



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:26 pm BST

PDB ID : 4JSU
Title : Yeast 20S proteasome in complex with the dimerized linear mimetic of TMC-95A - yCP:3a
Authors : Desvergne, A.; Genin, E.; Marechal, X.; Gallastegui, N.; Dufau, L.; Richy, N.; Groll, M.; Vidal, J.; Reboud-Ravaux, M.
Deposited on : 2013-03-22
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

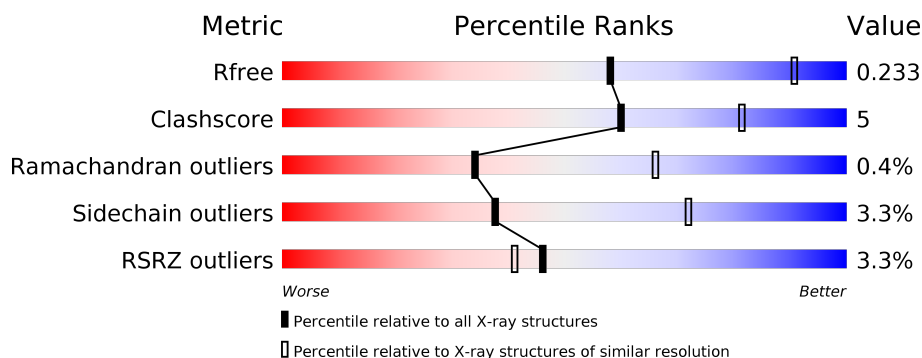
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 130704 | 1957 (2.90-2.90) |
| Clashscore | 141614 | 2172 (2.90-2.90) |
| Ramachandran outliers | 138981 | 2115 (2.90-2.90) |
| Sidechain outliers | 138945 | 2117 (2.90-2.90) |
| RSRZ outliers | 127900 | 1906 (2.90-2.90) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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 $\leq 5\%$. 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 | 250 | <div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div> |
| 1 | O | 250 | <div> <div>4%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div> |
| 2 | B | 258 | <div> <div>5%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5%</div> </div> </div> |
| 2 | P | 258 | <div> <div>6%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>5%</div> </div> </div> |
| 3 | C | 254 | <div> <div>6%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div> |
| 3 | Q | 254 | <div> <div>7%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div> </div> |


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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 4 | D | 260 | |
| 4 | R | 260 | |
| 5 | E | 234 | |
| 5 | S | 234 | |
| 6 | F | 288 | |
| 6 | T | 288 | |
| 7 | G | 252 | |
| 7 | U | 252 | |
| 8 | H | 232 | |
| 8 | V | 232 | |
| 9 | I | 205 | |
| 9 | W | 205 | |
| 10 | J | 198 | |
| 10 | X | 198 | |
| 11 | K | 212 | |
| 11 | Y | 212 | |
| 12 | L | 222 | |
| 12 | Z | 222 | |
| 13 | M | 233 | |
| 13 | a | 233 | |
| 14 | N | 196 | |
| 14 | b | 196 | |
| 15 | c | 8 | |
| 15 | d | 8 | |
| 15 | e | 8 | |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 15 | f | 8 |  |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 15 | RE0 | e | 7 | - | - | - | X |
| 15 | RE0 | f | 7 | - | - | - | X |

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 51118 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 Proteasome subunit alpha type-2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |
| 1 | O | 250 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1915 | 1219 | 315 | 377 | 4 | | | |

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 2 | B | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1904 | 1201 | 321 | 379 | 3 | | | |
| 2 | P | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1904 | 1201 | 321 | 379 | 3 | | | |

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 3 | C | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1890 | 1181 | 331 | 374 | 4 | | | |
| 3 | Q | 241 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1890 | 1181 | 331 | 374 | 4 | | | |

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 4 | D | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1861 | 1162 | 314 | 378 | 7 | | | |
| 4 | R | 242 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1861 | 1162 | 314 | 378 | 7 | | | |

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5 | E | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |
| 5 | S | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1795 | 1129 | 312 | 350 | 4 | | | |

- Molecule 6 is a protein called Probable proteasome subunit alpha type-7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 6 | F | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1896 | 1205 | 330 | 357 | 4 | | | |
| 6 | T | 244 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1896 | 1205 | 330 | 357 | 4 | | | |

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 7 | G | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |
| 7 | U | 243 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1921 | 1221 | 322 | 370 | 8 | | | |

- Molecule 8 is a protein called Proteasome subunit beta type-2.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 8 | H | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1684 | 1061 | 293 | 323 | 7 | | | |
| 8 | V | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1684 | 1061 | 293 | 323 | 7 | | | |

- Molecule 9 is a protein called Proteasome subunit beta type-3.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 9 | I | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |
| 9 | W | 204 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1581 | 1010 | 258 | 305 | 8 | | | |

- Molecule 10 is a protein called Proteasome subunit beta type-4.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | J | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 10 | X | 198 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1585 | 1005 | 269 | 305 | 6 | | | |

- Molecule 11 is a protein called Proteasome subunit beta type-5.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 11 | K | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |
| 11 | Y | 212 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1644 | 1045 | 280 | 312 | 7 | | | |

- Molecule 12 is a protein called Proteasome subunit beta type-6.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 12 | L | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |
| 12 | Z | 222 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1757 | 1115 | 303 | 335 | 4 | | | |

- Molecule 13 is a protein called Proteasome subunit beta type-7.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 13 | M | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |
| 13 | a | 233 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1824 | 1154 | 312 | 351 | 7 | | | |

- Molecule 14 is a protein called Proteasome subunit beta type-1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 14 | N | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |
| 14 | b | 196 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1512 | 955 | 250 | 300 | 7 | | | |

- Molecule 15 is a protein called TMC-95A mimic ligand yCP:3a.

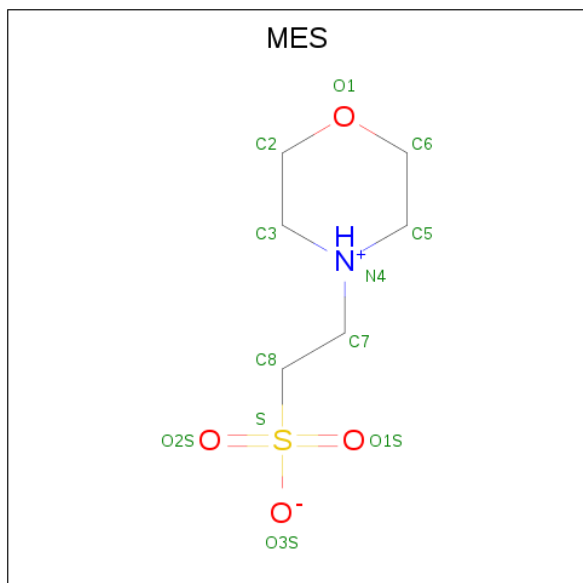
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 15 | c | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 56 | 43 | 6 | 7 | | | |
| 15 | d | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 56 | 43 | 6 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|---|---------|---------|-------|
| 15 | e | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 56 | 43 | 6 | 7 | | | |
| 15 | f | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 56 | 43 | 6 | 7 | | | |

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---|---------|---------|
| 16 | K | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 12 | 6 | 1 | 4 | 1 | | |
| 16 | Y | 1 | Total | C | N | O | S | 0 | 0 |
| | | | 12 | 6 | 1 | 4 | 1 | | |

- Molecule 17 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 17 | A | 58 | Total | O | 0 | 0 |
| | | | 58 | 58 | | |
| 17 | B | 40 | Total | O | 0 | 0 |
| | | | 40 | 40 | | |
| 17 | C | 40 | Total | O | 0 | 0 |
| | | | 40 | 40 | | |
| 17 | D | 37 | Total | O | 0 | 0 |
| | | | 37 | 37 | | |
| 17 | E | 22 | Total | O | 0 | 0 |
| | | | 22 | 22 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 17 | F | 47 | Total O 47 47 | 0 | 0 |
| 17 | G | 58 | Total O 58 58 | 0 | 0 |
| 17 | H | 53 | Total O 53 53 | 0 | 0 |
| 17 | I | 62 | Total O 62 62 | 0 | 0 |
| 17 | J | 53 | Total O 53 53 | 0 | 0 |
| 17 | K | 49 | Total O 49 49 | 0 | 0 |
| 17 | L | 58 | Total O 58 58 | 0 | 0 |
| 17 | M | 75 | Total O 75 75 | 0 | 0 |
| 17 | N | 57 | Total O 57 57 | 0 | 0 |
| 17 | O | 33 | Total O 33 33 | 0 | 0 |
| 17 | P | 29 | Total O 29 29 | 0 | 0 |
| 17 | Q | 29 | Total O 29 29 | 0 | 0 |
| 17 | R | 28 | Total O 28 28 | 0 | 0 |
| 17 | S | 18 | Total O 18 18 | 0 | 0 |
| 17 | T | 44 | Total O 44 44 | 0 | 0 |
| 17 | U | 58 | Total O 58 58 | 0 | 0 |
| 17 | V | 47 | Total O 47 47 | 0 | 0 |
| 17 | W | 58 | Total O 58 58 | 0 | 0 |
| 17 | X | 44 | Total O 44 44 | 0 | 0 |
| 17 | Y | 46 | Total O 46 46 | 0 | 0 |
| 17 | Z | 51 | Total O 51 51 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 17 | a | 79 | Total 79 | O 79 | 0 | 0 |
| 17 | b | 57 | Total 57 | O 57 | 0 | 0 |
| 17 | e | 1 | Total 1 | O 1 | 0 | 0 |
| 17 | f | 1 | Total 1 | O 1 | 0 | 0 |

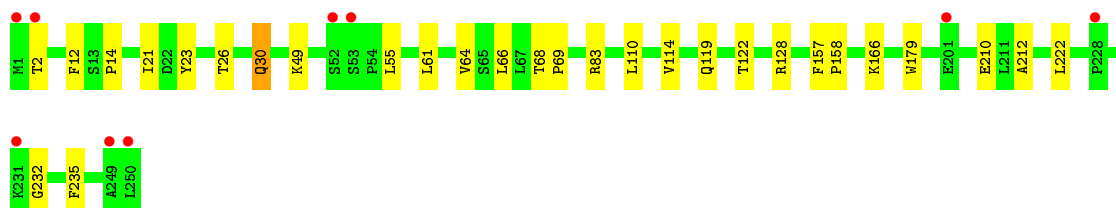
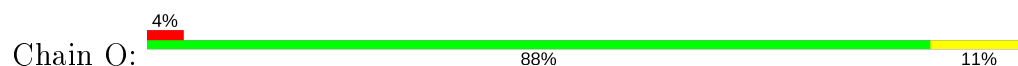
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

