# Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 02:55 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 2Q4P |
| Title | : | Ensemble refinement of the crystal structure of protein from Mus musculus Mm.29898 |
| Authors | : | Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG) |
| Deposited on | : | 2007-05-31 |
| Resolution | : | 2.32 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

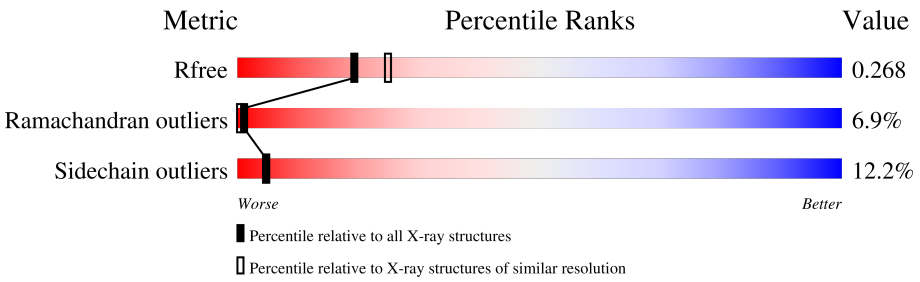
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.35 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 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 2.32 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 (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| $R_{free}$ | 130704 | 5974 (2.34-2.30) |
| Ramachandran outliers | 138981 | 6523 (2.34-2.30) |
| Sidechain outliers | 138945 | 6523 (2.34-2.30) |

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 >=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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1-A | 170 | 55% 11% • 34% |
| 1 | 1-B | 170 | 56% 8% 36% |
| 1 | 10-A | 170 | 55% 9% • 34% |
| 1 | 10-B | 170 | 54% 10% 36% |
| 1 | 11-A | 170 | 49% 16% • 34% |
| 1 | 11-B | 170 | 57% 6% • 36% |
| 1 | 12-A | 170 | 54% 11% • 34% |
| 1 | 12-B | 170 | 50% 14% • 36% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 13-A | 170 | 52% 14% • 34% |
| 1 | 13-B | 170 | 46% 15% • 36% |
| 1 | 14-A | 170 | 49% 16% • 34% |
| 1 | 14-B | 170 | 45% 16% • 36% |
| 1 | 15-A | 170 | 52% 14% • 34% |
| 1 | 15-B | 170 | 46% 16% • 36% |
| 1 | 16-A | 170 | 46% 15% 5% 34% |
| 1 | 16-B | 170 | 41% 21% • 36% |
| 1 | 2-A | 170 | 55% 11% • 34% |
| 1 | 2-B | 170 | 54% 9% • 36% |
| 1 | 3-A | 170 | 59% 6% • 34% |
| 1 | 3-B | 170 | 58% 6% 36% |
| 1 | 4-A | 170 | 58% 8% 34% |
| 1 | 4-B | 170 | 53% 10% • 36% |
| 1 | 5-A | 170 | 58% 8% 34% |
| 1 | 5-B | 170 | 54% 9% • 36% |
| 1 | 6-A | 170 | 58% 8% • 34% |
| 1 | 6-B | 170 | 53% 11% • 36% |
| 1 | 7-A | 170 | 58% 7% • 34% |
| 1 | 7-B | 170 | 53% 10% • 36% |
| 1 | 8-A | 170 | 59% 8% 34% |
| 1 | 8-B | 170 | 52% 11% • 36% |
| 1 | 9-A | 170 | 54% 11% • 34% |
| 1 | 9-B | 170 | 57% 6% • 36% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29392 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 Protein RS21-C6.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | Se | | | |
| 1 | 1-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 2-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 3-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 4-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 5-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 6-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 7-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 8-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 9-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 10-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 11-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 12-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 13-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 14-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 15-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |
| 1 | 16-A | 113 | 922 | 589 | 163 | 168 | 1 | 1 | 0 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | Se | | | |
| 1 | 1-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 2-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 3-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 4-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 5-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 6-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 7-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 8-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 9-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 10-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 11-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 12-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 13-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 14-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 15-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |
| 1 | 16-B | 109 | 891 | 569 | 157 | 163 | 1 | 1 | 0 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 1 | MSE | MET | modified residue | UNP Q9QY93 |
| A | 122 | MSE | MET | modified residue | UNP Q9QY93 |
| B | 1 | MSE | MET | modified residue | UNP Q9QY93 |
| B | 122 | MSE | MET | modified residue | UNP Q9QY93 |

- Molecule 2 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | 1-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 2-A | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 3-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 4-A | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 5-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 6-A | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 7-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 8-A | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 9-A | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 10-A | 10 | 10 | 10 | 0 | 0 |
| | | | Total | O | | |
| 2 | 11-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 12-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 13-A | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 14-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 15-A | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 16-A | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 1-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 2-B | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 3-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 4-B | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 5-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 6-B | 13 | 13 | 13 | 0 | 0 |

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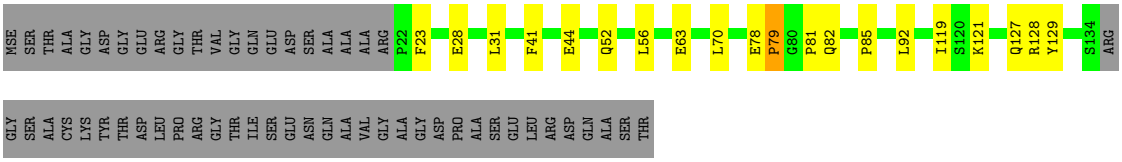
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | 7-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 8-B | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 9-B | 13 | 13 | 13 | 0 | 0 |
| | | | Total | O | | |
| 2 | 10-B | 14 | 14 | 14 | 0 | 0 |
| | | | Total | O | | |
| 2 | 11-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 12-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 13-B | 11 | 11 | 11 | 0 | 0 |
| | | | Total | O | | |
| 2 | 14-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 15-B | 12 | 12 | 12 | 0 | 0 |
| | | | Total | O | | |
| 2 | 16-B | 11 | 11 | 11 | 0 | 0 |

# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

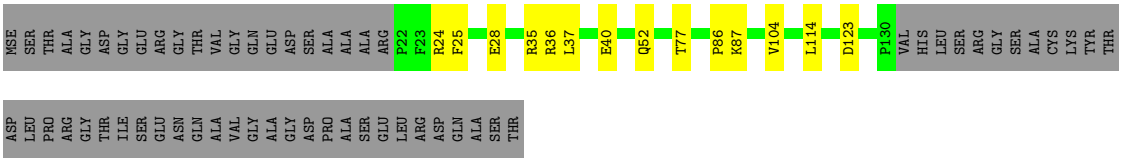
• Molecule 1: Protein RS21-C6

Chain 1-A:



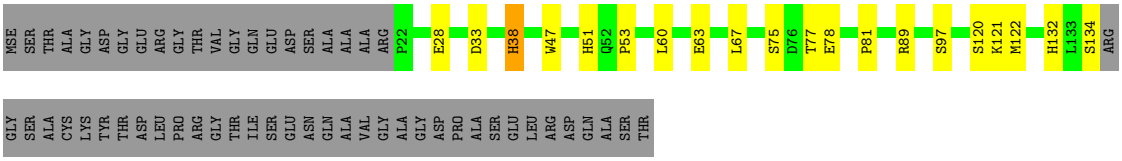

• Molecule 1: Protein RS21-C6

Chain 1-B:



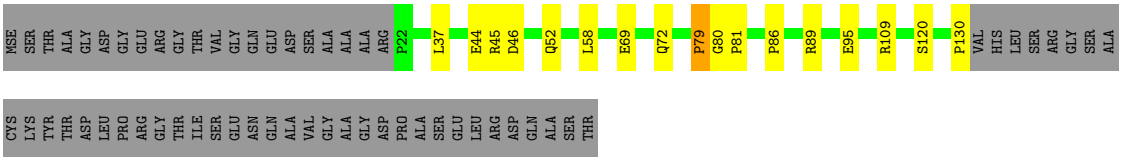

• Molecule 1: Protein RS21-C6

Chain 2-A:




• Molecule 1: Protein RS21-C6

Chain 2-B:




• Molecule 1: Protein RS21-C6

Chain 3-A: 59% 6% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 E40 F41 A42 E48 Q52 P53 R54 E63 L67 D76 T77 Q82 Y129 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE

SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 3-B: 58% 6% 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 H38 T77 E78 P79 W84 P85 P86 R89 E94 V104 I119 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG

GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 4-A: 58% 8% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 W47 R54 E63 V64 L67 T77 P81 W84 P85 P86 Y102 R109 M122 R126 Y129 S134 ARG GLY SER ALA CYS LYS TYR THR ASP

LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 4-B: 53% 10% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 L31 D46 Q49 R54 E63 Q72 T77 E78 P79 G80 P81 Q82 A83 R89 V104 R109 D113 I119 M122 P130 VAL HIS

LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

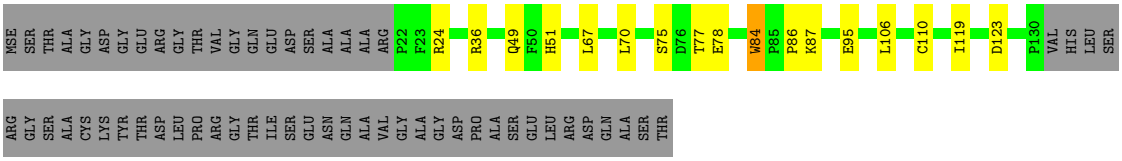
Chain 5-A: 58% 8% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 S26 P27 D33 E48 L67 Q72 P79 G80 P81 Q82 R89 I119 R128 Y129 H132 L133 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO

ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

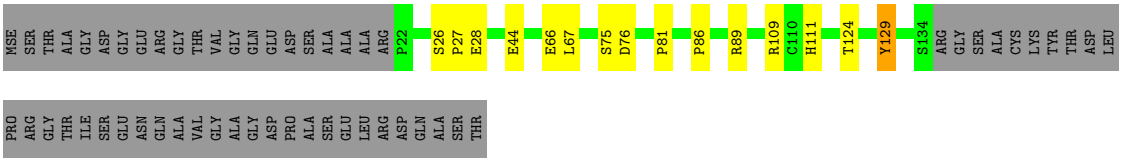
• Molecule 1: Protein RS21-C6

Chain 5-B: 54% 9% • 36%



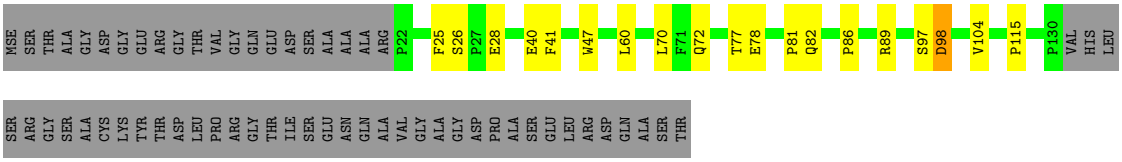

- Molecule 1: Protein RS21-C6

Chain 6-A:




