.41              |
| 2:D:159:VAL:HG22  | 2:D:178:LEU:HD13   | 2.03                     | 0.41              |
| 1:E:186:SER:HA    | 1:E:189:LEU:HD13   | 2.01                     | 0.41              |
| 2:I:33:VAL:HA     | 2:I:89:GLN:O       | 2.21                     | 0.41              |
| 2:I:153:SER:HA    | 2:I:154:PRO:HD3    | 1.84                     | 0.41              |

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| Atom-1             | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|-------------------|--------------------------|-------------------|
| 1:J:70:SER:O       | 1:J:78:LEU:HD12   | 2.21                     | 0.41              |
| 1:H:100(M):MET:SD  | 1:H:100(M):MET:N  | 2.94                     | 0.41              |
| 1:A:6:GLU:O        | 1:A:7:SER:HB3     | 2.20                     | 0.41              |
| 1:A:50:LEU:HD21    | 1:A:58:TYR:CD2    | 2.53                     | 0.41              |
| 1:G:87:THR:HG23    | 1:G:109:VAL:O     | 2.21                     | 0.41              |
| 1:J:184:VAL:HB     | 1:J:185:PRO:HD2   | 2.02                     | 0.41              |
| 2:K:36:TYR:O       | 2:K:86:TYR:HA     | 2.20                     | 0.41              |
| 1:C:66:ARG:C       | 1:C:67:PHE:HD1    | 2.29                     | 0.41              |
| 2:D:54:ARG:HG3     | 2:D:58:ILE:HB     | 2.01                     | 0.41              |
| 2:D:149:LYS:HD2    | 2:D:152:SER:O     | 2.21                     | 0.41              |
| 2:F:7:PRO:HA       | 2:F:8:PRO:HD3     | 1.95                     | 0.41              |
| 1:H:1:GLU:HG3      | 1:H:2:VAL:N       | 2.36                     | 0.41              |
| 1:H:124:LEU:HB3    | 2:L:118:PHE:CD1   | 2.55                     | 0.41              |
| 1:A:201:LYS:C      | 1:A:203:SER:N     | 2.79                     | 0.41              |
| 2:B:195:VAL:O      | 2:B:201:THR:HA    | 2.21                     | 0.41              |
| 1:J:38:ARG:HB3     | 1:J:90:TYR:CE1    | 2.55                     | 0.41              |
| 2:L:28:ILE:HG23    | 2:L:66:ASN:OD1    | 2.21                     | 0.40              |
| 1:A:143:LYS:HB2    | 1:A:143:LYS:HE3   | 1.84                     | 0.40              |
| 1:G:169:VAL:HG22   | 1:G:170:LEU:N     | 2.36                     | 0.40              |
| 2:I:162:THR:CG2    | 2:I:175:SER:HB2   | 2.51                     | 0.40              |
| 1:J:170:LEU:HD13   | 1:J:176:TYR:CE2   | 2.56                     | 0.40              |
| 2:K:145:THR:HB     | 2:K:196:THR:HB    | 2.04                     | 0.40              |
| 1:A:119:PRO:HB2    | 1:A:142:VAL:HG13  | 2.03                     | 0.40              |
| 1:A:185:PRO:HG2    | 1:A:188:SER:OG    | 2.21                     | 0.40              |
| 1:E:139:GLY:HA2    | 1:E:154:TRP:CH2   | 2.55                     | 0.40              |
| 1:J:64:LYS:HD2     | 1:J:65:GLY:N      | 2.37                     | 0.40              |
| 2:K:50:TYR:O       | 2:K:52:ASP:N      | 2.54                     | 0.40              |
| 2:F:166:LYS:HE3    | 2:F:166:LYS:HB2   | 1.86                     | 0.40              |
| 1:G:49:SER:HB2     | 1:G:59:TYR:HD1    | 1.86                     | 0.40              |
| 1:J:50:LEU:HD12    | 1:J:50:LEU:C      | 2.46                     | 0.40              |
| 2:K:113:PRO:HB3    | 2:K:136:ILE:CG2   | 2.52                     | 0.40              |
| 1:H:100(C):TYR:CD2 | 1:H:100(C):TYR:N  | 2.89                     | 0.40              |
| 2:L:59:PRO:C       | 2:L:61:ARG:N      | 2.79                     | 0.40              |
| 1:A:116:THR:HA     | 1:A:146:PHE:O     | 2.22                     | 0.40              |
| 1:A:185:PRO:C      | 1:A:187:SER:H     | 2.30                     | 0.40              |
| 1:J:94:LYS:O       | 1:J:100(M):MET:HA | 2.22                     | 0.40              |
| 2:L:34:HIS:CD2     | 2:L:49:TYR:HB2    | 2.57                     | 0.40              |
| 1:A:184:VAL:HB     | 1:A:185:PRO:HD2   | 2.04                     | 0.40              |
| 2:D:34:HIS:HD2     | 2:D:49:TYR:CA     | 2.34                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | A     | 208/231 (90%)   | 183 (88%)  | 23 (11%)  | 2 (1%)   | 12          | 41  |
| 1   | C     | 218/231 (94%)   | 193 (88%)  | 24 (11%)  | 1 (0%)   | 24          | 56  |
| 1   | E     | 208/231 (90%)   | 185 (89%)  | 23 (11%)  | 0        | 100         | 100 |
| 1   | G     | 218/231 (94%)   | 190 (87%)  | 25 (12%)  | 3 (1%)   | 9           | 34  |
| 1   | H     | 220/231 (95%)   | 195 (89%)  | 23 (10%)  | 2 (1%)   | 14          | 43  |
| 1   | J     | 219/231 (95%)   | 193 (88%)  | 23 (10%)  | 3 (1%)   | 9           | 34  |
| 2   | B     | 207/211 (98%)   | 180 (87%)  | 27 (13%)  | 0        | 100         | 100 |
| 2   | D     | 206/211 (98%)   | 177 (86%)  | 28 (14%)  | 1 (0%)   | 24          | 56  |
| 2   | F     | 206/211 (98%)   | 172 (84%)  | 31 (15%)  | 3 (2%)   | 8           | 33  |
| 2   | I     | 206/211 (98%)   | 176 (85%)  | 27 (13%)  | 3 (2%)   | 8           | 33  |
| 2   | K     | 206/211 (98%)   | 181 (88%)  | 24 (12%)  | 1 (0%)   | 24          | 56  |
| 2   | L     | 207/211 (98%)   | 179 (86%)  | 27 (13%)  | 1 (0%)   | 24          | 56  |
| All | All   | 2529/2652 (95%) | 2204 (87%) | 305 (12%) | 20 (1%)  | 16          | 45  |