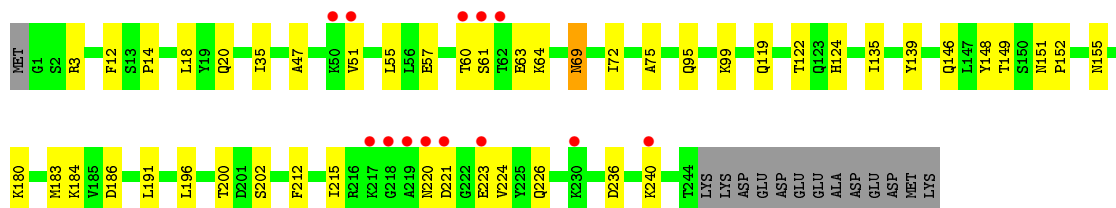
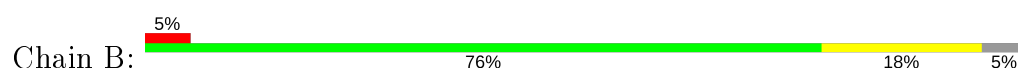
- Molecule 1: Proteasome subunit alpha type-2



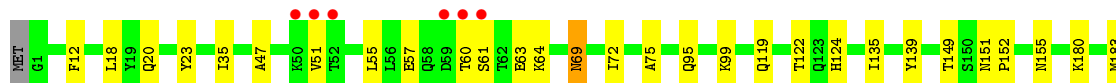
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-3

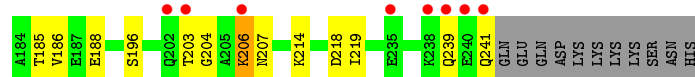
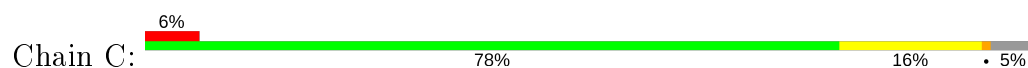


- Molecule 2: Proteasome subunit alpha type-3

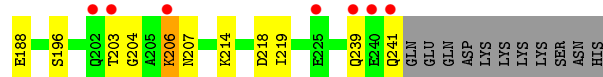
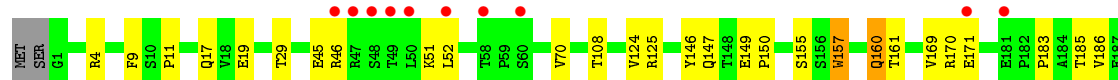
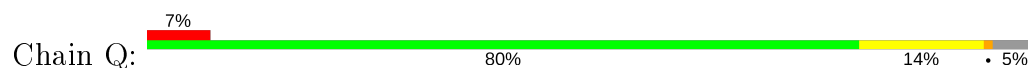




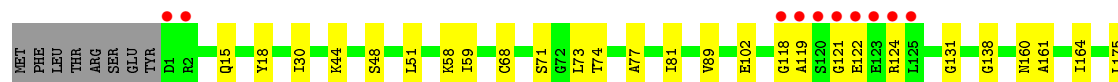
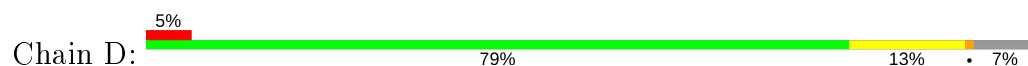
- Molecule 3: Proteasome subunit alpha type-4



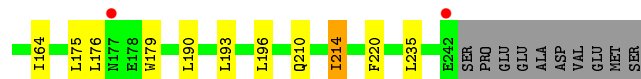
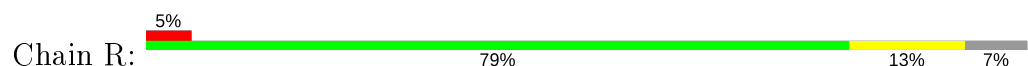
- Molecule 3: Proteasome subunit alpha type-4



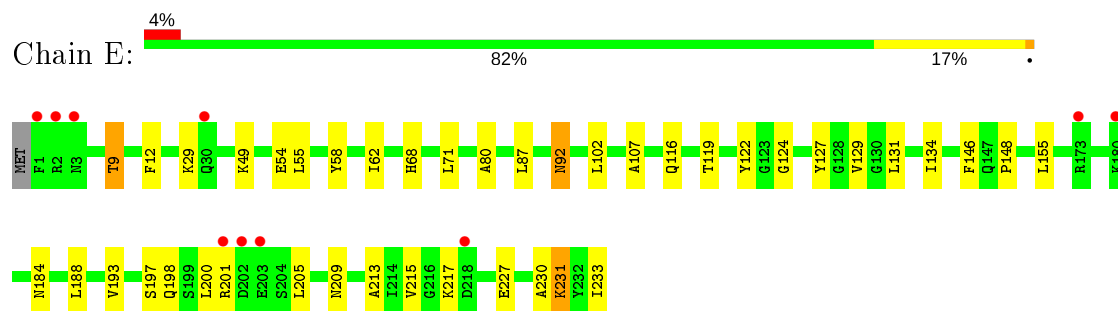
- Molecule 4: Proteasome subunit alpha type-5



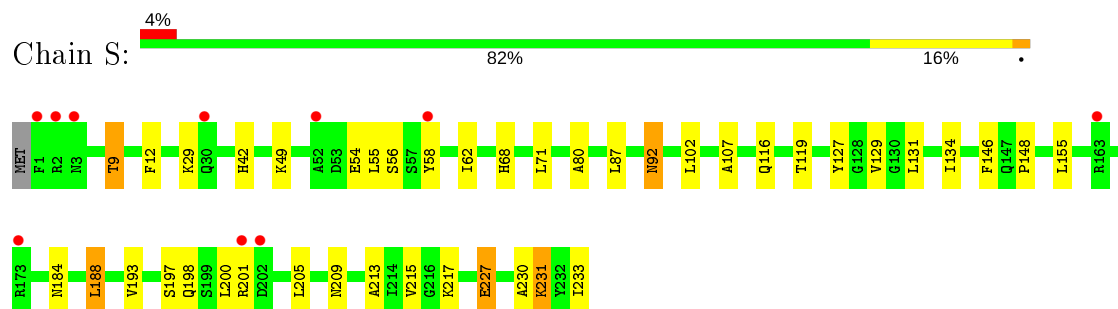
- Molecule 4: Proteasome subunit alpha type-5



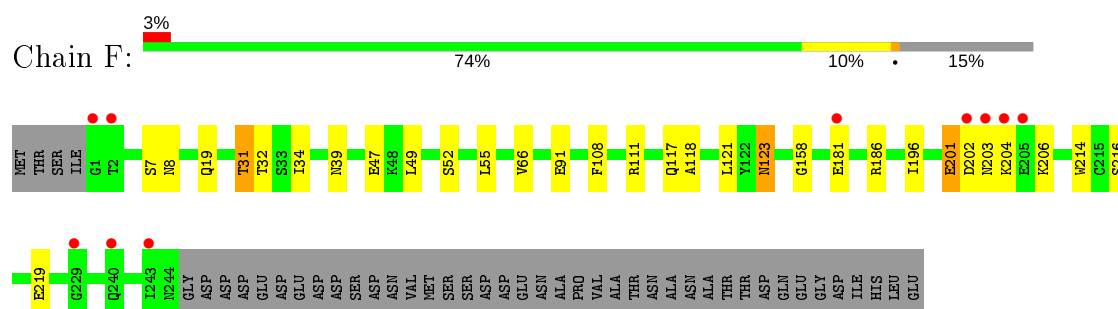
- Molecule 5: Proteasome subunit alpha type-6



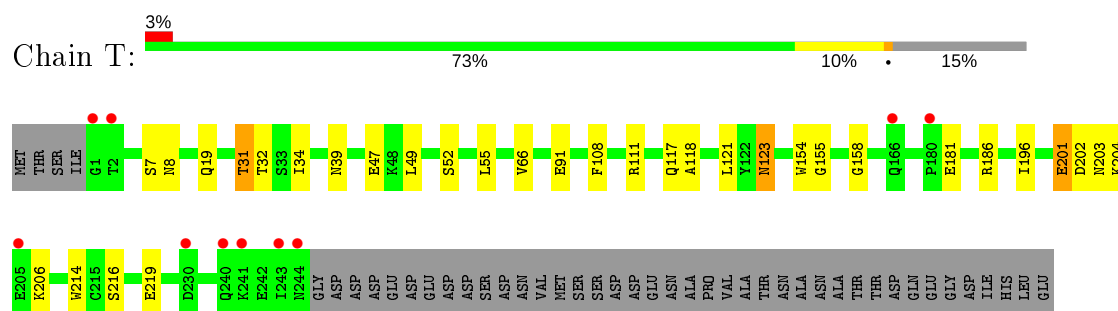
- Molecule 5: Proteasome subunit alpha type-6



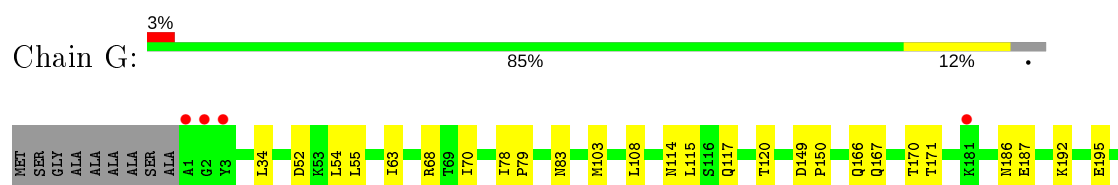
- Molecule 6: Probable proteasome subunit alpha type-7

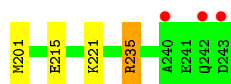


- Molecule 6: Probable proteasome subunit alpha type-7

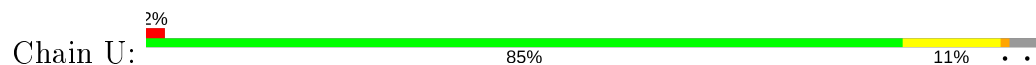


- Molecule 7: Proteasome subunit alpha type-1

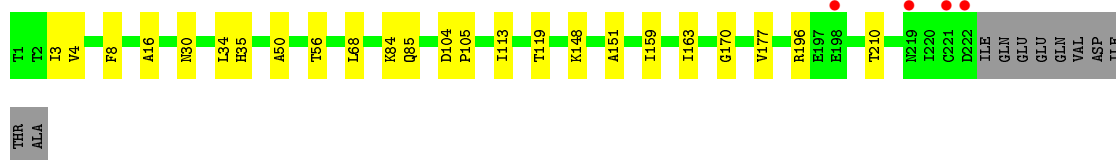
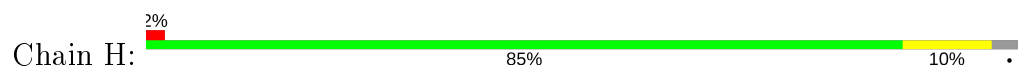




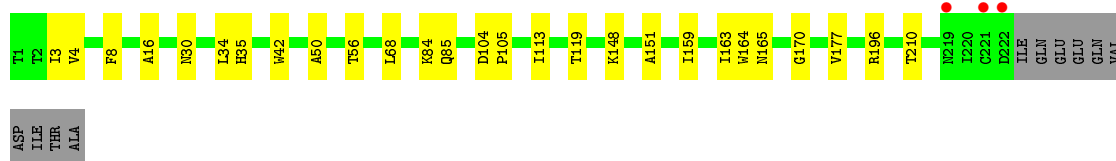
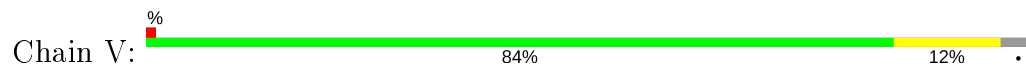
- Molecule 7: Proteasome subunit alpha type-1