- Molecule 1: Protein RS21-C6

Chain 6-B:

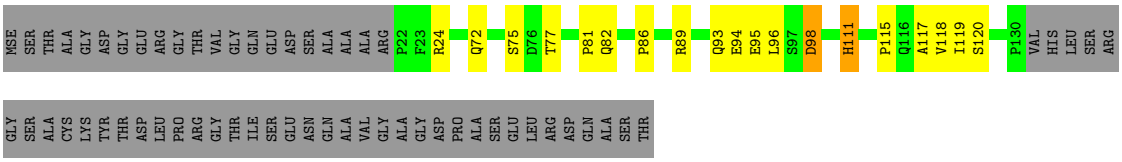



- Molecule 1: Protein RS21-C6

Chain 7-A:

- Molecule 1: Protein RS21-C6

Chain 7-B:




- Molecule 1: Protein RS21-C6

Chain 8-A:

GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 8-B: 52% 11% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 D33 R36 L37 R45 F50 L56 L60 E63 L67 A68 E69 Q72 P85 P86 K87 Q93 E94 E95 H111 V112 D113 L114 D123 Q127

P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 9-A: 54% 11% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 D46 W47 E48 F71 Q72 E78 Q82 P86 K87 E88 Q93 E94 E95 D98 V99 L100 P115 I119 M122 D123 Y129 S134 ARG GLY SER

ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 9-B: 57% 6% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 R36 D46 Q49 L67 Q72 S75 E78 P85 R89 A90 Q93 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU

PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

Chain 10-A: 55% 9% • 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 E28 L37 D46 W47 E48 V64 Q72 S75 E78 P81 Q82 A83 W84 P85 P86 Q93 E94 E95 Y102 Y129 H132 L133 S134 ARG

GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

• Molecule 1: Protein RS21-C6

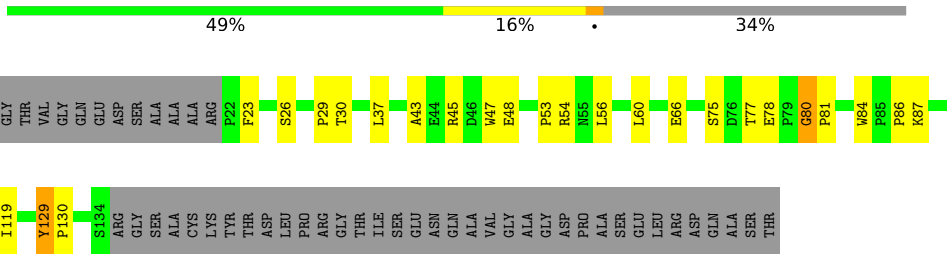
Chain 10-B: 54% 10% 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F25 S26 P27 E28 P29 T30 D33 W73 K74 S75 D76 T77 E78 P86 D98 V104 Q116 M122 D123 T124 N125 R126 P130 VAL HIS LEU SER ARG GLY

SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

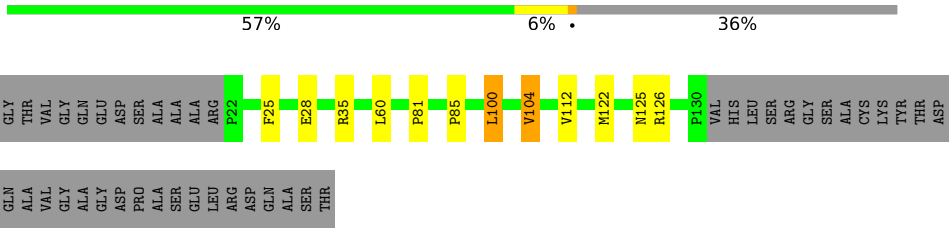
- Molecule 1: Protein RS21-C6

Chain 11-A:



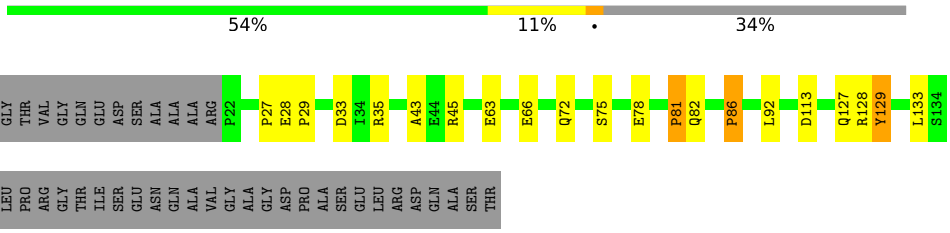

- Molecule 1: Protein RS21-C6

Chain 11-B:



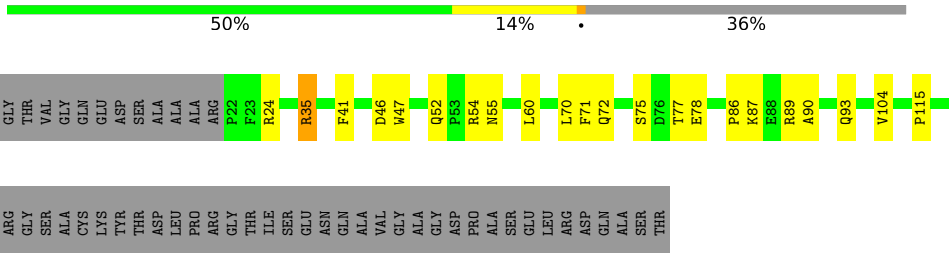

- Molecule 1: Protein RS21-C6

Chain 12-A:



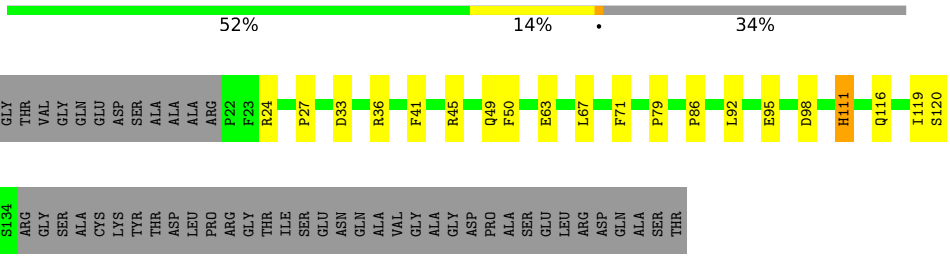

- Molecule 1: Protein RS21-C6

Chain 12-B:



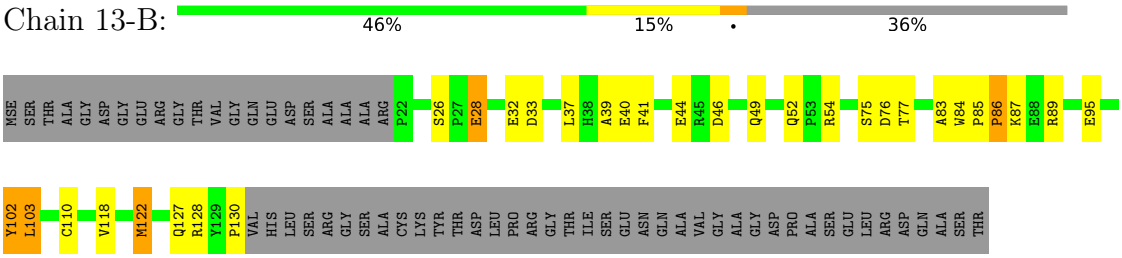

- Molecule 1: Protein RS21-C6

Chain 13-A:



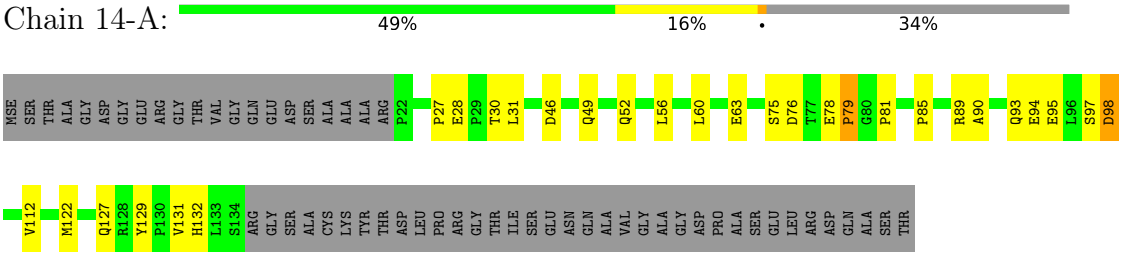

- Molecule 1: Protein RS21-C6

Chain 13-B:



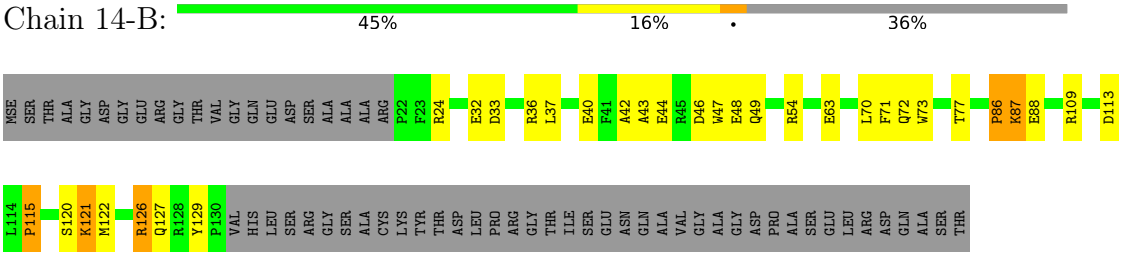

- Molecule 1: Protein RS21-C6

Chain 14-A:



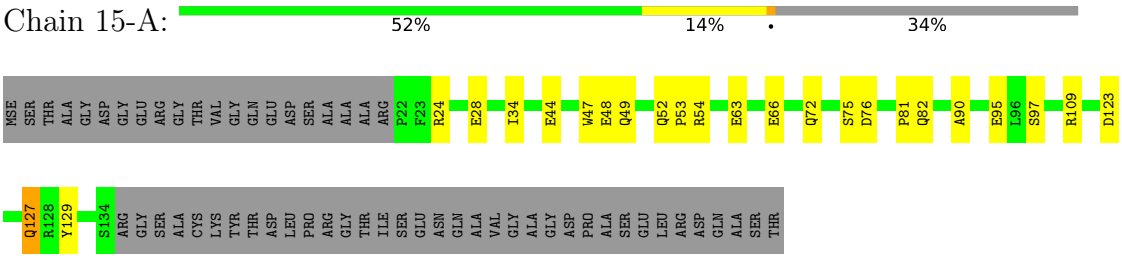

- Molecule 1: Protein RS21-C6

Chain 14-B:



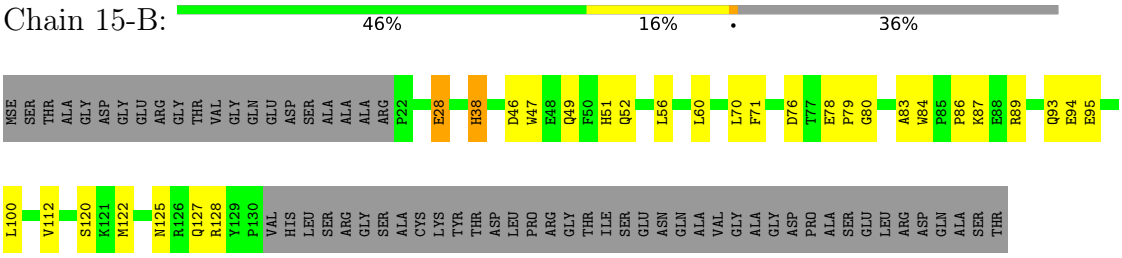

- Molecule 1: Protein RS21-C6

Chain 15-A:




- Molecule 1: Protein RS21-C6

Chain 15-B:




- Molecule 1: Protein RS21-C6

Chain 16-A: 46% 15% 5% 34%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 E28 E32 R35 R36 L37 R45 D46 W47 E48 Q49 F50 P53 R54 N55 L56 L57 L60 E66 L67 A68 E69 T77 E78 P79 G80 P81 Q82 A83 W84 P85

P86 Y102 L103 L106 H111 V112 D113 S120 T124 N125 R126 S134 ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA ALA GLY ASP PRO ALA SER GLU LEU ARG ASP GLN ALA SER THR

- Molecule 1: Protein RS21-C6

Chain 16-B: 41% 21% • 36%

MSE SER THR ALA GLY ASP GLY GLU ARG GLY THR VAL GLY GLN GLU ASP SER ALA ALA ALA ARG P22 F23 R24 F25 E28 P29 T30 L31 E32 R36 L37 H38 A39 E40 F41 A42 A43 E44 Q49 P53 R54 L67 A68 E69 L70 F71 Q72 W73 K74 S75 D76 T77 E78

K87 E88 R89 A90 A91 L92 Q93 E94 E95 L96 V104 C110 D113 Q116 M122 D123 T124 N125 R126 Y129 P130 VAL HIS LEU SER ARG GLY SER ALA CYS LYS TYR THR ASP LEU PRO ARG GLY THR ILE SER GLU ASN GLN ALA VAL GLY ALA GLY ASP PRO ALA SER GLU

LEU ARG ASP GLN ALA SER THR

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 65 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 73.54Å 73.54Å 236.08Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 37.93 – 2.32<br>43.29 – 2.32 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (37.93-2.32)<br>98.5 (43.29-2.32) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.69 (at 2.32Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.138 , 0.233<br>0.192 , 0.268 | Depositor<br>DCC |
| $R_{free}$ test set | 858 reflections (5.07%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 55.5 | Xtriage |
| Anisotropy | 0.134 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.40 , 652.5 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.49$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 29392 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 46.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 | 1-A | 0.83 | 0/947 | 1.09 | 1/1288 (0.1%) |
| 1 | 1-B | 0.93 | 0/915 | 1.02 | 2/1244 (0.2%) |
| 1 | 2-A | 0.92 | 0/947 | 1.08 | 2/1288 (0.2%) |
| 1 | 2-B | 0.94 | 1/915 (0.1%) | 1.01 | 1/1244 (0.1%) |
| 1 | 3-A | 0.87 | 0/947 | 0.94 | 0/1288 |
| 1 | 3-B | 0.99 | 0/915 | 0.95 | 0/1244 |
| 1 | 4-A | 0.94 | 0/947 | 0.98 | 0/1288 |
| 1 | 4-B | 1.01 | 0/915 | 1.11 | 3/1244 (0.2%) |
| 1 | 5-A | 0.89 | 0/947 | 0.91 | 0/1288 |
| 1 | 5-B | 0.93 | 1/915 (0.1%) | 0.98 | 3/1244 (0.2%) |
| 1 | 6-A | 0.87 | 0/947 | 0.98 | 0/1288 |
| 1 | 6-B | 1.05 | 2/915 (0.2%) | 1.11 | 4/1244 (0.3%) |
| 1 | 7-A | 0.90 | 0/947 | 0.99 | 2/1288 (0.2%) |
| 1 | 7-B | 0.92 | 0/915 | 0.98 | 1/1244 (0.1%) |
| 1 | 8-A | 0.86 | 0/947 | 0.99 | 1/1288 (0.1%) |
| 1 | 8-B | 0.99 | 2/915 (0.2%) | 1.09 | 2/1244 (0.2%) |
| 1 | 9-A | 0.94 | 2/947 (0.2%) | 0.98 | 0/1288 |
| 1 | 9-B | 0.90 | 0/915 | 0.94 | 1/1244 (0.1%) |
| 1 | 10-A | 0.93 | 1/947 (0.1%) | 1.01 | 2/1288 (0.2%) |
| 1 | 10-B | 0.98 | 0/915 | 1.04 | 4/1244 (0.3%) |
| 1 | 11-A | 0.95 | 1/947 (0.1%) | 1.12 | 7/1288 (0.5%) |
| 1 | 11-B | 0.99 | 1/915 (0.1%) | 1.22 | 4/1244 (0.3%) |
| 1 | 12-A | 0.96 | 1/947 (0.1%) | 1.02 | 2/1288 (0.2%) |
| 1 | 12-B | 0.91 | 1/915 (0.1%) | 1.07 | 3/1244 (0.2%) |
| 1 | 13-A | 1.05 | 0/947 | 1.15 | 2/1288 (0.2%) |
| 1 | 13-B | 1.28 | 5/915 (0.5%) | 1.26 | 7/1244 (0.6%) |
| 1 | 14-A | 1.05 | 1/947 (0.1%) | 1.23 | 4/1288 (0.3%) |
| 1 | 14-B | 1.10 | 2/915 (0.2%) | 1.13 | 3/1244 (0.2%) |
| 1 | 15-A | 0.98 | 1/947 (0.1%) | 1.10 | 2/1288 (0.2%) |
| 1 | 15-B | 1.16 | 2/915 (0.2%) | 1.16 | 4/1244 (0.3%) |
| 1 | 16-A | 1.11 | 2/947 (0.2%) | 1.31 | 10/1288 (0.8%) |
| 1 | 16-B | 1.39 | 9/915 (1.0%) | 1.41 | 13/1244 (1.0%) |
| All | All | 0.99 | 35/29792 (0.1%) | 1.08 | 90/40512 (0.2%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | 5-B | 0 | 1 |
| 1 | 9-A | 0 | 1 |
| 1 | 11-A | 0 | 1 |
| 1 | 12-A | 0 | 1 |
| 1 | 13-B | 0 | 2 |
| 1 | 16-A | 0 | 1 |
| 1 | 16-B | 0 | 1 |
| All | All | 0 | 8 |

All (35) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16-B | 42 | ALA | CA-CB | 13.50 | 1.80 | 1.52 |
| 1 | 16-B | 28 | GLU | CD-OE1 | -8.05 | 1.16 | 1.25 |
| 1 | 16-B | 28 | GLU | CG-CD | 7.98 | 1.64 | 1.51 |
| 1 | 13-B | 39 | ALA | CA-CB | -7.26 | 1.37 | 1.52 |
| 1 | 14-A | 94 | GLU | CG-CD | 7.26 | 1.62 | 1.51 |
| 1 | 9-A | 78 | GLU | CG-CD | 7.16 | 1.62 | 1.51 |
| 1 | 12-A | 113 | ASP | CB-CG | 7.02 | 1.66 | 1.51 |
| 1 | 16-B | 69 | GLU | CG-CD | 6.97 | 1.62 | 1.51 |
| 1 | 16-B | 69 | GLU | CB-CG | 6.86 | 1.65 | 1.52 |
| 1 | 13-B | 102 | TYR | CD2-CE2 | 6.27 | 1.48 | 1.39 |
| 1 | 14-B | 47 | TRP | CG-CD1 | 5.94 | 1.45 | 1.36 |
| 1 | 16-B | 104 | VAL | CB-CG1 | -5.85 | 1.40 | 1.52 |
| 1 | 5-B | 36 | ARG | CG-CD | 5.78 | 1.66 | 1.51 |
| 1 | 15-B | 28 | GLU | CG-CD | 5.64 | 1.60 | 1.51 |
| 1 | 15-B | 47 | TRP | CG-CD1 | 5.61 | 1.44 | 1.36 |
| 1 | 11-A | 102 | TYR | CD1-CE1 | 5.59 | 1.47 | 1.39 |
| 1 | 13-B | 28 | GLU | CG-CD | 5.57 | 1.60 | 1.51 |
| 1 | 16-A | 69 | GLU | CG-CD | 5.47 | 1.60 | 1.51 |
| 1 | 15-A | 109 | ARG | CZ-NH2 | 5.46 | 1.40 | 1.33 |
| 1 | 16-B | 28 | GLU | CB-CG | 5.42 | 1.62 | 1.52 |
| 1 | 13-B | 44 | GLU | CB-CG | 5.42 | 1.62 | 1.52 |
| 1 | 6-B | 41 | PHE | CE2-CZ | 5.41 | 1.47 | 1.37 |
| 1 | 13-B | 102 | TYR | CZ-OH | 5.35 | 1.47 | 1.37 |
| 1 | 8-B | 69 | GLU | CG-CD | 5.33 | 1.59 | 1.51 |
| 1 | 2-B | 69 | GLU | CG-CD | 5.25 | 1.59 | 1.51 |
| 1 | 14-B | 73 | TRP | CE3-CZ3 | 5.25 | 1.47 | 1.38 |
| 1 | 8-B | 33 | ASP | CB-CG | 5.24 | 1.62 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | 16-A | 32 | GLU | CG-CD | 5.23 | 1.59 | 1.51 |
| 1 | 10-A | 95 | GLU | CG-CD | 5.18 | 1.59 | 1.51 |
| 1 | 12-B | 47 | TRP | CB-CG | -5.18 | 1.41 | 1.50 |
| 1 | 16-B | 40 | GLU | CB-CG | -5.17 | 1.42 | 1.52 |
| 1 | 16-B | 104 | VAL | CA-CB | 5.16 | 1.65 | 1.54 |
| 1 | 9-A | 94 | GLU | CG-CD | 5.06 | 1.59 | 1.51 |
| 1 | 11-B | 104 | VAL | CA-CB | 5.05 | 1.65 | 1.54 |
| 1 | 6-B | 47 | TRP | CG-CD1 | 5.01 | 1.43 | 1.36 |