All (20) Ramachandran outliers are listed below:

| Mol | Chain | Res    | Type |
|-----|-------|--------|------|
| 1   | H     | 98     | ASP  |
| 2   | L     | 167    | GLN  |
| 2   | K     | 51     | ASP  |
| 1   | A     | 144    | ASP  |
| 1   | C     | 88     | ALA  |
| 2   | F     | 106(A) | LEU  |
| 1   | J     | 10     | ASN  |
| 2   | F     | 26     | ASN  |
| 1   | J     | 52     | SER  |
| 1   | H     | 14     | PRO  |
| 1   | A     | 14     | PRO  |
| 1   | G     | 14     | PRO  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | G     | 82(C) | LEU  |
| 2   | I     | 90    | VAL  |
| 2   | F     | 78    | VAL  |
| 2   | I     | 55    | PRO  |
| 1   | G     | 16    | GLY  |
| 2   | I     | 78    | VAL  |
| 2   | D     | 90    | VAL  |
| 1   | J     | 14    | PRO  |

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | A     | 182/197 (92%)   | 180 (99%)  | 2 (1%)   | 65          | 74  |
| 1   | C     | 189/197 (96%)   | 187 (99%)  | 2 (1%)   | 65          | 74  |
| 1   | E     | 182/197 (92%)   | 181 (100%) | 1 (0%)   | 81          | 82  |
| 1   | G     | 189/197 (96%)   | 187 (99%)  | 2 (1%)   | 65          | 74  |
| 1   | H     | 191/197 (97%)   | 186 (97%)  | 5 (3%)   | 40          | 64  |
| 1   | J     | 190/197 (96%)   | 186 (98%)  | 4 (2%)   | 47          | 66  |
| 2   | B     | 176/178 (99%)   | 174 (99%)  | 2 (1%)   | 65          | 74  |
| 2   | D     | 175/178 (98%)   | 174 (99%)  | 1 (1%)   | 78          | 80  |
| 2   | F     | 175/178 (98%)   | 175 (100%) | 0        | 100         | 100 |
| 2   | I     | 175/178 (98%)   | 174 (99%)  | 1 (1%)   | 78          | 80  |
| 2   | K     | 175/178 (98%)   | 175 (100%) | 0        | 100         | 100 |
| 2   | L     | 176/178 (99%)   | 174 (99%)  | 2 (1%)   | 65          | 74  |
| All | All   | 2175/2250 (97%) | 2153 (99%) | 22 (1%)  | 68          | 75  |