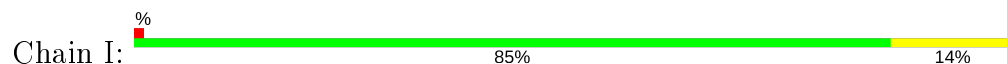
- Molecule 8: Proteasome subunit beta type-2



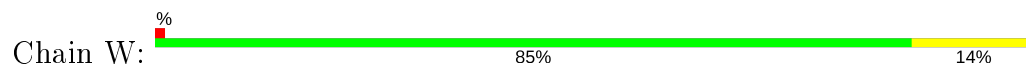
- Molecule 8: Proteasome subunit beta type-2



- Molecule 9: Proteasome subunit beta type-3



- Molecule 9: Proteasome subunit beta type-3



D204

- Molecule 10: Proteasome subunit beta type-4

Chain J: 3% 83% 17%

M1 D2 I3 V9 K19 T22 I25 S39 P40 L66 E71 S91 Y98 I119 K125 V126 E127 Y130 Y139 T140 F141 L144 H147 Y148 R149 P150 D151 M152 L158 D159 L160 L168 M172 P173 M174 I180 D194 F195 Q196 A197

Q198

- Molecule 10: Proteasome subunit beta type-4

Chain X: 4% 85% 15%

M1 D2 I3 V9 K19 T22 I25 S39 P40 E71 I119 K125 V126 E127 Y130 Y139 T140 F141 L144 H147 Y148 R149 P150 D151 M152 L158 D159 L160 L168 M172 P173 M174 I180 D194 F195 Q196 A197 Q198

- Molecule 11: Proteasome subunit beta type-5

Chain K: 4% 86% 11%

T1 L4 A5 F6 Q9 I12 I35 N38 P39 F40 A49 Q53 E56 L65 R73 V87 T99 M100 Y104 K107 P110 V115 D125 W146 D147 K158 L177 V180 T181 E182 D183 W198 K201 F207 N208 N209

G212

- Molecule 11: Proteasome subunit beta type-5

Chain Y: 4% 87% 10%

T1 L4 A5 F6 Q9 I12 I35 N38 P39 F40 A49 Q53 E56 L65 R73 V87 T99 M100 Y104 T105 K107 P110 V115 D125 W146 K158 L177 V180 T181 E182 D183 K201 F207 N208 N209 I211

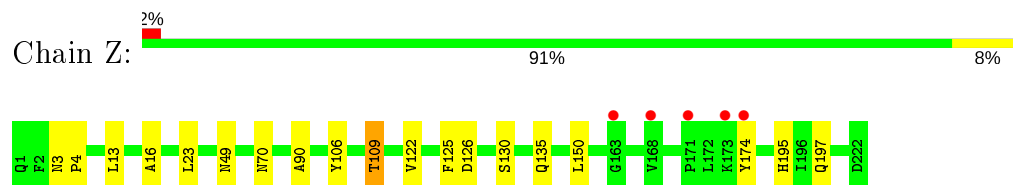
G212

- Molecule 12: Proteasome subunit beta type-6

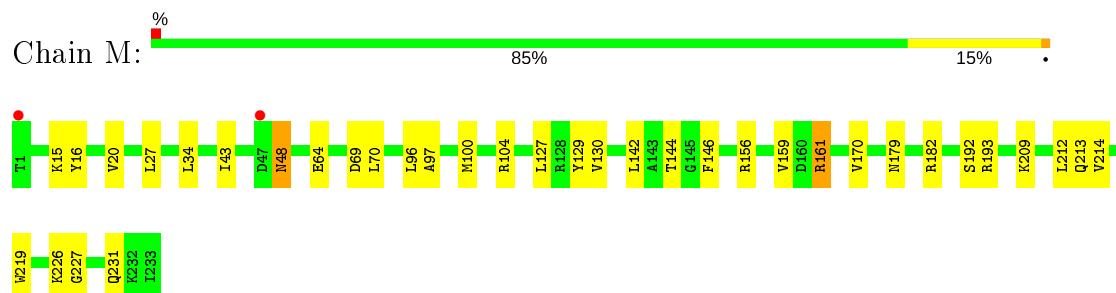
Chain L: 3% 91% 8%

Q1 F2 N3 P4 L13 A16 L23 N49 N70 N80 A90 Y106 T109 V122 F125 D126 S130 Q135 L150 N165 V168 P171 L172 K173 Y174 H195 I196 Q197 D222

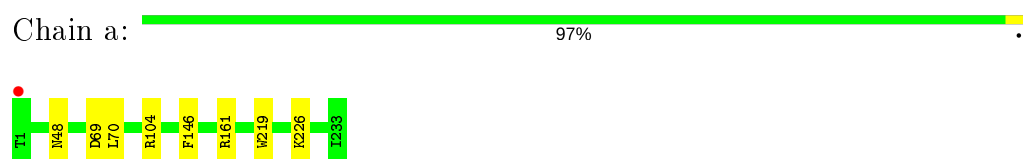
- Molecule 12: Proteasome subunit beta type-6



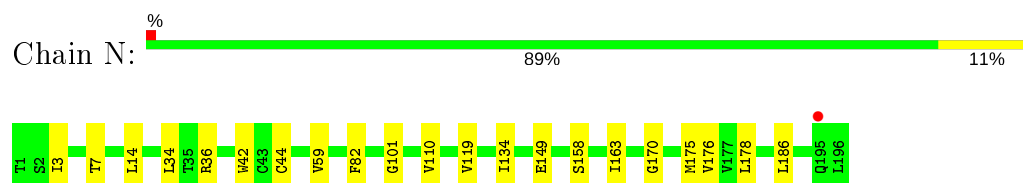
- Molecule 13: Proteasome subunit beta type-7



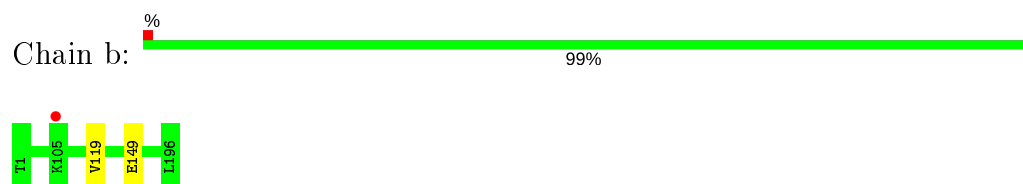
- Molecule 13: Proteasome subunit beta type-7



- Molecule 14: Proteasome subunit beta type-1



- Molecule 14: Proteasome subunit beta type-1

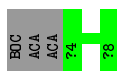


- Molecule 15: TMC-95A mimic ligand yCP:3a

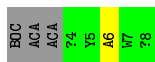


- Molecule 15: TMC-95A mimic ligand yCP:3a

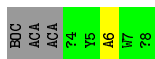




- Molecule 15: TMC-95A mimic ligand yCP:3a



- Molecule 15: TMC-95A mimic ligand yCP:3a



4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 1 21 1 | Depositor |
| Cell constants a, b, c, α , β , γ | 135.35Å 299.22Å 144.65Å 90.00° 112.97° 90.00° | Depositor |
| Resolution (Å) | 15.00 – 2.90 15.00 – 2.90 | Depositor EDS |
| % Data completeness (in resolution range) | 99.1 (15.00-2.90) 99.1 (15.00-2.90) | Depositor EDS |
| R_{merge} | 0.08 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.44 (at 2.91Å) | Xtriage |
| Refinement program | REFMAC | Depositor |
| R, R_{free} | 0.221 , 0.227 0.227 , 0.233 | Depositor DCC |
| R_{free} test set | 11475 reflections (5.00%) | wwPDB-VP |
| Wilson B-factor (Å ²) | 58.1 | Xtriage |
| Anisotropy | 0.159 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.32 , 59.8 | EDS |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| F_o, F_c correlation | 0.92 | EDS |
| Total number of atoms | 51118 | wwPDB-VP |
| Average B, all atoms (Å ²) | 67.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TY5, ACA, RE0, ABN, MES

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 | 0.37 | 2/1952 (0.1%) | 0.47 | 0/2642 |
| 1 | O | 0.37 | 1/1952 (0.1%) | 0.48 | 0/2642 |
| 2 | B | 0.33 | 0/1934 | 0.48 | 0/2618 |
| 2 | P | 0.33 | 0/1934 | 0.48 | 0/2618 |
| 3 | C | 0.34 | 0/1919 | 0.49 | 0/2598 |
| 3 | Q | 0.34 | 1/1919 (0.1%) | 0.49 | 0/2598 |
| 4 | D | 0.35 | 0/1886 | 0.49 | 0/2541 |
| 4 | R | 0.36 | 0/1886 | 0.49 | 0/2541 |
| 5 | E | 0.31 | 0/1823 | 0.47 | 0/2463 |
| 5 | S | 0.31 | 0/1823 | 0.47 | 0/2463 |
| 6 | F | 0.41 | 0/1936 | 0.47 | 0/2614 |
| 6 | T | 0.41 | 0/1936 | 0.47 | 0/2614 |
| 7 | G | 0.34 | 0/1959 | 0.47 | 0/2652 |
| 7 | U | 0.34 | 0/1959 | 0.47 | 0/2652 |
| 8 | H | 0.44 | 0/1715 | 0.48 | 0/2326 |
| 8 | V | 0.44 | 2/1715 (0.1%) | 0.48 | 0/2326 |
| 9 | I | 0.34 | 0/1611 | 0.49 | 0/2174 |
| 9 | W | 0.34 | 0/1611 | 0.49 | 0/2174 |
| 10 | J | 0.31 | 0/1613 | 0.48 | 0/2173 |
| 10 | X | 0.31 | 0/1613 | 0.48 | 0/2173 |
| 11 | K | 0.50 | 2/1681 (0.1%) | 0.51 | 1/2274 (0.0%) |
| 11 | Y | 0.50 | 1/1681 (0.1%) | 0.51 | 1/2274 (0.0%) |
| 12 | L | 0.36 | 0/1795 | 0.48 | 0/2420 |
| 12 | Z | 0.36 | 0/1795 | 0.48 | 0/2420 |
| 13 | M | 0.36 | 1/1855 (0.1%) | 0.49 | 0/2514 |
| 13 | a | 0.36 | 1/1855 (0.1%) | 0.50 | 0/2514 |
| 14 | N | 0.39 | 0/1541 | 0.45 | 0/2087 |
| 14 | b | 0.39 | 0/1541 | 0.45 | 0/2087 |
| 15 | c | 0.84 | 0/4 | 0.69 | 0/4 |
| 15 | d | 0.85 | 0/4 | 0.70 | 0/4 |
| 15 | e | 0.83 | 0/4 | 0.61 | 0/4 |
| 15 | f | 0.85 | 0/4 | 0.61 | 0/4 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| All | All | 0.37 | 11/50456 (0.0%) | 0.48 | 2/68208 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 15 | e | 0 | 1 |
| 15 | f | 0 | 1 |
| All | All | 0 | 2 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 11 | K | 146 | TRP | CD2-CE2 | 5.05 | 1.47 | 1.41 |
| 13 | M | 219 | TRP | CD2-CE2 | 5.04 | 1.47 | 1.41 |
| 1 | A | 179 | TRP | CD2-CE2 | 5.04 | 1.47 | 1.41 |
| 11 | Y | 146 | TRP | CD2-CE2 | 5.03 | 1.47 | 1.41 |
| 8 | V | 42 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | A | 159 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 1 | O | 179 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 13 | a | 219 | TRP | CD2-CE2 | 5.02 | 1.47 | 1.41 |
| 11 | K | 198 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |
| 3 | Q | 157 | TRP | CD2-CE2 | 5.01 | 1.47 | 1.41 |
| 8 | V | 164 | TRP | CD2-CE2 | 5.00 | 1.47 | 1.41 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11 | Y | 4 | LEU | CA-CB-CG | 5.34 | 127.59 | 115.30 |
| 11 | K | 4 | LEU | CA-CB-CG | 5.33 | 127.55 | 115.30 |

There are no chirality outliers.