All (90) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 11-B | 35 | ARG | NE-CZ-NH1 | 15.25 | 127.92 | 120.30 |
| 1 | 11-B | 35 | ARG | NE-CZ-NH2 | -14.82 | 112.89 | 120.30 |
| 1 | 12-B | 35 | ARG | NE-CZ-NH2 | -10.14 | 115.23 | 120.30 |
| 1 | 6-B | 89 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | 5-B | 36 | ARG | NE-CZ-NH1 | 8.12 | 124.36 | 120.30 |
| 1 | 12-B | 35 | ARG | NE-CZ-NH1 | 8.12 | 124.36 | 120.30 |
| 1 | 5-B | 67 | LEU | CA-CB-CG | 7.83 | 133.32 | 115.30 |
| 1 | 11-A | 56 | LEU | CA-CB-CG | 7.65 | 132.90 | 115.30 |
| 1 | 13-B | 54 | ARG | NE-CZ-NH1 | 7.51 | 124.06 | 120.30 |
| 1 | 6-B | 89 | ARG | NE-CZ-NH2 | -7.46 | 116.57 | 120.30 |
| 1 | 16-A | 37 | LEU | CA-CB-CG | -7.19 | 98.76 | 115.30 |
| 1 | 8-B | 56 | LEU | CA-CB-CG | 7.17 | 131.79 | 115.30 |
| 1 | 7-A | 31 | LEU | N-CA-C | -7.14 | 91.72 | 111.00 |
| 1 | 15-A | 109 | ARG | NE-CZ-NH1 | -7.13 | 116.73 | 120.30 |
| 1 | 11-A | 37 | LEU | CA-CB-CG | -7.03 | 99.14 | 115.30 |
| 1 | 2-A | 38 | HIS | N-CA-C | -7.00 | 92.11 | 111.00 |
| 1 | 16-B | 39 | ALA | C-N-CA | 6.99 | 139.19 | 121.70 |
| 1 | 8-A | 113 | ASP | CB-CG-OD1 | -6.96 | 112.04 | 118.30 |
| 1 | 4-B | 109 | ARG | NE-CZ-NH1 | -6.89 | 116.86 | 120.30 |
| 1 | 12-B | 46 | ASP | CB-CG-OD1 | 6.89 | 124.50 | 118.30 |
| 1 | 7-A | 31 | LEU | CA-CB-CG | 6.87 | 131.10 | 115.30 |
| 1 | 13-B | 54 | ARG | NE-CZ-NH2 | -6.86 | 116.87 | 120.30 |
| 1 | 1-B | 28 | GLU | N-CA-C | -6.76 | 92.76 | 111.00 |
| 1 | 16-B | 39 | ALA | CA-C-N | -6.74 | 102.38 | 117.20 |
| 1 | 10-B | 30 | THR | N-CA-C | -6.67 | 92.99 | 111.00 |
| 1 | 16-A | 47 | TRP | N-CA-C | 6.66 | 128.97 | 111.00 |
| 1 | 10-B | 26 | SER | C-N-CD | -6.65 | 105.96 | 120.60 |
| 1 | 14-B | 54 | ARG | NE-CZ-NH2 | -6.62 | 116.99 | 120.30 |
| 1 | 16-A | 45 | ARG | NE-CZ-NH2 | 6.59 | 123.60 | 120.30 |
| 1 | 16-B | 91 | ALA | N-CA-C | -6.45 | 93.60 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 15-A | 54 | ARG | NE-CZ-NH1 | 6.43 | 123.52 | 120.30 |
| 1 | 13-B | 49 | GLN | N-CA-C | -6.40 | 93.73 | 111.00 |
| 1 | 16-B | 39 | ALA | N-CA-C | 6.39 | 128.25 | 111.00 |
| 1 | 10-A | 24 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | 14-B | 109 | ARG | NE-CZ-NH1 | -6.36 | 117.12 | 120.30 |
| 1 | 5-B | 36 | ARG | NE-CZ-NH2 | -6.32 | 117.14 | 120.30 |
| 1 | 13-B | 130 | PRO | N-CA-C | 6.30 | 128.48 | 112.10 |
| 1 | 11-B | 100 | LEU | CA-CB-CG | 6.24 | 129.64 | 115.30 |
| 1 | 6-B | 26 | SER | C-N-CD | -6.18 | 107.00 | 120.60 |
| 1 | 13-A | 36 | ARG | NE-CZ-NH1 | -6.16 | 117.22 | 120.30 |
| 1 | 10-B | 26 | SER | C-N-CA | 6.14 | 147.77 | 122.00 |
| 1 | 16-A | 103 | LEU | CA-CB-CG | -6.07 | 101.34 | 115.30 |
| 1 | 16-A | 54 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 1 | 2-B | 109 | ARG | NE-CZ-NH1 | -5.98 | 117.31 | 120.30 |
| 1 | 16-A | 45 | ARG | CG-CD-NE | 5.93 | 124.24 | 111.80 |
| 1 | 12-A | 43 | ALA | N-CA-C | -5.92 | 95.02 | 111.00 |
| 1 | 16-B | 110 | CYS | CA-CB-SG | -5.90 | 103.38 | 114.00 |
| 1 | 16-B | 36 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | 9-B | 67 | LEU | CA-CB-CG | 5.84 | 128.73 | 115.30 |
| 1 | 14-A | 49 | GLN | N-CA-C | -5.84 | 95.24 | 111.00 |
| 1 | 1-B | 25 | PHE | N-CA-C | -5.83 | 95.26 | 111.00 |
| 1 | 12-A | 113 | ASP | CB-CG-OD2 | 5.76 | 123.48 | 118.30 |
| 1 | 16-B | 39 | ALA | O-C-N | 5.69 | 131.80 | 122.70 |
| 1 | 2-A | 33 | ASP | CB-CG-OD1 | 5.67 | 123.41 | 118.30 |
| 1 | 14-A | 76 | ASP | CB-CG-OD1 | 5.62 | 123.36 | 118.30 |
| 1 | 16-A | 113 | ASP | N-CA-C | -5.61 | 95.85 | 111.00 |
| 1 | 11-A | 80 | GLY | N-CA-C | 5.61 | 127.12 | 113.10 |
| 1 | 13-B | 103 | LEU | CA-CB-CG | -5.55 | 102.53 | 115.30 |
| 1 | 16-B | 70 | LEU | CB-CG-CD1 | -5.55 | 101.57 | 111.00 |
| 1 | 13-A | 36 | ARG | NE-CZ-NH2 | 5.54 | 123.07 | 120.30 |
| 1 | 16-A | 46 | ASP | CB-CG-OD2 | 5.52 | 123.27 | 118.30 |
| 1 | 11-A | 84 | TRP | N-CA-C | -5.45 | 96.29 | 111.00 |
| 1 | 11-A | 45 | ARG | NE-CZ-NH1 | -5.44 | 117.58 | 120.30 |
| 1 | 16-B | 70 | LEU | C-N-CA | -5.42 | 108.14 | 121.70 |
| 1 | 16-B | 96 | LEU | CA-CB-CG | -5.39 | 102.90 | 115.30 |
| 1 | 16-B | 69 | GLU | OE1-CD-OE2 | -5.36 | 116.86 | 123.30 |
| 1 | 16-B | 25 | PHE | CB-CA-C | -5.36 | 99.68 | 110.40 |
| 1 | 14-B | 36 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 1 | 11-A | 102 | TYR | CA-CB-CG | 5.33 | 123.53 | 113.40 |
| 1 | 13-B | 26 | SER | N-CA-C | -5.29 | 96.72 | 111.00 |
| 1 | 16-A | 46 | ASP | CB-CG-OD1 | -5.28 | 113.55 | 118.30 |
| 1 | 11-B | 112 | VAL | N-CA-C | -5.26 | 96.81 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | 14-A | 131 | VAL | CB-CA-C | -5.25 | 101.42 | 111.40 |
| 1 | 15-B | 56 | LEU | CA-CB-CG | -5.24 | 103.24 | 115.30 |
| 1 | 1-A | 56 | LEU | CA-CB-CG | 5.23 | 127.32 | 115.30 |
| 1 | 7-B | 98 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | 13-B | 122 | MSE | N-CA-C | -5.20 | 96.96 | 111.00 |
| 1 | 15-B | 112 | VAL | CB-CA-C | -5.19 | 101.54 | 111.40 |
| 1 | 8-B | 36 | ARG | NE-CZ-NH1 | 5.17 | 122.88 | 120.30 |
| 1 | 10-A | 37 | LEU | CA-CB-CG | -5.17 | 103.42 | 115.30 |
| 1 | 4-B | 31 | LEU | N-CA-C | -5.16 | 97.08 | 111.00 |
| 1 | 15-B | 70 | LEU | CA-CB-CG | 5.14 | 127.12 | 115.30 |
| 1 | 15-B | 38 | HIS | N-CA-C | 5.14 | 124.87 | 111.00 |
| 1 | 16-B | 38 | HIS | N-CA-C | 5.13 | 124.87 | 111.00 |
| 1 | 14-A | 112 | VAL | N-CA-C | -5.06 | 97.35 | 111.00 |
| 1 | 4-B | 119 | ILE | N-CA-C | -5.04 | 97.41 | 111.00 |
| 1 | 16-A | 46 | ASP | CB-CA-C | 5.04 | 120.47 | 110.40 |
| 1 | 6-B | 98 | ASP | CB-CG-OD1 | 5.03 | 122.83 | 118.30 |
| 1 | 10-B | 30 | THR | CB-CA-C | -5.01 | 98.06 | 111.60 |
| 1 | 11-A | 60 | LEU | CA-CB-CG | 5.01 | 126.83 | 115.30 |

There are no chirality outliers.