All (22) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 3   | GLN  |
| 1   | H     | 32  | SER  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | H     | 68  | THR  |
| 1   | H     | 116 | THR  |
| 1   | H     | 182 | VAL  |
| 2   | L     | 49  | TYR  |
| 2   | L     | 136 | ILE  |
| 1   | A     | 50  | LEU  |
| 1   | A     | 116 | THR  |
| 2   | B     | 3   | VAL  |
| 2   | B     | 136 | ILE  |
| 1   | C     | 30  | ASP  |
| 1   | C     | 116 | THR  |
| 2   | D     | 136 | ILE  |
| 1   | E     | 116 | THR  |
| 1   | G     | 27  | PHE  |
| 1   | G     | 64  | LYS  |
| 2   | I     | 22  | THR  |
| 1   | J     | 12  | VAL  |
| 1   | J     | 31  | ASP  |
| 1   | J     | 53  | ASN  |
| 1   | J     | 56  | ARG  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | H     | 13    | GLN  |
| 1   | H     | 200   | HIS  |
| 2   | L     | 34    | HIS  |
| 2   | L     | 69    | ASN  |
| 2   | L     | 108   | GLN  |
| 2   | L     | 126   | GLN  |
| 2   | L     | 188   | HIS  |
| 2   | L     | 197   | HIS  |
| 1   | A     | 13    | GLN  |
| 1   | A     | 164   | HIS  |
| 1   | A     | 200   | HIS  |
| 2   | B     | 27    | ASN  |
| 2   | B     | 34    | HIS  |
| 2   | B     | 69    | ASN  |
| 2   | B     | 89    | GLN  |
| 2   | B     | 95(B) | HIS  |
| 2   | B     | 108   | GLN  |
| 2   | B     | 188   | HIS  |

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| Mol | Chain | Res   | Type |
|-----|-------|-------|------|
| 1   | C     | 13    | GLN  |
| 1   | C     | 81    | GLN  |
| 1   | C     | 82(A) | ASN  |
| 1   | C     | 164   | HIS  |
| 1   | C     | 192   | GLN  |
| 2   | D     | 27    | ASN  |
| 2   | D     | 30    | ASN  |
| 2   | D     | 32    | ASN  |
| 2   | D     | 34    | HIS  |
| 2   | D     | 188   | HIS  |
| 1   | E     | 13    | GLN  |
| 1   | E     | 164   | HIS  |
| 2   | F     | 34    | HIS  |
| 2   | F     | 69    | ASN  |
| 2   | F     | 89    | GLN  |
| 2   | F     | 108   | GLN  |
| 2   | F     | 170   | ASN  |
| 2   | F     | 188   | HIS  |
| 1   | G     | 13    | GLN  |
| 1   | G     | 164   | HIS  |
| 2   | I     | 26    | ASN  |
| 2   | I     | 30    | ASN  |
| 2   | I     | 34    | HIS  |
| 2   | I     | 108   | GLN  |
| 2   | I     | 188   | HIS  |
| 1   | J     | 13    | GLN  |
| 1   | J     | 53    | ASN  |
| 1   | J     | 76    | ASN  |
| 2   | K     | 30    | ASN  |
| 2   | K     | 108   | GLN  |
| 2   | K     | 170   | 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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

| Mol | Chain | Analysed        | <RSRZ> | #RSRZ>2       | OWAB(Å <sup>2</sup> ) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|-------|
| 1   | A     | 214/231 (92%)   | 0.20   | 1 (0%) 87 76  | 73, 119, 176, 274     | 0     |
| 1   | C     | 222/231 (96%)   | 0.24   | 6 (2%) 56 37  | 52, 112, 219, 322     | 0     |
| 1   | E     | 214/231 (92%)   | -0.10  | 1 (0%) 87 76  | 33, 76, 123, 155      | 0     |
| 1   | G     | 222/231 (96%)   | 0.41   | 6 (2%) 56 37  | 65, 123, 204, 311     | 0     |
| 1   | H     | 224/231 (96%)   | 0.11   | 6 (2%) 56 37  | 32, 78, 142, 249      | 0     |
| 1   | J     | 223/231 (96%)   | 0.64   | 18 (8%) 18 13 | 60, 140, 252, 443     | 0     |
| 2   | B     | 209/211 (99%)   | 0.07   | 4 (1%) 66 47  | 65, 115, 177, 250     | 0     |
| 2   | D     | 208/211 (98%)   | 0.22   | 1 (0%) 87 76  | 56, 118, 204, 295     | 0     |
| 2   | F     | 208/211 (98%)   | -0.07  | 3 (1%) 73 55  | 44, 91, 146, 261      | 0     |
| 2   | I     | 208/211 (98%)   | 0.14   | 3 (1%) 73 55  | 50, 109, 180, 234     | 0     |
| 2   | K     | 208/211 (98%)   | 0.38   | 11 (5%) 32 22 | 77, 135, 208, 274     | 0     |
| 2   | L     | 209/211 (99%)   | -0.12  | 0 100 100     | 34, 87, 136, 201      | 0     |
| All | All   | 2569/2652 (96%) | 0.18   | 60 (2%) 61 42 | 32, 108, 197, 443     | 0     |