All (2) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 15 | e | 6 | ALA | Peptide |
| 15 | f | 6 | ALA | Peptide |

5.2 Too-close contacts ⓘ

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 1915 | 0 | 1929 | 14 | 0 |
| 1 | O | 1915 | 0 | 1929 | 19 | 0 |
| 2 | B | 1904 | 0 | 1904 | 27 | 0 |
| 2 | P | 1904 | 0 | 1904 | 25 | 0 |
| 3 | C | 1890 | 0 | 1903 | 29 | 0 |
| 3 | Q | 1890 | 0 | 1903 | 23 | 0 |
| 4 | D | 1861 | 0 | 1839 | 19 | 0 |
| 4 | R | 1861 | 0 | 1839 | 18 | 0 |
| 5 | E | 1795 | 0 | 1800 | 26 | 0 |
| 5 | S | 1795 | 0 | 1800 | 25 | 0 |
| 6 | F | 1896 | 0 | 1889 | 17 | 0 |
| 6 | T | 1896 | 0 | 1889 | 18 | 0 |
| 7 | G | 1921 | 0 | 1913 | 16 | 0 |
| 7 | U | 1921 | 0 | 1913 | 19 | 0 |
| 8 | H | 1684 | 0 | 1688 | 13 | 0 |
| 8 | V | 1684 | 0 | 1688 | 14 | 0 |
| 9 | I | 1581 | 0 | 1574 | 20 | 0 |
| 9 | W | 1581 | 0 | 1574 | 19 | 0 |
| 10 | J | 1585 | 0 | 1590 | 23 | 0 |
| 10 | X | 1585 | 0 | 1590 | 19 | 0 |
| 11 | K | 1644 | 0 | 1595 | 15 | 0 |
| 11 | Y | 1644 | 0 | 1595 | 15 | 0 |
| 12 | L | 1757 | 0 | 1711 | 11 | 0 |
| 12 | Z | 1757 | 0 | 1711 | 11 | 0 |
| 13 | M | 1824 | 0 | 1832 | 20 | 0 |
| 13 | a | 1824 | 0 | 1832 | 0 | 0 |
| 14 | N | 1512 | 0 | 1481 | 11 | 0 |
| 14 | b | 1512 | 0 | 1481 | 0 | 0 |
| 15 | c | 56 | 0 | 48 | 0 | 0 |
| 15 | d | 56 | 0 | 48 | 0 | 0 |
| 15 | e | 56 | 0 | 48 | 0 | 0 |
| 15 | f | 56 | 0 | 48 | 0 | 0 |
| 16 | K | 12 | 0 | 13 | 0 | 0 |
| 16 | Y | 12 | 0 | 13 | 0 | 0 |
| 17 | A | 58 | 0 | 0 | 0 | 0 |
| 17 | B | 40 | 0 | 0 | 0 | 0 |
| 17 | C | 40 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 17 | D | 37 | 0 | 0 | 0 | 0 |
| 17 | E | 22 | 0 | 0 | 0 | 0 |
| 17 | F | 47 | 0 | 0 | 0 | 0 |
| 17 | G | 58 | 0 | 0 | 0 | 0 |
| 17 | H | 53 | 0 | 0 | 0 | 0 |
| 17 | I | 62 | 0 | 0 | 0 | 0 |
| 17 | J | 53 | 0 | 0 | 2 | 0 |
| 17 | K | 49 | 0 | 0 | 0 | 0 |
| 17 | L | 58 | 0 | 0 | 0 | 0 |
| 17 | M | 75 | 0 | 0 | 0 | 0 |
| 17 | N | 57 | 0 | 0 | 0 | 0 |
| 17 | O | 33 | 0 | 0 | 0 | 0 |
| 17 | P | 29 | 0 | 0 | 0 | 0 |
| 17 | Q | 29 | 0 | 0 | 0 | 0 |
| 17 | R | 28 | 0 | 0 | 0 | 0 |
| 17 | S | 18 | 0 | 0 | 0 | 0 |
| 17 | T | 44 | 0 | 0 | 0 | 0 |
| 17 | U | 58 | 0 | 0 | 0 | 0 |
| 17 | V | 47 | 0 | 0 | 0 | 0 |
| 17 | W | 58 | 0 | 0 | 0 | 0 |
| 17 | X | 44 | 0 | 0 | 0 | 0 |
| 17 | Y | 46 | 0 | 0 | 0 | 0 |
| 17 | Z | 51 | 0 | 0 | 0 | 0 |
| 17 | a | 79 | 0 | 0 | 0 | 0 |
| 17 | b | 57 | 0 | 0 | 0 | 0 |
| 17 | e | 1 | 0 | 0 | 0 | 0 |
| 17 | f | 1 | 0 | 0 | 0 | 0 |
| All | All | 51118 | 0 | 49514 | 409 | 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 5.