All (8) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 11-A | 102 | TYR | Sidechain |
| 1 | 12-A | 129 | TYR | Sidechain |
| 1 | 13-B | 102 | TYR | Sidechain |
| 1 | 13-B | 41 | PHE | Sidechain |
| 1 | 16-A | 102 | TYR | Sidechain |
| 1 | 16-B | 41 | PHE | Sidechain |
| 1 | 5-B | 51 | HIS | Sidechain |
| 1 | 9-A | 71 | PHE | Sidechain |

## 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 | 1-A | 922 | 0 | 901 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 1-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 2-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 2-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 3-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 3-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 4-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 4-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 5-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 5-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 6-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 6-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 7-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 7-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 8-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 8-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 9-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 9-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 10-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 10-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 11-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 11-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 12-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 12-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 13-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 13-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 14-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 14-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 15-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 15-B | 891 | 0 | 869 | 0 | 0 |
| 1 | 16-A | 922 | 0 | 901 | 0 | 0 |
| 1 | 16-B | 891 | 0 | 869 | 0 | 0 |
| 2 | 1-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 1-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 2-A | 11 | 0 | 0 | 0 | 0 |
| 2 | 2-B | 13 | 0 | 0 | 0 | 0 |
| 2 | 3-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 3-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 4-A | 11 | 0 | 0 | 0 | 0 |
| 2 | 4-B | 13 | 0 | 0 | 0 | 0 |
| 2 | 5-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 5-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 6-A | 11 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | 6-B | 13 | 0 | 0 | 0 | 0 |
| 2 | 7-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 7-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 8-A | 13 | 0 | 0 | 0 | 0 |
| 2 | 8-B | 11 | 0 | 0 | 0 | 0 |
| 2 | 9-A | 11 | 0 | 0 | 0 | 0 |
| 2 | 9-B | 13 | 0 | 0 | 0 | 0 |
| 2 | 10-A | 10 | 0 | 0 | 0 | 0 |
| 2 | 10-B | 14 | 0 | 0 | 0 | 0 |
| 2 | 11-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 11-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 12-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 12-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 13-A | 13 | 0 | 0 | 0 | 0 |
| 2 | 13-B | 11 | 0 | 0 | 0 | 0 |
| 2 | 14-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 14-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 15-A | 12 | 0 | 0 | 0 | 0 |
| 2 | 15-B | 12 | 0 | 0 | 0 | 0 |
| 2 | 16-A | 13 | 0 | 0 | 0 | 0 |
| 2 | 16-B | 11 | 0 | 0 | 0 | 0 |
| All | All | 29392 | 0 | 28320 | 0 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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 | 1-A | 111/170 (65%) | 83 (75%) | 23 (21%) | 5 (4%) | 2 1 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 1-B | 107/170 (63%) | 83 (78%) | 22 (21%) | 2 (2%) | 8 | 6 |
| 1 | 2-A | 111/170 (65%) | 89 (80%) | 18 (16%) | 4 (4%) | 3 | 2 |
| 1 | 2-B | 107/170 (63%) | 90 (84%) | 10 (9%) | 7 (6%) | 1 | 0 |
| 1 | 3-A | 111/170 (65%) | 97 (87%) | 9 (8%) | 5 (4%) | 2 | 1 |
| 1 | 3-B | 107/170 (63%) | 98 (92%) | 6 (6%) | 3 (3%) | 5 | 3 |
| 1 | 4-A | 111/170 (65%) | 92 (83%) | 14 (13%) | 5 (4%) | 2 | 1 |
| 1 | 4-B | 107/170 (63%) | 85 (79%) | 14 (13%) | 8 (8%) | 1 | 0 |
| 1 | 5-A | 111/170 (65%) | 95 (86%) | 12 (11%) | 4 (4%) | 3 | 2 |
| 1 | 5-B | 107/170 (63%) | 98 (92%) | 6 (6%) | 3 (3%) | 5 | 3 |
| 1 | 6-A | 111/170 (65%) | 91 (82%) | 13 (12%) | 7 (6%) | 1 | 0 |
| 1 | 6-B | 107/170 (63%) | 85 (79%) | 16 (15%) | 6 (6%) | 2 | 0 |
| 1 | 7-A | 111/170 (65%) | 85 (77%) | 18 (16%) | 8 (7%) | 1 | 0 |
| 1 | 7-B | 107/170 (63%) | 85 (79%) | 10 (9%) | 12 (11%) | 0 | 0 |
| 1 | 8-A | 111/170 (65%) | 96 (86%) | 12 (11%) | 3 (3%) | 5 | 3 |
| 1 | 8-B | 107/170 (63%) | 80 (75%) | 18 (17%) | 9 (8%) | 1 | 0 |
| 1 | 9-A | 111/170 (65%) | 80 (72%) | 22 (20%) | 9 (8%) | 1 | 0 |
| 1 | 9-B | 107/170 (63%) | 92 (86%) | 11 (10%) | 4 (4%) | 3 | 1 |
| 1 | 10-A | 111/170 (65%) | 90 (81%) | 16 (14%) | 5 (4%) | 2 | 1 |
| 1 | 10-B | 107/170 (63%) | 85 (79%) | 15 (14%) | 7 (6%) | 1 | 0 |
| 1 | 11-A | 111/170 (65%) | 79 (71%) | 17 (15%) | 15 (14%) | 0 | 0 |
| 1 | 11-B | 107/170 (63%) | 87 (81%) | 14 (13%) | 6 (6%) | 2 | 0 |
| 1 | 12-A | 111/170 (65%) | 82 (74%) | 19 (17%) | 10 (9%) | 1 | 0 |
| 1 | 12-B | 107/170 (63%) | 75 (70%) | 22 (21%) | 10 (9%) | 0 | 0 |
| 1 | 13-A | 111/170 (65%) | 85 (77%) | 19 (17%) | 7 (6%) | 1 | 0 |
| 1 | 13-B | 107/170 (63%) | 82 (77%) | 16 (15%) | 9 (8%) | 1 | 0 |
| 1 | 14-A | 111/170 (65%) | 77 (69%) | 21 (19%) | 13 (12%) | 0 | 0 |
| 1 | 14-B | 107/170 (63%) | 81 (76%) | 14 (13%) | 12 (11%) | 0 | 0 |
| 1 | 15-A | 111/170 (65%) | 80 (72%) | 20 (18%) | 11 (10%) | 0 | 0 |
| 1 | 15-B | 107/170 (63%) | 84 (78%) | 16 (15%) | 7 (6%) | 1 | 0 |
| 1 | 16-A | 111/170 (65%) | 75 (68%) | 23 (21%) | 13 (12%) | 0 | 0 |
| 1 | 16-B | 107/170 (63%) | 76 (71%) | 19 (18%) | 12 (11%) | 0 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| All | All | 3488/5440 (64%) | 2742 (79%) | 505 (14%) | 241 (7%) | 1 0 |