All (60) RSRZ outliers are listed below:

| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | J     | 100(A) | TYR  | 3.7  |
| 1   | J     | 112    | SER  | 3.6  |
| 1   | J     | 23     | THR  | 3.6  |
| 1   | H     | 100(A) | TYR  | 3.5  |
| 1   | J     | 194    | TYR  | 3.5  |
| 1   | J     | 24     | ALA  | 3.5  |
| 2   | K     | 26     | ASN  | 3.4  |
| 1   | G     | 76     | ASN  | 3.4  |
| 1   | G     | 41     | PRO  | 3.2  |
| 2   | K     | 22     | THR  | 3.2  |
| 2   | K     | 3      | VAL  | 3.1  |

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| Mol | Chain | Res    | Type | RSRZ |
|-----|-------|--------|------|------|
| 1   | A     | 118    | GLY  | 3.0  |
| 1   | C     | 30     | ASP  | 3.0  |
| 1   | C     | 159    | LEU  | 3.0  |
| 2   | K     | 191    | TYR  | 3.0  |
| 1   | J     | 100(G) | TYR  | 2.9  |
| 2   | F     | 189    | ARG  | 2.9  |
| 1   | G     | 194    | TYR  | 2.9  |
| 2   | B     | 50     | TYR  | 2.9  |
| 2   | F     | 108    | GLN  | 2.8  |
| 2   | K     | 202    | VAL  | 2.7  |
| 2   | K     | 186    | LYS  | 2.6  |
| 1   | C     | 100(C) | TYR  | 2.6  |
| 1   | J     | 158    | ALA  | 2.6  |
| 1   | G     | 107    | THR  | 2.6  |
| 1   | G     | 159    | LEU  | 2.5  |
| 2   | B     | 191    | TYR  | 2.5  |
| 2   | K     | 200    | SER  | 2.5  |
| 2   | I     | 47     | VAL  | 2.5  |
| 1   | J     | 159    | LEU  | 2.5  |
| 2   | K     | 187    | SER  | 2.5  |
| 1   | H     | 1      | GLU  | 2.5  |
| 1   | H     | 164    | HIS  | 2.5  |
| 2   | K     | 143    | ALA  | 2.4  |
| 2   | I     | 108    | GLN  | 2.4  |
| 2   | B     | 22     | THR  | 2.4  |
| 1   | H     | 192    | GLN  | 2.4  |
| 2   | D     | 152    | SER  | 2.4  |
| 1   | C     | 194    | TYR  | 2.4  |
| 1   | J     | 210    | ARG  | 2.4  |
| 1   | H     | 100(G) | TYR  | 2.4  |
| 1   | H     | 33     | THR  | 2.3  |
| 2   | K     | 113    | PRO  | 2.3  |
| 1   | J     | 193    | THR  | 2.3  |
| 1   | G     | 100(C) | TYR  | 2.3  |
| 2   | B     | 202    | VAL  | 2.3  |
| 1   | J     | 30     | ASP  | 2.3  |
| 1   | J     | 31     | ASP  | 2.3  |
| 1   | C     | 100(A) | TYR  | 2.2  |
| 1   | J     | 123    | PRO  | 2.2  |
| 2   | K     | 60     | ASP  | 2.2  |
| 1   | C     | 163    | VAL  | 2.1  |
| 2   | F     | 188    | HIS  | 2.1  |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | J     | 97  | GLY  | 2.1  |
| 2   | I     | 152 | SER  | 2.1  |
| 1   | J     | 156 | SER  | 2.1  |
| 1   | E     | 30  | ASP  | 2.1  |
| 1   | J     | 107 | THR  | 2.0  |
| 1   | J     | 176 | TYR  | 2.0  |
| 1   | J     | 143 | LYS  | 2.0  |

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.