All (409) 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) |
|------------------|-------------------|--------------------------|-------------------|
| 12:Z:13:LEU:HD11 | 12:Z:150:LEU:HD21 | 1.55 | 0.88 |
| 6:F:91:GLU:HG2 | 6:F:111:ARG:HB3 | 1.57 | 0.86 |
| 6:T:91:GLU:HG2 | 6:T:111:ARG:HB3 | 1.57 | 0.86 |
| 12:L:13:LEU:HD11 | 12:L:150:LEU:HD21 | 1.55 | 0.86 |
| 1:O:12:PHE:H | 2:P:20:GLN:HE22 | 1.29 | 0.80 |
| 2:B:12:PHE:H | 3:C:17:GLN:HE22 | 1.28 | 0.79 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:160:GLN:HE21 | 3:C:160:GLN:HA | 1.50 | 0.76 |
| 3:Q:160:GLN:HE21 | 3:Q:160:GLN:HA | 1.50 | 0.75 |
| 2:B:122:THR:HG22 | 3:C:125:ARG:HH21 | 1.54 | 0.73 |
| 3:Q:9:PHE:H | 4:R:15:GLN:HE22 | 1.36 | 0.72 |
| 1:O:128:ARG:HH21 | 7:U:120:THR:HG22 | 1.55 | 0.72 |
| 1:A:12:PHE:H | 2:B:20:GLN:HE22 | 1.36 | 0.72 |
| 7:G:187:GLU:HG2 | 7:G:192:LYS:HB2 | 1.72 | 0.71 |
| 3:C:9:PHE:H | 4:D:15:GLN:HE22 | 1.38 | 0.71 |
| 7:U:187:GLU:HG2 | 7:U:192:LYS:HB2 | 1.72 | 0.70 |
| 5:S:12:PHE:H | 6:T:19:GLN:HE22 | 1.38 | 0.70 |
| 2:P:200:THR:HG22 | 2:P:202:SER:H | 1.57 | 0.69 |
| 2:B:200:THR:HG22 | 2:B:202:SER:H | 1.57 | 0.69 |
| 2:P:124:HIS:HB3 | 3:Q:124:VAL:HG12 | 1.75 | 0.69 |
| 13:M:161:ARG:HH11 | 13:M:161:ARG:HG3 | 1.60 | 0.67 |
| 5:E:12:PHE:H | 6:F:19:GLN:HE22 | 1.42 | 0.66 |
| 2:P:122:THR:HG22 | 3:Q:125:ARG:HH21 | 1.60 | 0.65 |
| 12:L:13:LEU:CD1 | 12:L:150:LEU:HD21 | 2.28 | 0.64 |
| 10:J:168:LEU:O | 10:J:172:MET:HB2 | 1.99 | 0.63 |
| 2:P:12:PHE:H | 3:Q:17:GLN:HE22 | 1.47 | 0.63 |
| 2:B:95:GLN:HE22 | 9:I:71:ASN:HD22 | 1.45 | 0.63 |
| 1:A:128:ARG:HH21 | 7:G:120:THR:HG22 | 1.64 | 0.62 |
| 10:J:139:TYR:OH | 10:X:25:ILE:HG12 | 1.99 | 0.62 |
| 12:L:16:ALA:HB2 | 12:L:122:VAL:HG23 | 1.81 | 0.62 |
| 2:B:124:HIS:HB3 | 3:C:124:VAL:HG12 | 1.82 | 0.62 |
| 10:J:25:ILE:HG12 | 10:X:139:TYR:OH | 1.99 | 0.62 |
| 5:E:87:LEU:HD11 | 5:E:107:ALA:HB1 | 1.82 | 0.62 |
| 2:P:95:GLN:HE22 | 9:W:71:ASN:HD22 | 1.48 | 0.62 |
| 3:Q:214:LYS:HB2 | 3:Q:218:ASP:HB3 | 1.82 | 0.62 |
| 4:R:73:LEU:HD12 | 4:R:131:GLY:HA3 | 1.82 | 0.62 |
| 10:X:168:LEU:O | 10:X:172:MET:HB2 | 1.99 | 0.62 |
| 12:Z:13:LEU:CD1 | 12:Z:150:LEU:HD21 | 2.28 | 0.62 |
| 3:C:214:LYS:HB2 | 3:C:218:ASP:HB3 | 1.81 | 0.61 |
| 11:K:107:LYS:H | 11:K:107:LYS:HD2 | 1.66 | 0.61 |
| 12:Z:16:ALA:HB2 | 12:Z:122:VAL:HG23 | 1.81 | 0.61 |
| 4:D:73:LEU:HD12 | 4:D:131:GLY:HA3 | 1.82 | 0.61 |
| 9:I:35:VAL:HG13 | 17:J:240:HOH:O | 2.01 | 0.61 |
| 6:F:31:THR:HG21 | 6:F:47:GLU:O | 2.01 | 0.61 |
| 5:S:87:LEU:HD11 | 5:S:107:ALA:HB1 | 1.82 | 0.61 |
| 13:M:127:LEU:HG | 13:M:142:LEU:HD12 | 1.83 | 0.61 |
| 4:D:119:ALA:HA | 5:E:124:GLY:HA2 | 1.83 | 0.60 |
| 6:T:31:THR:HG21 | 6:T:47:GLU:O | 2.01 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:107:LYS:H | 11:Y:107:LYS:HD2 | 1.66 | 0.60 |
| 3:C:161:THR:HG21 | 3:C:169:VAL:HG13 | 1.84 | 0.60 |
| 12:Z:126:ASP:HB2 | 12:Z:130:SER:HB3 | 1.83 | 0.60 |
| 12:L:109:THR:HG23 | 12:L:125:PHE:HB2 | 1.82 | 0.60 |
| 7:U:195:GLU:HG3 | 7:U:235:ARG:HG3 | 1.83 | 0.60 |
| 7:G:195:GLU:HG3 | 7:G:235:ARG:HG3 | 1.83 | 0.59 |
| 12:L:195:HIS:HD2 | 12:L:197:GLN:H | 1.51 | 0.59 |
| 3:Q:161:THR:HG21 | 3:Q:169:VAL:HG13 | 1.84 | 0.59 |
| 2:P:151:ASN:HB2 | 2:P:152:PRO:HD2 | 1.84 | 0.59 |
| 3:C:169:VAL:HG23 | 3:C:196:SER:HB2 | 1.84 | 0.59 |
| 14:N:175:MET:HB2 | 14:N:186:LEU:HB2 | 1.83 | 0.59 |
| 3:Q:169:VAL:HG23 | 3:Q:196:SER:HB2 | 1.84 | 0.59 |
| 2:B:63:GLU:HG3 | 2:B:64:LYS:HG3 | 1.86 | 0.58 |
| 10:J:3:ILE:HD13 | 10:J:168:LEU:HD13 | 1.85 | 0.58 |
| 12:Z:195:HIS:HD2 | 12:Z:197:GLN:H | 1.50 | 0.58 |
| 3:C:155:SER:HB2 | 4:D:51:LEU:HD21 | 1.84 | 0.58 |
| 12:L:126:ASP:HB2 | 12:L:130:SER:HB3 | 1.84 | 0.58 |
| 8:H:35:HIS:CB | 8:H:56:THR:HG21 | 2.34 | 0.58 |
| 10:X:3:ILE:HD13 | 10:X:168:LEU:HD13 | 1.86 | 0.58 |
| 12:Z:109:THR:HG23 | 12:Z:125:PHE:HB2 | 1.85 | 0.57 |
| 9:I:9:GLY:HA3 | 9:I:41:LYS:HE2 | 1.86 | 0.57 |
| 2:B:151:ASN:HB2 | 2:B:152:PRO:HD2 | 1.84 | 0.57 |
| 2:P:63:GLU:HG3 | 2:P:64:LYS:HG3 | 1.86 | 0.57 |
| 8:V:35:HIS:CB | 8:V:56:THR:HG21 | 2.34 | 0.57 |
| 2:P:215:ILE:HG12 | 2:P:226:GLN:HG2 | 1.87 | 0.57 |
| 10:J:174:MET:HE1 | 10:X:173:PRO:HB2 | 1.86 | 0.57 |
| 13:M:179:ASN:HD22 | 13:M:182:ARG:HH11 | 1.52 | 0.57 |
| 2:B:215:ILE:HG12 | 2:B:226:GLN:HG2 | 1.87 | 0.56 |
| 5:E:68:HIS:HE1 | 5:E:102:LEU:O | 1.88 | 0.56 |
| 4:R:161:ALA:HB3 | 5:S:55:LEU:HD23 | 1.88 | 0.56 |
| 9:W:9:GLY:HA3 | 9:W:41:LYS:HE2 | 1.86 | 0.56 |
| 4:D:77:ALA:O | 4:D:81:ILE:HG12 | 2.06 | 0.56 |
| 4:R:77:ALA:O | 4:R:81:ILE:HG12 | 2.06 | 0.56 |
| 10:J:173:PRO:HB2 | 10:X:174:MET:HE1 | 1.87 | 0.56 |
| 7:G:103:MET:HE3 | 7:G:108:LEU:HD13 | 1.88 | 0.55 |
| 1:O:83:ARG:HE | 7:U:114:ASN:HD21 | 1.53 | 0.55 |
| 8:V:163:ILE:HG23 | 8:V:170:GLY:HA2 | 1.89 | 0.55 |
| 10:J:119:ILE:HG12 | 10:J:125:LYS:HG3 | 1.88 | 0.55 |
| 5:E:205:LEU:HA | 5:E:209:ASN:HD22 | 1.72 | 0.54 |
| 8:H:163:ILE:HG23 | 8:H:170:GLY:HA2 | 1.89 | 0.54 |
| 5:S:68:HIS:HE1 | 5:S:102:LEU:O | 1.88 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 10:X:119:ILE:HG12 | 10:X:125:LYS:HG3 | 1.88 | 0.54 |
| 11:Y:158:LYS:HB2 | 11:Y:177:LEU:HD11 | 1.90 | 0.54 |
| 2:B:35:ILE:HD12 | 2:B:196:LEU:HG | 1.88 | 0.54 |
| 11:K:208:ASN:HD21 | 10:X:150:PRO:HG3 | 1.73 | 0.54 |
| 9:W:94:LEU:HD11 | 9:W:106:PRO:HG2 | 1.90 | 0.54 |
| 2:P:35:ILE:HD12 | 2:P:196:LEU:HG | 1.88 | 0.54 |
| 5:S:205:LEU:HA | 5:S:209:ASN:HD22 | 1.72 | 0.54 |
| 9:I:94:LEU:HD11 | 9:I:106:PRO:HG2 | 1.90 | 0.54 |
| 11:K:73:ARG:NH2 | 11:K:104:TYR:O | 2.41 | 0.53 |
| 2:P:75:ALA:HB3 | 2:P:135:ILE:HB | 1.90 | 0.53 |
| 11:Y:73:ARG:NH2 | 11:Y:104:TYR:O | 2.41 | 0.53 |
| 12:Z:135:GLN:HG3 | 12:Z:174:TYR:OH | 2.08 | 0.53 |
| 7:U:103:MET:HE3 | 7:U:108:LEU:HD13 | 1.89 | 0.53 |
| 3:Q:157:TRP:CE2 | 4:R:51:LEU:HD23 | 2.43 | 0.53 |
| 1:A:83:ARG:HE | 7:G:114:ASN:HD21 | 1.56 | 0.53 |
| 7:U:63:ILE:HD12 | 7:U:215:GLU:HG2 | 1.90 | 0.53 |
| 2:B:75:ALA:HB3 | 2:B:135:ILE:HB | 1.90 | 0.53 |
| 2:B:151:ASN:HB2 | 2:B:152:PRO:CD | 2.39 | 0.53 |
| 8:H:35:HIS:HB2 | 8:H:56:THR:HG21 | 1.89 | 0.53 |
| 2:P:151:ASN:HB2 | 2:P:152:PRO:CD | 2.39 | 0.53 |
| 12:L:135:GLN:HG3 | 12:L:174:TYR:OH | 2.08 | 0.53 |
| 6:T:91:GLU:HG3 | 6:T:111:ARG:HH11 | 1.74 | 0.53 |
| 1:O:83:ARG:HE | 7:U:114:ASN:ND2 | 2.06 | 0.53 |
| 8:V:35:HIS:HB2 | 8:V:56:THR:HG21 | 1.89 | 0.53 |