All (241) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1-A | 78 | GLU |
| 1 | 1-A | 128 | ARG |
| 1 | 1-B | 86 | PRO |
| 1 | 2-A | 81 | PRO |
| 1 | 2-B | 72 | GLN |
| 1 | 2-B | 81 | PRO |
| 1 | 2-B | 86 | PRO |
| 1 | 3-A | 41 | PHE |
| 1 | 4-A | 47 | TRP |
| 1 | 4-B | 72 | GLN |
| 1 | 4-B | 79 | PRO |
| 1 | 4-B | 81 | PRO |
| 1 | 5-A | 26 | SER |
| 1 | 5-B | 78 | GLU |
| 1 | 5-B | 86 | PRO |
| 1 | 6-A | 27 | PRO |
| 1 | 6-A | 76 | ASP |
| 1 | 6-A | 111 | HIS |
| 1 | 6-A | 124 | THR |
| 1 | 6-A | 129 | TYR |
| 1 | 6-B | 72 | GLN |
| 1 | 6-B | 82 | GLN |
| 1 | 6-B | 86 | PRO |
| 1 | 7-A | 30 | THR |
| 1 | 7-A | 74 | LYS |
| 1 | 7-A | 88 | GLU |
| 1 | 7-B | 75 | SER |
| 1 | 7-B | 81 | PRO |
| 1 | 7-B | 95 | GLU |
| 1 | 7-B | 96 | LEU |
| 1 | 7-B | 111 | HIS |
| 1 | 7-B | 118 | VAL |
| 1 | 7-B | 119 | ILE |
| 1 | 7-B | 120 | SER |
| 1 | 8-B | 72 | GLN |
| 1 | 8-B | 85 | PRO |
| 1 | 8-B | 86 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 8-B | 87 | LYS |
| 1 | 8-B | 111 | HIS |
| 1 | 9-A | 23 | PHE |
| 1 | 9-A | 47 | TRP |
| 1 | 9-A | 82 | GLN |
| 1 | 9-A | 93 | GLN |
| 1 | 9-A | 94 | GLU |
| 1 | 9-B | 72 | GLN |
| 1 | 10-A | 72 | GLN |
| 1 | 10-A | 81 | PRO |
| 1 | 10-A | 86 | PRO |
| 1 | 10-B | 25 | PHE |
| 1 | 10-B | 78 | GLU |
| 1 | 10-B | 122 | MSE |
| 1 | 11-A | 23 | PHE |
| 1 | 11-A | 47 | TRP |
| 1 | 11-A | 48 | GLU |
| 1 | 11-A | 80 | GLY |
| 1 | 11-A | 107 | ALA |
| 1 | 12-A | 81 | PRO |
| 1 | 12-B | 72 | GLN |
| 1 | 12-B | 75 | SER |
| 1 | 12-B | 86 | PRO |
| 1 | 12-B | 87 | LYS |
| 1 | 13-A | 49 | GLN |
| 1 | 13-A | 111 | HIS |
| 1 | 13-B | 76 | ASP |
| 1 | 13-B | 83 | ALA |
| 1 | 13-B | 110 | CYS |
| 1 | 14-A | 30 | THR |
| 1 | 14-A | 78 | GLU |
| 1 | 14-A | 81 | PRO |
| 1 | 14-A | 97 | SER |
| 1 | 14-A | 98 | ASP |
| 1 | 14-B | 42 | ALA |
| 1 | 14-B | 43 | ALA |
| 1 | 14-B | 70 | LEU |
| 1 | 14-B | 121 | LYS |
| 1 | 14-B | 126 | ARG |
| 1 | 14-B | 129 | TYR |
| 1 | 15-A | 28 | GLU |
| 1 | 15-A | 47 | TRP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 15-A | 48 | GLU |
| 1 | 15-A | 75 | SER |
| 1 | 15-A | 76 | ASP |
| 1 | 15-A | 81 | PRO |
| 1 | 15-A | 90 | ALA |
| 1 | 15-B | 86 | PRO |
| 1 | 15-B | 87 | LYS |
| 1 | 16-A | 49 | GLN |
| 1 | 16-A | 53 | PRO |
| 1 | 16-A | 54 | ARG |
| 1 | 16-A | 69 | GLU |
| 1 | 16-A | 81 | PRO |
| 1 | 16-A | 82 | GLN |
| 1 | 16-A | 83 | ALA |
| 1 | 16-A | 111 | HIS |
| 1 | 16-B | 24 | ARG |
| 1 | 16-B | 30 | THR |
| 1 | 16-B | 129 | TYR |
| 1 | 1-A | 119 | ILE |
| 1 | 1-A | 127 | GLN |
| 1 | 2-A | 47 | TRP |
| 1 | 4-B | 78 | GLU |
| 1 | 4-B | 83 | ALA |
| 1 | 6-B | 81 | PRO |
| 1 | 7-A | 87 | LYS |
| 1 | 7-B | 117 | ALA |
| 1 | 8-A | 47 | TRP |
| 1 | 8-A | 62 | GLY |
| 1 | 8-B | 37 | LEU |
| 1 | 9-A | 87 | LYS |
| 1 | 9-B | 89 | ARG |
| 1 | 10-B | 74 | LYS |
| 1 | 10-B | 86 | PRO |
| 1 | 11-A | 81 | PRO |
| 1 | 11-A | 87 | LYS |
| 1 | 11-A | 108 | ALA |
| 1 | 11-B | 25 | PHE |
| 1 | 11-B | 85 | PRO |
| 1 | 12-A | 45 | ARG |
| 1 | 12-A | 86 | PRO |
| 1 | 12-A | 127 | GLN |
| 1 | 12-A | 128 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 12-B | 41 | PHE |
| 1 | 12-B | 122 | MSE |
| 1 | 13-A | 50 | PHE |
| 1 | 13-B | 127 | GLN |
| 1 | 14-A | 132 | HIS |
| 1 | 14-B | 120 | SER |
| 1 | 15-A | 72 | GLN |
| 1 | 15-B | 46 | ASP |
| 1 | 15-B | 80 | GLY |
| 1 | 15-B | 83 | ALA |
| 1 | 16-B | 53 | PRO |
| 1 | 16-B | 54 | ARG |
| 1 | 16-B | 72 | GLN |
| 1 | 16-B | 113 | ASP |
| 1 | 1-A | 79 | PRO |
| 1 | 1-B | 87 | LYS |
| 1 | 2-B | 80 | GLY |
| 1 | 3-A | 76 | ASP |
| 1 | 4-A | 77 | THR |
| 1 | 4-A | 81 | PRO |
| 1 | 4-B | 46 | ASP |
| 1 | 5-A | 132 | HIS |
| 1 | 6-B | 25 | PHE |
| 1 | 7-A | 75 | SER |
| 1 | 7-A | 76 | ASP |
| 1 | 7-B | 94 | GLU |
| 1 | 8-B | 50 | PHE |
| 1 | 9-A | 88 | GLU |
| 1 | 9-B | 85 | PRO |
| 1 | 9-B | 90 | ALA |
| 1 | 10-A | 84 | TRP |
| 1 | 11-A | 75 | SER |
| 1 | 11-B | 81 | PRO |
| 1 | 12-A | 72 | GLN |
| 1 | 12-B | 90 | ALA |
| 1 | 13-A | 27 | PRO |
| 1 | 14-A | 79 | PRO |
| 1 | 14-A | 95 | GLU |
| 1 | 14-A | 127 | GLN |
| 1 | 14-B | 46 | ASP |
| 1 | 14-B | 87 | LYS |
| 1 | 15-B | 79 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16-A | 45 | ARG |
| 1 | 16-A | 47 | TRP |
| 1 | 16-A | 57 | LEU |
| 1 | 16-B | 67 | LEU |
| 1 | 16-B | 89 | ARG |
| 1 | 2-A | 60 | LEU |
| 1 | 2-B | 45 | ARG |
| 1 | 2-B | 58 | LEU |
| 1 | 3-A | 40 | GLU |
| 1 | 3-B | 85 | PRO |
| 1 | 4-B | 77 | THR |
| 1 | 4-B | 113 | ASP |
| 1 | 6-B | 70 | LEU |
| 1 | 7-A | 25 | PHE |
| 1 | 7-B | 72 | GLN |
| 1 | 7-B | 115 | PRO |
| 1 | 8-B | 45 | ARG |
| 1 | 10-B | 28 | GLU |
| 1 | 10-B | 77 | THR |
| 1 | 11-A | 43 | ALA |
| 1 | 11-A | 86 | PRO |
| 1 | 13-B | 46 | ASP |
| 1 | 13-B | 85 | PRO |
| 1 | 14-A | 75 | SER |
| 1 | 14-A | 90 | ALA |
| 1 | 14-B | 88 | GLU |
| 1 | 14-B | 115 | PRO |
| 1 | 15-A | 53 | PRO |
| 1 | 15-A | 97 | SER |
| 1 | 16-B | 76 | ASP |
| 1 | 2-A | 53 | PRO |
| 1 | 2-B | 79 | PRO |
| 1 | 3-A | 42 | ALA |
| 1 | 3-B | 84 | TRP |
| 1 | 3-B | 86 | PRO |
| 1 | 4-A | 84 | TRP |
| 1 | 4-A | 126 | ARG |
| 1 | 7-A | 72 | GLN |
| 1 | 10-A | 93 | GLN |
| 1 | 11-A | 91 | ALA |
| 1 | 11-A | 115 | PRO |
| 1 | 12-A | 27 | PRO |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 12-A | 82 | GLN |
| 1 | 12-B | 115 | PRO |
| 1 | 14-A | 27 | PRO |
| 1 | 14-A | 56 | LEU |
| 1 | 14-B | 86 | PRO |
| 1 | 15-A | 127 | GLN |
| 1 | 16-B | 87 | LYS |
| 1 | 16-B | 95 | GLU |
| 1 | 5-A | 27 | PRO |
| 1 | 11-B | 125 | ASN |
| 1 | 11-B | 126 | ARG |
| 1 | 12-A | 133 | LEU |
| 1 | 12-B | 55 | ASN |
| 1 | 12-B | 78 | GLU |
| 1 | 13-A | 131 | VAL |
| 1 | 13-B | 33 | ASP |
| 1 | 13-B | 84 | TRP |
| 1 | 13-B | 86 | PRO |
| 1 | 15-B | 84 | TRP |
| 1 | 3-A | 53 | PRO |
| 1 | 6-A | 81 | PRO |
| 1 | 8-A | 86 | PRO |
| 1 | 13-A | 119 | ILE |
| 1 | 5-A | 81 | PRO |
| 1 | 6-A | 86 | PRO |
| 1 | 8-B | 114 | LEU |
| 1 | 9-A | 86 | PRO |
| 1 | 9-A | 115 | PRO |
| 1 | 11-A | 53 | PRO |
| 1 | 16-A | 79 | PRO |
| 1 | 12-A | 78 | GLU |
| 1 | 16-A | 86 | PRO |
| 1 | 11-A | 129 | TYR |
| 1 | 11-B | 28 | GLU |
| 1 | 13-A | 79 | PRO |
| 1 | 5-B | 84 | TRP |

### 5.3.2 Protein sidechains (i)

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 | 1-A | 98/136 (72%) | 83 (85%) | 15 (15%) | 2 | 2 |
| 1 | 1-B | 94/136 (69%) | 84 (89%) | 10 (11%) | 6 | 7 |
| 1 | 2-A | 98/136 (72%) | 83 (85%) | 15 (15%) | 2 | 2 |
| 1 | 2-B | 94/136 (69%) | 85 (90%) | 9 (10%) | 8 | 9 |
| 1 | 3-A | 98/136 (72%) | 88 (90%) | 10 (10%) | 7 | 8 |
| 1 | 3-B | 94/136 (69%) | 86 (92%) | 8 (8%) | 10 | 12 |
| 1 | 4-A | 98/136 (72%) | 89 (91%) | 9 (9%) | 9 | 10 |
| 1 | 4-B | 94/136 (69%) | 84 (89%) | 10 (11%) | 6 | 7 |
| 1 | 5-A | 98/136 (72%) | 88 (90%) | 10 (10%) | 7 | 8 |
| 1 | 5-B | 94/136 (69%) | 82 (87%) | 12 (13%) | 4 | 4 |
| 1 | 6-A | 98/136 (72%) | 89 (91%) | 9 (9%) | 9 | 10 |
| 1 | 6-B | 94/136 (69%) | 85 (90%) | 9 (10%) | 8 | 9 |
| 1 | 7-A | 98/136 (72%) | 89 (91%) | 9 (9%) | 9 | 10 |
| 1 | 7-B | 94/136 (69%) | 86 (92%) | 8 (8%) | 10 | 12 |
| 1 | 8-A | 98/136 (72%) | 89 (91%) | 9 (9%) | 9 | 10 |
| 1 | 8-B | 94/136 (69%) | 84 (89%) | 10 (11%) | 6 | 7 |
| 1 | 9-A | 98/136 (72%) | 87 (89%) | 11 (11%) | 6 | 6 |
| 1 | 9-B | 94/136 (69%) | 86 (92%) | 8 (8%) | 10 | 12 |
| 1 | 10-A | 98/136 (72%) | 84 (86%) | 14 (14%) | 3 | 3 |
| 1 | 10-B | 94/136 (69%) | 86 (92%) | 8 (8%) | 10 | 12 |
| 1 | 11-A | 98/136 (72%) | 88 (90%) | 10 (10%) | 7 | 8 |
| 1 | 11-B | 94/136 (69%) | 90 (96%) | 4 (4%) | 29 | 40 |
| 1 | 12-A | 98/136 (72%) | 87 (89%) | 11 (11%) | 6 | 6 |
| 1 | 12-B | 94/136 (69%) | 82 (87%) | 12 (13%) | 4 | 4 |
| 1 | 13-A | 98/136 (72%) | 80 (82%) | 18 (18%) | 1 | 1 |
| 1 | 13-B | 94/136 (69%) | 79 (84%) | 15 (16%) | 2 | 2 |
| 1 | 14-A | 98/136 (72%) | 85 (87%) | 13 (13%) | 4 | 4 |
| 1 | 14-B | 94/136 (69%) | 74 (79%) | 20 (21%) | 1 | 1 |
| 1 | 15-A | 98/136 (72%) | 86 (88%) | 12 (12%) | 5 | 5 |
| 1 | 15-B | 94/136 (69%) | 75 (80%) | 19 (20%) | 1 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 16-A | 98/136 (72%) | 79 (81%) | 19 (19%) | 1 1 |
| 1 | 16-B | 94/136 (69%) | 76 (81%) | 18 (19%) | 1 1 |
| All | All | 3072/4352 (71%) | 2698 (88%) | 374 (12%) | 5 5 |