| 8:V:104:ASP:HB2 | 8:V:105:PRO:HD2 | 1.91 | 0.52 |
| 1:A:55:LEU:HD12 | 7:G:170:THR:HG23 | 1.90 | 0.52 |
| 13:M:27:LEU:HB2 | 13:M:192:SER:HB2 | 1.90 | 0.52 |
| 10:J:39:SER:HB2 | 10:J:40:PRO:HD2 | 1.92 | 0.52 |
| 6:T:32:THR:HG22 | 6:T:47:GLU:OE2 | 2.10 | 0.52 |
| 7:G:63:ILE:HD12 | 7:G:215:GLU:HG2 | 1.90 | 0.52 |
| 11:K:158:LYS:HB2 | 11:K:177:LEU:HD11 | 1.91 | 0.52 |
| 6:F:32:THR:HG22 | 6:F:47:GLU:OE2 | 2.09 | 0.52 |
| 10:J:150:PRO:HG3 | 11:Y:208:ASN:HD21 | 1.74 | 0.52 |
| 12:Z:3:ASN:HD22 | 12:Z:4:PRO:HD2 | 1.75 | 0.52 |
| 2:B:3:ARG:HB2 | 5:E:122:TYR:OH | 2.10 | 0.52 |
| 4:D:138:GLY:HA2 | 4:D:214:ILE:HG12 | 1.92 | 0.52 |
| 8:H:104:ASP:HB2 | 8:H:105:PRO:HD2 | 1.91 | 0.52 |
| 13:M:48:ASN:H | 13:M:48:ASN:HD22 | 1.57 | 0.52 |
| 4:R:44:LYS:HE3 | 4:R:210:GLN:HB2 | 1.92 | 0.52 |
| 3:C:204:GLY:HA3 | 3:C:207:ASN:HB2 | 1.92 | 0.51 |
| 4:D:44:LYS:HE3 | 4:D:210:GLN:HB2 | 1.92 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 9:I:28:LEU:HB3 | 9:I:36:SER:HB3 | 1.92 | 0.51 |
| 3:C:157:TRP:CE2 | 4:D:51:LEU:HD23 | 2.45 | 0.51 |
| 4:R:159:TYR:CE2 | 5:S:56:SER:HB3 | 2.45 | 0.51 |
| 10:J:139:TYR:HD1 | 17:J:226:HOH:O | 1.94 | 0.51 |
| 6:F:91:GLU:HG3 | 6:F:111:ARG:HH11 | 1.75 | 0.51 |
| 5:S:127:TYR:O | 5:S:148:PRO:HB3 | 2.09 | 0.51 |
| 10:X:39:SER:HB2 | 10:X:40:PRO:HD2 | 1.92 | 0.51 |
| 5:E:127:TYR:O | 5:E:148:PRO:HB3 | 2.10 | 0.51 |
| 11:K:38:ASN:HB2 | 11:K:39:PRO:HD2 | 1.93 | 0.51 |
| 1:A:30:GLN:HE21 | 1:A:30:GLN:HA | 1.75 | 0.51 |
| 4:D:59:ILE:HG22 | 4:D:220:PHE:HZ | 1.76 | 0.51 |
| 12:L:3:ASN:HD22 | 12:L:4:PRO:HD2 | 1.75 | 0.51 |
| 7:G:78:ILE:N | 7:G:79:PRO:HD2 | 2.26 | 0.51 |
| 10:X:149:ARG:HB2 | 10:X:152:MET:HG3 | 1.93 | 0.51 |
| 11:Y:38:ASN:HB2 | 11:Y:39:PRO:HD2 | 1.93 | 0.51 |
| 3:Q:155:SER:HB2 | 4:R:51:LEU:HD21 | 1.93 | 0.50 |
| 1:O:30:GLN:HE21 | 1:O:30:GLN:HA | 1.76 | 0.50 |
| 4:R:138:GLY:HA2 | 4:R:214:ILE:HG12 | 1.93 | 0.50 |
| 5:S:9:THR:HG21 | 5:S:119:THR:HA | 1.94 | 0.50 |
| 13:M:27:LEU:HD21 | 13:M:34:LEU:HD22 | 1.93 | 0.50 |
| 2:P:57:GLU:O | 2:P:61:SER:HB2 | 2.11 | 0.50 |
| 2:B:57:GLU:O | 2:B:61:SER:HB2 | 2.11 | 0.50 |
| 13:M:15:LYS:HB3 | 13:M:20:VAL:HG12 | 1.92 | 0.50 |
| 9:W:28:LEU:HB3 | 9:W:36:SER:HB3 | 1.93 | 0.50 |
| 4:R:59:ILE:HG22 | 4:R:220:PHE:HZ | 1.76 | 0.50 |
| 9:W:52:ILE:HB | 9:W:59:VAL:HG13 | 1.94 | 0.50 |
| 5:E:9:THR:HG21 | 5:E:119:THR:HA | 1.93 | 0.50 |
| 7:U:78:ILE:N | 7:U:79:PRO:HD2 | 2.26 | 0.50 |
| 5:E:205:LEU:HD23 | 5:E:205:LEU:H | 1.77 | 0.50 |
| 5:S:205:LEU:HD23 | 5:S:205:LEU:H | 1.77 | 0.50 |
| 3:Q:185:THR:HB | 3:Q:188:GLU:HG2 | 1.94 | 0.49 |
| 3:Q:204:GLY:HA3 | 3:Q:207:ASN:HB2 | 1.92 | 0.49 |
| 1:O:23:TYR:CD1 | 7:U:12:PRO:HA | 2.47 | 0.49 |
| 9:I:52:ILE:HB | 9:I:59:VAL:HG13 | 1.94 | 0.49 |
| 10:J:149:ARG:HB2 | 10:J:152:MET:HG3 | 1.93 | 0.49 |
| 4:D:89:VAL:HG21 | 11:K:65:LEU:HD13 | 1.94 | 0.49 |
| 5:S:231:LYS:HD2 | 5:S:231:LYS:H | 1.78 | 0.49 |
| 3:C:160:GLN:HE21 | 3:C:160:GLN:CA | 2.24 | 0.49 |
| 3:C:185:THR:HB | 3:C:188:GLU:HG2 | 1.94 | 0.49 |
| 5:S:197:SER:HA | 5:S:200:LEU:HG | 1.95 | 0.49 |
| 13:M:156:ARG:HH11 | 8:V:165:ASN:HD22 | 1.61 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 13:M:97:ALA:HA | 13:M:130:VAL:HG21 | 1.95 | 0.49 |
| 5:E:231:LYS:H | 5:E:231:LYS:HD2 | 1.78 | 0.49 |
| 4:D:176:LEU:HD22 | 5:E:55:LEU:HD13 | 1.95 | 0.48 |
| 6:T:201:GLU:O | 6:T:204:LYS:HD2 | 2.13 | 0.48 |
| 3:Q:160:GLN:HE22 | 3:Q:170:ARG:HE | 1.61 | 0.48 |
| 3:Q:186:VAL:HG21 | 3:Q:214:LYS:HE2 | 1.95 | 0.48 |
| 5:S:155:LEU:HD23 | 6:T:55:LEU:HA | 1.95 | 0.48 |
| 5:S:200:LEU:HD11 | 5:S:205:LEU:HD22 | 1.95 | 0.48 |
| 5:S:80:ALA:HB2 | 5:S:129:VAL:HG21 | 1.95 | 0.48 |
| 8:V:113:ILE:HG12 | 8:V:119:THR:HG22 | 1.94 | 0.48 |
| 8:V:210:THR:HG21 | 9:W:167:SER:HB3 | 1.94 | 0.48 |
| 1:A:83:ARG:HE | 7:G:114:ASN:ND2 | 2.11 | 0.48 |
| 8:H:113:ILE:HG12 | 8:H:119:THR:HG22 | 1.94 | 0.48 |
| 10:X:147:HIS:HB2 | 10:X:160:LEU:HD11 | 1.95 | 0.48 |
| 5:E:193:VAL:HG13 | 5:E:205:LEU:HD11 | 1.95 | 0.48 |
| 11:K:35:ILE:HG21 | 11:K:56:GLU:HB3 | 1.96 | 0.48 |
| 6:F:31:THR:HG23 | 6:F:47:GLU:HB3 | 1.95 | 0.48 |
| 13:M:129:TYR:HE1 | 13:M:144:THR:HG22 | 1.78 | 0.48 |
| 3:C:186:VAL:HG21 | 3:C:214:LYS:HE2 | 1.95 | 0.48 |
| 5:E:197:SER:HA | 5:E:200:LEU:HG | 1.94 | 0.48 |
| 5:E:200:LEU:HD11 | 5:E:205:LEU:HD22 | 1.95 | 0.48 |
| 8:H:8:PHE:HB3 | 8:H:151:ALA:HB2 | 1.96 | 0.48 |
| 13:M:227:GLY:HA3 | 13:M:231:GLN:HB3 | 1.95 | 0.48 |
| 2:P:180:LYS:HG3 | 2:P:183:MET:HG3 | 1.95 | 0.48 |
| 3:Q:46:ARG:HD2 | 3:Q:206:LYS:O | 2.14 | 0.48 |
| 4:R:89:VAL:HG21 | 11:Y:65:LEU:HD13 | 1.95 | 0.48 |
| 2:B:180:LYS:HG3 | 2:B:183:MET:HG3 | 1.96 | 0.48 |
| 11:K:99:THR:HG22 | 11:K:115:VAL:O | 2.14 | 0.48 |
| 5:S:193:VAL:HG13 | 5:S:205:LEU:HD11 | 1.96 | 0.48 |
| 9:I:36:SER:HB2 | 10:J:126:VAL:HG21 | 1.96 | 0.47 |
| 3:C:160:GLN:HE22 | 3:C:170:ARG:HE | 1.61 | 0.47 |
| 5:E:80:ALA:HB2 | 5:E:129:VAL:HG21 | 1.95 | 0.47 |
| 3:Q:46:ARG:HB2 | 3:Q:207:ASN:HA | 1.96 | 0.47 |
| 1:A:222:LEU:HD13 | 1:A:232:GLY:HA2 | 1.96 | 0.47 |
| 6:T:31:THR:HG23 | 6:T:47:GLU:HB3 | 1.95 | 0.47 |
| 9:W:10:ILE:HD11 | 9:W:174:ALA:HB2 | 1.96 | 0.47 |
| 2:B:139:TYR:CD1 | 2:B:224:VAL:HG21 | 2.49 | 0.47 |
| 8:V:8:PHE:HB3 | 8:V:151:ALA:HB2 | 1.96 | 0.47 |
| 11:Y:201:LYS:HG3 | 11:Y:207:PHE:HB2 | 1.97 | 0.47 |
| 10:J:147:HIS:HB2 | 10:J:160:LEU:HD11 | 1.95 | 0.47 |
| 3:C:46:ARG:HD2 | 3:C:206:LYS:O | 2.14 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 9:I:14:MET:HB3 | 9:I:162:LEU:HD11 | 1.97 | 0.47 |
| 9:I:10:ILE:HD11 | 9:I:174:ALA:HB2 | 1.95 | 0.47 |
| 11:K:201:LYS:HG3 | 11:K:207:PHE:HB2 | 1.97 | 0.47 |
| 2:P:236:ASP:O | 2:P:240:LYS:HG2 | 2.15 | 0.47 |
| 13:M:193:ARG:HG3 | 13:M:214:VAL:HB | 1.96 | 0.47 |
| 9:W:14:MET:HB3 | 9:W:162:LEU:HD11 | 1.97 | 0.47 |
| 11:Y:35:ILE:HG21 | 11:Y:56:GLU:HB3 | 1.96 | 0.47 |
| 2:P:139:TYR:CD1 | 2:P:224:VAL:HG21 | 2.49 | 0.47 |
| 3:Q:70:VAL:HG13 | 3:Q:219:ILE:HD13 | 1.97 | 0.47 |
| 8:V:4:VAL:HG22 | 8:V:159:ILE:HD11 | 1.97 | 0.47 |
| 13:M:16:TYR:CE2 | 13:M:170:VAL:HG22 | 2.50 | 0.47 |
| 6:T:216:SER:HB3 | 6:T:219:GLU:HB2 | 1.97 | 0.47 |
| 1:O:55:LEU:HB3 | 7:U:159:ALA:O | 2.15 | 0.47 |
| 2:B:236:ASP:O | 2:B:240:LYS:HG2 | 2.15 | 0.46 |
| 5:E:155:LEU:HD23 | 6:F:55:LEU:HA | 1.96 | 0.46 |
| 8:H:210:THR:HG21 | 9:I:167:SER:HB3 | 1.96 | 0.46 |
| 1:A:68:THR:HB | 1:A:69:PRO:HD2 | 1.97 | 0.46 |