All (374) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1-A | 23 | PHE |
| 1 | 1-A | 28 | GLU |
| 1 | 1-A | 31 | LEU |
| 1 | 1-A | 41 | PHE |
| 1 | 1-A | 44 | GLU |
| 1 | 1-A | 52 | GLN |
| 1 | 1-A | 63 | GLU |
| 1 | 1-A | 70 | LEU |
| 1 | 1-A | 79 | PRO |
| 1 | 1-A | 81 | PRO |
| 1 | 1-A | 82 | GLN |
| 1 | 1-A | 85 | PRO |
| 1 | 1-A | 92 | LEU |
| 1 | 1-A | 121 | LYS |
| 1 | 1-A | 129 | TYR |
| 1 | 1-B | 24 | ARG |
| 1 | 1-B | 35 | ARG |
| 1 | 1-B | 36 | ARG |
| 1 | 1-B | 37 | LEU |
| 1 | 1-B | 40 | GLU |
| 1 | 1-B | 52 | GLN |
| 1 | 1-B | 77 | THR |
| 1 | 1-B | 104 | VAL |
| 1 | 1-B | 114 | LEU |
| 1 | 1-B | 123 | ASP |
| 1 | 2-A | 28 | GLU |
| 1 | 2-A | 38 | HIS |
| 1 | 2-A | 51 | HIS |
| 1 | 2-A | 63 | GLU |
| 1 | 2-A | 67 | LEU |
| 1 | 2-A | 75 | SER |
| 1 | 2-A | 77 | THR |
| 1 | 2-A | 78 | GLU |
| 1 | 2-A | 89 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 2-A | 97 | SER |
| 1 | 2-A | 120 | SER |
| 1 | 2-A | 121 | LYS |
| 1 | 2-A | 122 | MSE |
| 1 | 2-A | 132 | HIS |
| 1 | 2-A | 134 | SER |
| 1 | 2-B | 37 | LEU |
| 1 | 2-B | 44 | GLU |
| 1 | 2-B | 46 | ASP |
| 1 | 2-B | 52 | GLN |
| 1 | 2-B | 79 | PRO |
| 1 | 2-B | 89 | ARG |
| 1 | 2-B | 95 | GLU |
| 1 | 2-B | 120 | SER |
| 1 | 2-B | 130 | PRO |
| 1 | 3-A | 48 | GLU |
| 1 | 3-A | 52 | GLN |
| 1 | 3-A | 53 | PRO |
| 1 | 3-A | 54 | ARG |
| 1 | 3-A | 63 | GLU |
| 1 | 3-A | 67 | LEU |
| 1 | 3-A | 76 | ASP |
| 1 | 3-A | 77 | THR |
| 1 | 3-A | 82 | GLN |
| 1 | 3-A | 129 | TYR |
| 1 | 3-B | 24 | ARG |
| 1 | 3-B | 38 | HIS |
| 1 | 3-B | 77 | THR |
| 1 | 3-B | 79 | PRO |
| 1 | 3-B | 89 | ARG |
| 1 | 3-B | 94 | GLU |
| 1 | 3-B | 104 | VAL |
| 1 | 3-B | 119 | ILE |
| 1 | 4-A | 54 | ARG |
| 1 | 4-A | 63 | GLU |
| 1 | 4-A | 64 | VAL |
| 1 | 4-A | 67 | LEU |
| 1 | 4-A | 86 | PRO |
| 1 | 4-A | 102 | TYR |
| 1 | 4-A | 109 | ARG |
| 1 | 4-A | 122 | MSE |
| 1 | 4-A | 129 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 4-B | 24 | ARG |
| 1 | 4-B | 49 | GLN |
| 1 | 4-B | 54 | ARG |
| 1 | 4-B | 63 | GLU |
| 1 | 4-B | 81 | PRO |
| 1 | 4-B | 82 | GLN |
| 1 | 4-B | 89 | ARG |
| 1 | 4-B | 104 | VAL |
| 1 | 4-B | 119 | ILE |
| 1 | 4-B | 122 | MSE |
| 1 | 5-A | 33 | ASP |
| 1 | 5-A | 48 | GLU |
| 1 | 5-A | 67 | LEU |
| 1 | 5-A | 72 | GLN |
| 1 | 5-A | 79 | PRO |
| 1 | 5-A | 82 | GLN |
| 1 | 5-A | 89 | ARG |
| 1 | 5-A | 119 | ILE |
| 1 | 5-A | 128 | ARG |
| 1 | 5-A | 129 | TYR |
| 1 | 5-B | 24 | ARG |
| 1 | 5-B | 49 | GLN |
| 1 | 5-B | 70 | LEU |
| 1 | 5-B | 75 | SER |
| 1 | 5-B | 77 | THR |
| 1 | 5-B | 84 | TRP |
| 1 | 5-B | 87 | LYS |
| 1 | 5-B | 95 | GLU |
| 1 | 5-B | 106 | LEU |
| 1 | 5-B | 110 | CYS |
| 1 | 5-B | 119 | ILE |
| 1 | 5-B | 123 | ASP |
| 1 | 6-A | 26 | SER |
| 1 | 6-A | 28 | GLU |
| 1 | 6-A | 44 | GLU |
| 1 | 6-A | 66 | GLU |
| 1 | 6-A | 67 | LEU |
| 1 | 6-A | 75 | SER |
| 1 | 6-A | 89 | ARG |
| 1 | 6-A | 109 | ARG |
| 1 | 6-A | 129 | TYR |
| 1 | 6-B | 28 | GLU |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 6-B | 40 | GLU |
| 1 | 6-B | 60 | LEU |
| 1 | 6-B | 77 | THR |
| 1 | 6-B | 78 | GLU |
| 1 | 6-B | 97 | SER |
| 1 | 6-B | 98 | ASP |
| 1 | 6-B | 104 | VAL |
| 1 | 6-B | 115 | PRO |
| 1 | 7-A | 25 | PHE |
| 1 | 7-A | 51 | HIS |
| 1 | 7-A | 63 | GLU |
| 1 | 7-A | 67 | LEU |
| 1 | 7-A | 75 | SER |
| 1 | 7-A | 82 | GLN |
| 1 | 7-A | 87 | LYS |
| 1 | 7-A | 129 | TYR |
| 1 | 7-A | 133 | LEU |
| 1 | 7-B | 24 | ARG |
| 1 | 7-B | 77 | THR |
| 1 | 7-B | 82 | GLN |
| 1 | 7-B | 86 | PRO |
| 1 | 7-B | 89 | ARG |
| 1 | 7-B | 93 | GLN |
| 1 | 7-B | 98 | ASP |
| 1 | 7-B | 111 | HIS |
| 1 | 8-A | 26 | SER |
| 1 | 8-A | 28 | GLU |
| 1 | 8-A | 63 | GLU |
| 1 | 8-A | 66 | GLU |
| 1 | 8-A | 74 | LYS |
| 1 | 8-A | 75 | SER |
| 1 | 8-A | 98 | ASP |
| 1 | 8-A | 129 | TYR |
| 1 | 8-A | 132 | HIS |
| 1 | 8-B | 50 | PHE |
| 1 | 8-B | 60 | LEU |
| 1 | 8-B | 63 | GLU |
| 1 | 8-B | 67 | LEU |
| 1 | 8-B | 87 | LYS |
| 1 | 8-B | 93 | GLN |
| 1 | 8-B | 95 | GLU |
| 1 | 8-B | 113 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 8-B | 123 | ASP |
| 1 | 8-B | 127 | GLN |
| 1 | 9-A | 46 | ASP |
| 1 | 9-A | 47 | TRP |
| 1 | 9-A | 48 | GLU |
| 1 | 9-A | 72 | GLN |
| 1 | 9-A | 95 | GLU |
| 1 | 9-A | 98 | ASP |
| 1 | 9-A | 100 | LEU |
| 1 | 9-A | 119 | ILE |
| 1 | 9-A | 122 | MSE |
| 1 | 9-A | 123 | ASP |
| 1 | 9-A | 129 | TYR |
| 1 | 9-B | 36 | ARG |
| 1 | 9-B | 46 | ASP |
| 1 | 9-B | 49 | GLN |
| 1 | 9-B | 75 | SER |
| 1 | 9-B | 78 | GLU |
| 1 | 9-B | 89 | ARG |
| 1 | 9-B | 93 | GLN |
| 1 | 9-B | 129 | TYR |
| 1 | 10-A | 28 | GLU |
| 1 | 10-A | 46 | ASP |
| 1 | 10-A | 48 | GLU |
| 1 | 10-A | 64 | VAL |
| 1 | 10-A | 72 | GLN |
| 1 | 10-A | 75 | SER |
| 1 | 10-A | 78 | GLU |
| 1 | 10-A | 82 | GLN |
| 1 | 10-A | 86 | PRO |
| 1 | 10-A | 94 | GLU |
| 1 | 10-A | 95 | GLU |
| 1 | 10-A | 102 | TYR |
| 1 | 10-A | 129 | TYR |
| 1 | 10-A | 132 | HIS |
| 1 | 10-B | 33 | ASP |
| 1 | 10-B | 73 | TRP |
| 1 | 10-B | 75 | SER |
| 1 | 10-B | 98 | ASP |
| 1 | 10-B | 104 | VAL |
| 1 | 10-B | 116 | GLN |
| 1 | 10-B | 124 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 10-B | 126 | ARG |
| 1 | 11-A | 26 | SER |
| 1 | 11-A | 29 | PRO |
| 1 | 11-A | 30 | THR |
| 1 | 11-A | 54 | ARG |
| 1 | 11-A | 66 | GLU |
| 1 | 11-A | 77 | THR |
| 1 | 11-A | 78 | GLU |
| 1 | 11-A | 119 | ILE |
| 1 | 11-A | 129 | TYR |
| 1 | 11-A | 130 | PRO |
| 1 | 11-B | 60 | LEU |
| 1 | 11-B | 100 | LEU |
| 1 | 11-B | 104 | VAL |
| 1 | 11-B | 122 | MSE |
| 1 | 12-A | 28 | GLU |
| 1 | 12-A | 29 | PRO |
| 1 | 12-A | 33 | ASP |
| 1 | 12-A | 35 | ARG |
| 1 | 12-A | 63 | GLU |
| 1 | 12-A | 66 | GLU |
| 1 | 12-A | 75 | SER |
| 1 | 12-A | 81 | PRO |
| 1 | 12-A | 86 | PRO |
| 1 | 12-A | 92 | LEU |
| 1 | 12-A | 129 | TYR |
| 1 | 12-B | 24 | ARG |
| 1 | 12-B | 35 | ARG |
| 1 | 12-B | 52 | GLN |
| 1 | 12-B | 54 | ARG |
| 1 | 12-B | 60 | LEU |
| 1 | 12-B | 70 | LEU |
| 1 | 12-B | 71 | PHE |
| 1 | 12-B | 77 | THR |
| 1 | 12-B | 89 | ARG |
| 1 | 12-B | 93 | GLN |
| 1 | 12-B | 104 | VAL |
| 1 | 12-B | 124 | THR |
| 1 | 13-A | 24 | ARG |
| 1 | 13-A | 33 | ASP |
| 1 | 13-A | 41 | PHE |
| 1 | 13-A | 45 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 13-A | 63 | GLU |
| 1 | 13-A | 67 | LEU |
| 1 | 13-A | 71 | PHE |
| 1 | 13-A | 86 | PRO |
| 1 | 13-A | 92 | LEU |
| 1 | 13-A | 95 | GLU |
| 1 | 13-A | 98 | ASP |
| 1 | 13-A | 111 | HIS |
| 1 | 13-A | 116 | GLN |
| 1 | 13-A | 120 | SER |
| 1 | 13-A | 121 | LYS |
| 1 | 13-A | 125 | ASN |
| 1 | 13-A | 129 | TYR |
| 1 | 13-A | 132 | HIS |
| 1 | 13-B | 28 | GLU |
| 1 | 13-B | 32 | GLU |
| 1 | 13-B | 37 | LEU |
| 1 | 13-B | 40 | GLU |
| 1 | 13-B | 52 | GLN |
| 1 | 13-B | 75 | SER |
| 1 | 13-B | 77 | THR |
| 1 | 13-B | 86 | PRO |
| 1 | 13-B | 87 | LYS |
| 1 | 13-B | 89 | ARG |
| 1 | 13-B | 95 | GLU |
| 1 | 13-B | 103 | LEU |
| 1 | 13-B | 118 | VAL |
| 1 | 13-B | 122 | MSE |
| 1 | 13-B | 128 | ARG |
| 1 | 14-A | 28 | GLU |
| 1 | 14-A | 31 | LEU |
| 1 | 14-A | 46 | ASP |
| 1 | 14-A | 52 | GLN |
| 1 | 14-A | 60 | LEU |
| 1 | 14-A | 63 | GLU |
| 1 | 14-A | 79 | PRO |
| 1 | 14-A | 85 | PRO |
| 1 | 14-A | 89 | ARG |
| 1 | 14-A | 93 | GLN |
| 1 | 14-A | 98 | ASP |
| 1 | 14-A | 122 | MSE |
| 1 | 14-A | 129 | TYR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 14-B | 24 | ARG |
| 1 | 14-B | 32 | GLU |
| 1 | 14-B | 33 | ASP |
| 1 | 14-B | 37 | LEU |
| 1 | 14-B | 40 | GLU |
| 1 | 14-B | 44 | GLU |
| 1 | 14-B | 48 | GLU |
| 1 | 14-B | 49 | GLN |
| 1 | 14-B | 63 | GLU |
| 1 | 14-B | 71 | PHE |
| 1 | 14-B | 72 | GLN |
| 1 | 14-B | 77 | THR |
| 1 | 14-B | 86 | PRO |
| 1 | 14-B | 87 | LYS |
| 1 | 14-B | 113 | ASP |
| 1 | 14-B | 115 | PRO |
| 1 | 14-B | 121 | LYS |
| 1 | 14-B | 122 | MSE |
| 1 | 14-B | 126 | ARG |
| 1 | 14-B | 127 | GLN |
| 1 | 15-A | 24 | ARG |
| 1 | 15-A | 34 | ILE |
| 1 | 15-A | 44 | GLU |
| 1 | 15-A | 49 | GLN |
| 1 | 15-A | 52 | GLN |
| 1 | 15-A | 63 | GLU |
| 1 | 15-A | 66 | GLU |
| 1 | 15-A | 82 | GLN |
| 1 | 15-A | 95 | GLU |
| 1 | 15-A | 123 | ASP |
| 1 | 15-A | 127 | GLN |
| 1 | 15-A | 129 | TYR |
| 1 | 15-B | 28 | GLU |
| 1 | 15-B | 38 | HIS |
| 1 | 15-B | 49 | GLN |
| 1 | 15-B | 51 | HIS |
| 1 | 15-B | 52 | GLN |
| 1 | 15-B | 60 | LEU |
| 1 | 15-B | 71 | PHE |
| 1 | 15-B | 76 | ASP |
| 1 | 15-B | 78 | GLU |
| 1 | 15-B | 89 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 15-B | 93 | GLN |
| 1 | 15-B | 94 | GLU |
| 1 | 15-B | 95 | GLU |
| 1 | 15-B | 100 | LEU |
| 1 | 15-B | 120 | SER |
| 1 | 15-B | 122 | MSE |
| 1 | 15-B | 125 | ASN |
| 1 | 15-B | 127 | GLN |
| 1 | 15-B | 128 | ARG |
| 1 | 16-A | 28 | GLU |
| 1 | 16-A | 35 | ARG |
| 1 | 16-A | 46 | ASP |
| 1 | 16-A | 48 | GLU |
| 1 | 16-A | 50 | PHE |
| 1 | 16-A | 53 | PRO |
| 1 | 16-A | 56 | LEU |
| 1 | 16-A | 60 | LEU |
| 1 | 16-A | 66 | GLU |
| 1 | 16-A | 67 | LEU |
| 1 | 16-A | 77 | THR |
| 1 | 16-A | 79 | PRO |
| 1 | 16-A | 84 | TRP |
| 1 | 16-A | 102 | TYR |
| 1 | 16-A | 106 | LEU |
| 1 | 16-A | 120 | SER |
| 1 | 16-A | 124 | THR |
| 1 | 16-A | 125 | ASN |
| 1 | 16-A | 126 | ARG |
| 1 | 16-B | 29 | PRO |
| 1 | 16-B | 32 | GLU |
| 1 | 16-B | 37 | LEU |
| 1 | 16-B | 41 | PHE |
| 1 | 16-B | 44 | GLU |
| 1 | 16-B | 49 | GLN |
| 1 | 16-B | 54 | ARG |
| 1 | 16-B | 67 | LEU |
| 1 | 16-B | 73 | TRP |
| 1 | 16-B | 75 | SER |
| 1 | 16-B | 77 | THR |
| 1 | 16-B | 78 | GLU |
| 1 | 16-B | 93 | GLN |
| 1 | 16-B | 110 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 16-B | 116 | GLN |
| 1 | 16-B | 122 | MSE |
| 1 | 16-B | 124 | THR |
| 1 | 16-B | 126 | ARG |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1-A | 93 | GLN |
| 1 | 1-A | 127 | GLN |
| 1 | 1-B | 93 | GLN |
| 1 | 2-A | 38 | HIS |
| 1 | 2-A | 52 | GLN |
| 1 | 2-A | 55 | ASN |
| 1 | 2-A | 82 | GLN |
| 1 | 2-A | 93 | GLN |
| 1 | 2-B | 52 | GLN |
| 1 | 2-B | 72 | GLN |
| 1 | 2-B | 125 | ASN |
| 1 | 3-A | 38 | HIS |
| 1 | 3-A | 93 | GLN |
| 1 | 3-A | 111 | HIS |
| 1 | 3-A | 127 | GLN |
| 1 | 3-A | 132 | HIS |
| 1 | 3-B | 49 | GLN |
| 1 | 3-B | 52 | GLN |
| 1 | 3-B | 111 | HIS |
| 1 | 4-A | 93 | GLN |
| 1 | 4-A | 127 | GLN |
| 1 | 4-B | 38 | HIS |
| 1 | 4-B | 72 | GLN |
| 1 | 4-B | 82 | GLN |
| 1 | 4-B | 93 | GLN |
| 1 | 4-B | 111 | HIS |
| 1 | 5-B | 55 | ASN |
| 1 | 5-B | 93 | GLN |
| 1 | 5-B | 111 | HIS |
| 1 | 5-B | 116 | GLN |
| 1 | 5-B | 125 | ASN |
| 1 | 5-B | 127 | GLN |
| 1 | 6-A | 49 | GLN |
| 1 | 6-A | 82 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 6-A | 93 | GLN |
| 1 | 6-A | 127 | GLN |
| 1 | 6-B | 38 | HIS |
| 1 | 6-B | 82 | GLN |
| 1 | 6-B | 93 | GLN |
| 1 | 6-B | 127 | GLN |
| 1 | 7-A | 49 | GLN |
| 1 | 7-A | 111 | HIS |
| 1 | 7-A | 116 | GLN |
| 1 | 7-A | 127 | GLN |
| 1 | 7-B | 49 | GLN |
| 1 | 7-B | 52 | GLN |
| 1 | 7-B | 82 | GLN |
| 1 | 7-B | 111 | HIS |
| 1 | 8-A | 55 | ASN |
| 1 | 8-A | 111 | HIS |
| 1 | 8-B | 38 | HIS |
| 1 | 8-B | 51 | HIS |
| 1 | 8-B | 82 | GLN |
| 1 | 8-B | 93 | GLN |
| 1 | 8-B | 127 | GLN |
| 1 | 9-A | 72 | GLN |
| 1 | 9-A | 111 | HIS |
| 1 | 9-B | 52 | GLN |
| 1 | 9-B | 125 | ASN |
| 1 | 10-A | 38 | HIS |
| 1 | 10-A | 127 | GLN |
| 1 | 10-B | 93 | GLN |
| 1 | 10-B | 116 | GLN |
| 1 | 10-B | 125 | ASN |
| 1 | 10-B | 127 | GLN |
| 1 | 11-A | 55 | ASN |
| 1 | 11-A | 72 | GLN |
| 1 | 11-A | 93 | GLN |
| 1 | 11-A | 127 | GLN |
| 1 | 11-B | 38 | HIS |
| 1 | 11-B | 93 | GLN |
| 1 | 11-B | 111 | HIS |
| 1 | 11-B | 116 | GLN |
| 1 | 11-B | 125 | ASN |
| 1 | 12-A | 55 | ASN |
| 1 | 12-A | 82 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 12-A | 111 | HIS |
| 1 | 12-B | 51 | HIS |
| 1 | 12-B | 52 | GLN |
| 1 | 12-B | 82 | GLN |
| 1 | 12-B | 93 | GLN |
| 1 | 12-B | 116 | GLN |
| 1 | 12-B | 125 | ASN |
| 1 | 13-A | 38 | HIS |
| 1 | 13-A | 52 | GLN |
| 1 | 13-A | 55 | ASN |
| 1 | 13-A | 72 | GLN |
| 1 | 13-A | 93 | GLN |
| 1 | 13-A | 111 | HIS |
| 1 | 13-B | 51 | HIS |
| 1 | 13-B | 52 | GLN |
| 1 | 13-B | 55 | ASN |
| 1 | 13-B | 111 | HIS |
| 1 | 14-A | 55 | ASN |
| 1 | 14-A | 93 | GLN |
| 1 | 14-A | 116 | GLN |
| 1 | 14-A | 127 | GLN |
| 1 | 14-B | 38 | HIS |
| 1 | 14-B | 51 | HIS |
| 1 | 14-B | 52 | GLN |
| 1 | 14-B | 93 | GLN |
| 1 | 15-A | 49 | GLN |
| 1 | 15-A | 52 | GLN |
| 1 | 15-A | 72 | GLN |
| 1 | 15-A | 127 | GLN |
| 1 | 15-B | 38 | HIS |
| 1 | 15-B | 52 | GLN |
| 1 | 15-B | 111 | HIS |
| 1 | 15-B | 127 | GLN |
| 1 | 16-A | 51 | HIS |
| 1 | 16-A | 52 | GLN |
| 1 | 16-A | 111 | HIS |
| 1 | 16-B | 72 | GLN |
| 1 | 16-B | 93 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.