| 14:N:34:LEU:HD13 | 14:N:176:VAL:HG23 | 1.98 | 0.46 |
| 1:O:68:THR:HB | 1:O:69:PRO:HD2 | 1.97 | 0.46 |
| 5:S:230:ALA:HA | 5:S:233:ILE:HD12 | 1.98 | 0.46 |
| 5:S:92:ASN:HD21 | 12:Z:70:ASN:ND2 | 2.13 | 0.46 |
| 9:W:36:SER:HB2 | 10:X:126:VAL:HG21 | 1.97 | 0.46 |
| 6:F:216:SER:HB3 | 6:F:219:GLU:HB2 | 1.97 | 0.46 |
| 9:W:62:LEU:HD11 | 9:W:104:VAL:HG21 | 1.98 | 0.46 |
| 3:C:46:ARG:HB2 | 3:C:207:ASN:HA | 1.96 | 0.46 |
| 10:J:173:PRO:HB3 | 10:X:22:THR:HG21 | 1.98 | 0.46 |
| 1:O:158:PRO:HB2 | 2:P:57:GLU:HB3 | 1.97 | 0.46 |
| 1:A:110:LEU:O | 1:A:114:VAL:HG23 | 2.16 | 0.46 |
| 13:M:96:LEU:O | 13:M:100:MET:HG2 | 2.16 | 0.46 |
| 1:O:222:LEU:HD13 | 1:O:232:GLY:HA2 | 1.97 | 0.46 |
| 1:O:110:LEU:O | 1:O:114:VAL:HG23 | 2.16 | 0.46 |
| 5:S:131:LEU:HB2 | 5:S:146:PHE:HB3 | 1.97 | 0.46 |
| 8:V:50:ALA:HB2 | 9:W:128:CYS:HB2 | 1.97 | 0.46 |
| 5:E:131:LEU:HB2 | 5:E:146:PHE:HB3 | 1.97 | 0.46 |
| 5:E:49:LYS:HB3 | 5:E:58:TYR:HB3 | 1.98 | 0.46 |
| 7:U:167:GLN:HE21 | 7:U:171:THR:HG23 | 1.81 | 0.46 |
| 11:Y:99:THR:HG22 | 11:Y:115:VAL:O | 2.14 | 0.46 |
| 5:E:230:ALA:HA | 5:E:233:ILE:HD12 | 1.98 | 0.45 |
| 7:G:167:GLN:HE21 | 7:G:171:THR:HG23 | 1.81 | 0.45 |
| 10:X:19:LYS:HD3 | 10:X:180:ILE:HG13 | 1.99 | 0.45 |
| 3:C:108:THR:HG21 | 3:C:146:TYR:HB3 | 1.98 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 8:H:4:VAL:HG22 | 8:H:159:ILE:HD11 | 1.96 | 0.45 |
| 13:M:179:ASN:HD22 | 13:M:182:ARG:NH1 | 2.15 | 0.45 |
| 6:T:52:SER:H | 6:T:55:LEU:HD13 | 1.80 | 0.45 |
| 9:W:10:ILE:HG21 | 9:W:141:ALA:HB3 | 1.98 | 0.45 |
| 1:A:119:GLN:O | 1:A:122:THR:HB | 2.16 | 0.45 |
| 6:F:52:SER:H | 6:F:55:LEU:HD13 | 1.80 | 0.45 |
| 6:F:201:GLU:O | 6:F:204:LYS:HD2 | 2.16 | 0.45 |
| 3:C:70:VAL:HG13 | 3:C:219:ILE:HD13 | 1.97 | 0.45 |
| 8:H:35:HIS:HB3 | 8:H:56:THR:HG21 | 1.99 | 0.45 |
| 11:K:38:ASN:O | 11:K:40:PHE:N | 2.49 | 0.45 |
| 8:V:35:HIS:HB3 | 8:V:56:THR:HG21 | 1.99 | 0.45 |
| 9:I:10:ILE:HG21 | 9:I:141:ALA:HB3 | 1.98 | 0.45 |
| 10:J:22:THR:HG21 | 10:X:173:PRO:HB3 | 1.97 | 0.45 |
| 10:J:19:LYS:HD3 | 10:J:180:ILE:HG13 | 1.99 | 0.45 |
| 2:P:69:ASN:HB3 | 2:P:72:ILE:H | 1.82 | 0.45 |
| 5:S:49:LYS:HB3 | 5:S:58:TYR:HB3 | 1.99 | 0.45 |
| 5:E:92:ASN:HD21 | 12:L:70:ASN:ND2 | 2.13 | 0.45 |
| 3:Q:239:GLN:C | 3:Q:241:GLN:H | 2.21 | 0.45 |
| 3:C:239:GLN:C | 3:C:241:GLN:H | 2.20 | 0.44 |
| 3:C:157:TRP:CZ3 | 4:D:48:SER:HB3 | 2.51 | 0.44 |
| 8:H:84:LYS:HG3 | 8:H:85:GLN:N | 2.32 | 0.44 |
| 14:N:14:LEU:O | 14:N:175:MET:HA | 2.17 | 0.44 |
| 1:O:14:PRO:HA | 2:P:23:TYR:CD1 | 2.52 | 0.44 |
| 2:P:18:LEU:HD13 | 2:P:122:THR:HG23 | 1.99 | 0.44 |
| 4:R:30:ILE:HD12 | 4:R:196:LEU:HG | 1.99 | 0.44 |
| 6:T:49:LEU:HD22 | 6:T:206:LYS:HB2 | 1.99 | 0.44 |
| 3:C:149:GLU:HB2 | 3:C:150:PRO:HD2 | 1.98 | 0.44 |
| 1:O:21:ILE:HD11 | 1:O:122:THR:HG21 | 2.00 | 0.44 |
| 9:W:20:VAL:HG13 | 9:W:118:PRO:HB3 | 1.99 | 0.44 |
| 9:W:33:LEU:HD11 | 10:X:141:PHE:HD2 | 1.81 | 0.44 |
| 11:Y:38:ASN:O | 11:Y:40:PHE:N | 2.50 | 0.44 |
| 2:B:99:LYS:HG3 | 9:I:64:GLU:HB3 | 1.98 | 0.44 |
| 9:I:62:LEU:HD11 | 9:I:104:VAL:HG21 | 1.98 | 0.44 |
| 14:N:101:GLY:HA2 | 14:N:178:LEU:HD23 | 1.98 | 0.44 |
| 2:B:18:LEU:HD13 | 2:B:122:THR:HG23 | 1.99 | 0.44 |
| 5:E:92:ASN:HD21 | 12:L:70:ASN:HD21 | 1.66 | 0.44 |
| 3:Q:149:GLU:HB2 | 3:Q:150:PRO:HD2 | 1.98 | 0.44 |
| 1:A:26:THR:O | 1:A:30:GLN:HG2 | 2.18 | 0.44 |
| 4:D:30:ILE:HD12 | 4:D:196:LEU:HG | 1.99 | 0.44 |
| 9:I:33:LEU:HD11 | 10:J:141:PHE:HD2 | 1.82 | 0.44 |
| 13:M:209:LYS:HB3 | 13:M:212:LEU:HD11 | 1.99 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 1:O:119:GLN:O | 1:O:122:THR:HB | 2.16 | 0.44 |
| 6:T:118:ALA:HA | 6:T:121:LEU:HD12 | 1.99 | 0.44 |
| 3:C:29:THR:HB | 3:C:45:GLU:HG3 | 2.00 | 0.44 |
| 11:K:6:PHE:HA | 11:K:125:ASP:O | 2.18 | 0.44 |
| 6:F:118:ALA:HA | 6:F:121:LEU:HD12 | 1.99 | 0.43 |
| 1:A:21:ILE:HD11 | 1:A:122:THR:HG21 | 2.00 | 0.43 |
| 5:E:134:ILE:HD12 | 5:E:215:VAL:HG12 | 2.00 | 0.43 |
| 6:F:49:LEU:HD22 | 6:F:206:LYS:HB2 | 1.99 | 0.43 |
| 6:T:158:GLY:O | 7:U:54:LEU:HB3 | 2.18 | 0.43 |
| 8:V:148:LYS:HE3 | 8:V:177:VAL:HG11 | 1.99 | 0.43 |
| 10:J:1:MET:HG2 | 10:J:2:ASP:N | 2.33 | 0.43 |
| 5:S:92:ASN:HD21 | 12:Z:70:ASN:HD21 | 1.66 | 0.43 |
| 9:I:20:VAL:HG13 | 9:I:118:PRO:HB3 | 2.00 | 0.43 |
| 1:O:21:ILE:HD11 | 1:O:122:THR:CG2 | 2.49 | 0.43 |
| 3:Q:11:PRO:HA | 4:R:18:TYR:CD1 | 2.54 | 0.43 |
| 5:S:134:ILE:HD12 | 5:S:215:VAL:HG12 | 2.00 | 0.43 |
| 12:L:90:ALA:HA | 12:L:125:PHE:HZ | 1.84 | 0.43 |
| 14:N:7:THR:HG23 | 14:N:110:VAL:HG23 | 2.00 | 0.43 |
| 8:V:84:LYS:HG3 | 8:V:85:GLN:N | 2.32 | 0.43 |
| 11:Y:6:PHE:HA | 11:Y:125:ASP:O | 2.18 | 0.43 |
| 3:Q:108:THR:HG21 | 3:Q:146:TYR:HB3 | 1.99 | 0.43 |
| 5:S:205:LEU:HA | 5:S:209:ASN:ND2 | 2.34 | 0.43 |
| 1:A:21:ILE:HD11 | 1:A:122:THR:CG2 | 2.48 | 0.43 |
| 2:B:69:ASN:HB3 | 2:B:72:ILE:H | 1.82 | 0.43 |
| 6:F:66:VAL:HG11 | 6:F:108:PHE:CE1 | 2.53 | 0.43 |
| 8:H:148:LYS:HE3 | 8:H:177:VAL:HG11 | 1.99 | 0.43 |
| 1:O:26:THR:O | 1:O:30:GLN:HG2 | 2.18 | 0.43 |
| 10:X:1:MET:HG2 | 10:X:2:ASP:N | 2.34 | 0.43 |
| 6:T:66:VAL:HG11 | 6:T:108:PHE:CE1 | 2.53 | 0.43 |
| 6:T:155:GLY:HA3 | 7:U:59:THR:HG21 | 2.01 | 0.43 |
| 6:T:154:TRP:CZ3 | 7:U:60:VAL:HA | 2.54 | 0.43 |
| 10:J:158:LEU:HD13 | 10:J:198:GLN:HE22 | 1.84 | 0.43 |
| 14:N:176:VAL:HG12 | 14:N:178:LEU:HD13 | 1.99 | 0.43 |
| 5:E:205:LEU:HA | 5:E:209:ASN:ND2 | 2.33 | 0.42 |
| 6:F:158:GLY:O | 7:G:54:LEU:HB3 | 2.19 | 0.42 |
| 3:Q:29:THR:HB | 3:Q:45:GLU:HG3 | 2.00 | 0.42 |
| 7:U:149:ASP:HB2 | 7:U:150:PRO:HD2 | 2.00 | 0.42 |
| 12:Z:90:ALA:HA | 12:Z:125:PHE:HZ | 1.83 | 0.42 |
| 6:F:34:ILE:HG12 | 6:F:196:ILE:HD11 | 2.01 | 0.42 |
| 2:P:99:LYS:HG3 | 9:W:64:GLU:HB3 | 2.00 | 0.42 |
| 3:C:92:GLN:HG3 | 10:J:66:LEU:HB2 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 11:Y:12:ILE:HB | 11:Y:180:VAL:HB | 2.02 | 0.42 |
| 14:N:36:ARG:HG3 | 14:N:42:TRP:CE2 | 2.54 | 0.42 |
| 4:D:160:ASN:HB3 | 4:D:179:TRP:CE2 | 2.54 | 0.42 |
| 8:H:50:ALA:HB2 | 9:I:128:CYS:HB2 | 2.01 | 0.42 |
| 4:R:160:ASN:HB3 | 4:R:179:TRP:CE2 | 2.54 | 0.42 |
| 2:B:47:ALA:HB1 | 2:B:64:LYS:HD3 | 2.02 | 0.42 |
| 7:G:149:ASP:HB2 | 7:G:150:PRO:HD2 | 2.00 | 0.42 |
| 14:N:59:VAL:HG11 | 14:N:82:PHE:CE2 | 2.55 | 0.42 |
| 4:R:161:ALA:HB1 | 4:R:175:LEU:HD22 | 2.02 | 0.42 |
| 3:C:155:SER:CB | 4:D:51:LEU:HD21 | 2.49 | 0.42 |
| 6:F:8:ASN:HB3 | 6:F:123:ASN:HA | 2.01 | 0.42 |
| 11:K:12:ILE:HB | 11:K:180:VAL:HB | 2.02 | 0.42 |
| 2:P:223:GLU:HG2 | 2:P:224:VAL:H | 1.85 | 0.42 |
| 2:P:223:GLU:HG2 | 2:P:224:VAL:N | 2.35 | 0.42 |
| 2:P:47:ALA:HB1 | 2:P:64:LYS:HD3 | 2.02 | 0.42 |
| 5:S:62:ILE:HG21 | 5:S:213:ALA:HB2 | 2.02 | 0.42 |
| 10:X:158:LEU:HD13 | 10:X:198:GLN:HE22 | 1.84 | 0.42 |
| 2:B:223:GLU:HG2 | 2:B:224:VAL:N | 2.35 | 0.42 |
| 5:E:62:ILE:HG21 | 5:E:213:ALA:HB2 | 2.02 | 0.42 |
| 7:G:52:ASP:HB3 | 7:G:55:LEU:HG | 2.02 | 0.42 |
| 11:Y:104:TYR:CE2 | 11:Y:110:PRO:HG3 | 2.55 | 0.42 |
| 2:B:196:LEU:O | 2:B:200:THR:OG1 | 2.35 | 0.42 |
| 6:T:34:ILE:HG12 | 6:T:196:ILE:HD11 | 2.01 | 0.42 |
| 2:B:146:GLN:HG2 | 3:C:57:ILE:HG21 | 2.00 | 0.41 |
| 10:J:91:SER:HG | 10:J:98:TYR:H | 1.65 | 0.41 |
| 4:D:161:ALA:HB1 | 4:D:175:LEU:HD22 | 2.01 | 0.41 |
| 5:E:12:PHE:HB2 | 6:F:19:GLN:HE22 | 1.84 | 0.41 |
| 1:O:64:VAL:HG11 | 1:O:212:ALA:HB3 | 2.02 | 0.41 |
| 9:I:36:SER:CB | 10:J:126:VAL:HG21 | 2.50 | 0.41 |
| 14:N:163:ILE:HG23 | 14:N:170:GLY:HA2 | 2.02 | 0.41 |
| 3:Q:157:TRP:CZ3 | 4:R:48:SER:HB3 | 2.56 | 0.41 |
| 10:X:130:TYR:HB2 | 10:X:144:LEU:HD13 | 2.02 | 0.41 |
| 13:M:129:TYR:CE1 | 13:M:144:THR:HG22 | 2.55 | 0.41 |
| 14:N:3:ILE:HB | 14:N:44:CYS:HB3 | 2.02 | 0.41 |
| 7:U:70:ILE:HG21 | 7:U:108:LEU:HD23 | 2.02 | 0.41 |
| 5:E:92:ASN:HA | 5:E:92:ASN:HD22 | 1.73 | 0.41 |
| 4:R:71:SER:HB3 | 4:R:164:ILE:HD12 | 2.03 | 0.41 |
| 2:B:223:GLU:HG2 | 2:B:224:VAL:H | 1.85 | 0.41 |
| 11:K:104:TYR:CE2 | 11:K:110:PRO:HG3 | 2.55 | 0.41 |
| 13:M:161:ARG:NH1 | 13:M:161:ARG:HG3 | 2.32 | 0.41 |
| 13:M:213:GLN:HE21 | 13:M:213:GLN:HB3 | 1.69 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-------------------|--------------------------|-------------------|
| 3:C:11:PRO:HA | 4:D:18:TYR:CD1 | 2.55 | 0.41 |
| 4:D:58:LYS:HE2 | 4:D:74:THR:HG21 | 2.03 | 0.41 |
| 10:J:130:TYR:HB2 | 10:J:144:LEU:HD13 | 2.02 | 0.41 |
| 2:P:95:GLN:HE21 | 9:W:68:TYR:HA | 1.86 | 0.41 |
| 11:Y:49:ALA:O | 11:Y:53:GLN:HB2 | 2.21 | 0.41 |
| 14:N:134:ILE:HG21 | 14:N:158:SER:O | 2.21 | 0.41 |
| 5:S:227:GLU:CD | 5:S:227:GLU:H | 2.25 | 0.41 |
| 7:U:52:ASP:HB3 | 7:U:55:LEU:HG | 2.03 | 0.41 |
| 8:V:3:ILE:HG22 | 8:V:16:ALA:HB2 | 2.02 | 0.41 |
| 11:K:49:ALA:O | 11:K:53:GLN:HB2 | 2.21 | 0.41 |
| 4:R:58:LYS:HE2 | 4:R:74:THR:HG21 | 2.03 | 0.41 |
| 8:H:3:ILE:HG22 | 8:H:16:ALA:HB2 | 2.03 | 0.40 |
| 9:I:7:ASN:HA | 9:I:29:GLY:O | 2.22 | 0.40 |
| 13:M:43:ILE:HG12 | 13:M:64:GLU:HG2 | 2.03 | 0.40 |
| 9:W:141:ALA:HB2 | 9:W:177:ASP:HB2 | 2.03 | 0.40 |
| 11:Y:38:ASN:C | 11:Y:40:PHE:H | 2.25 | 0.40 |
| 1:A:64:VAL:HG11 | 1:A:212:ALA:HB3 | 2.02 | 0.40 |
| 4:D:71:SER:HB3 | 4:D:164:ILE:HD12 | 2.03 | 0.40 |
| 7:G:149:ASP:HB2 | 7:G:150:PRO:CD | 2.51 | 0.40 |
| 7:G:70:ILE:HG21 | 7:G:108:LEU:HD23 | 2.02 | 0.40 |
| 9:I:62:LEU:CD1 | 9:I:104:VAL:HG21 | 2.51 | 0.40 |
| 5:S:42:HIS:HB2 | 5:S:188:LEU:HD12 | 2.04 | 0.40 |
| 6:T:8:ASN:HB3 | 6:T:123:ASN:HA | 2.01 | 0.40 |
| 9:W:62:LEU:CD1 | 9:W:104:VAL:HG21 | 2.51 | 0.40 |
| 2:B:148:TYR:OH | 3:C:57:ILE:HB | 2.22 | 0.40 |
| 2:B:14:PRO:HA | 3:C:20:TYR:CD1 | 2.57 | 0.40 |
| 9:I:141:ALA:HB2 | 9:I:177:ASP:HB2 | 2.03 | 0.40 |
| 9:W:111:ILE:HG21 | 9:W:191:LYS:HG2 | 2.04 | 0.40 |
| 7:G:34:LEU:HD23 | 7:G:201:MET:HE3 | 2.04 | 0.40 |
| 11:K:38:ASN:C | 11:K:40:PHE:H | 2.25 | 0.40 |
| 1:O:49:LYS:HG3 | 1:O:210:GLU:HB2 | 2.03 | 0.40 |
| 1:O:66:LEU:HD12 | 1:O:235:PHE:CD2 | 2.57 | 0.40 |
| 7:U:117:GLN:O | 7:U:120:THR:HB | 2.22 | 0.40 |
| 7:U:149:ASP:HB2 | 7:U:150:PRO:CD | 2.51 | 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 | 248/250 (99%) | 242 (98%) | 4 (2%) | 2 (1%) | 19 | 51 |
| 1 | O | 248/250 (99%) | 242 (98%) | 4 (2%) | 2 (1%) | 19 | 51 |
| 2 | B | 242/258 (94%) | 230 (95%) | 10 (4%) | 2 (1%) | 19 | 51 |
| 2 | P | 242/258 (94%) | 230 (95%) | 10 (4%) | 2 (1%) | 19 | 51 |
| 3 | C | 239/254 (94%) | 229 (96%) | 7 (3%) | 3 (1%) | 12 | 37 |
| 3 | Q | 239/254 (94%) | 230 (96%) | 6 (2%) | 3 (1%) | 12 | 37 |
| 4 | D | 240/260 (92%) | 231 (96%) | 6 (2%) | 3 (1%) | 12 | 37 |
| 4 | R | 240/260 (92%) | 230 (96%) | 7 (3%) | 3 (1%) | 12 | 37 |
| 5 | E | 231/234 (99%) | 221 (96%) | 8 (4%) | 2 (1%) | 17 | 48 |
| 5 | S | 231/234 (99%) | 221 (96%) | 8 (4%) | 2 (1%) | 17 | 48 |
| 6 | F | 242/288 (84%) | 235 (97%) | 7 (3%) | 0 | 100 | 100 |
| 6 | T | 242/288 (84%) | 235 (97%) | 7 (3%) | 0 | 100 | 100 |
| 7 | G | 241/252 (96%) | 233 (97%) | 8 (3%) | 0 | 100 | 100 |
| 7 | U | 241/252 (96%) | 233 (97%) | 8 (3%) | 0 | 100 | 100 |
| 8 | H | 220/232 (95%) | 212 (96%) | 8 (4%) | 0 | 100 | 100 |
| 8 | V | 220/232 (95%) | 212 (96%) | 8 (4%) | 0 | 100 | 100 |
| 9 | I | 202/205 (98%) | 193 (96%) | 9 (4%) | 0 | 100 | 100 |
| 9 | W | 202/205 (98%) | 194 (96%) | 8 (4%) | 0 | 100 | 100 |
| 10 | J | 196/198 (99%) | 189 (96%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 10 | X | 196/198 (99%) | 189 (96%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 11 | K | 210/212 (99%) | 203 (97%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 11 | Y | 210/212 (99%) | 203 (97%) | 6 (3%) | 1 (0%) | 29 | 61 |
| 12 | L | 220/222 (99%) | 213 (97%) | 7 (3%) | 0 | 100 | 100 |
| 12 | Z | 220/222 (99%) | 213 (97%) | 7 (3%) | 0 | 100 | 100 |
| 13 | M | 231/233 (99%) | 222 (96%) | 9 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 13 | a | 231/233 (99%) | 221 (96%) | 10 (4%) | 0 | 100 | 100 |
| 14 | N | 194/196 (99%) | 187 (96%) | 7 (4%) | 0 | 100 | 100 |
| 14 | b | 194/196 (99%) | 187 (96%) | 7 (4%) | 0 | 100 | 100 |
| 15 | c | 1/8 (12%) | 1 (100%) | 0 | 0 | 100 | 100 |
| 15 | d | 1/8 (12%) | 1 (100%) | 0 | 0 | 100 | 100 |
| 15 | e | 1/8 (12%) | 1 (100%) | 0 | 0 | 100 | 100 |
| 15 | f | 1/8 (12%) | 1 (100%) | 0 | 0 | 100 | 100 |
| All | All | 6316/6620 (95%) | 6084 (96%) | 204 (3%) | 28 (0%) | 34 | 66 |

All (28) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3 | C | 52 | LEU |
| 3 | Q | 52 | LEU |
| 1 | A | 166 | LYS |
| 5 | E | 201 | ARG |
| 11 | K | 39 | PRO |
| 1 | O | 166 | LYS |
| 5 | S | 201 | ARG |
| 11 | Y | 39 | PRO |
| 1 | A | 2 | THR |
| 2 | B | 221 | ASP |
| 4 | D | 121 | GLY |
| 4 | D | 122 | GLU |
| 1 | O | 2 | THR |
| 2 | P | 221 | ASP |
| 4 | R | 121 | GLY |
| 4 | R | 122 | GLU |
| 2 | B | 51 | VAL |
| 3 | C | 183 | PRO |
| 3 | C | 203 | THR |
| 5 | E | 217 | LYS |
| 2 | P | 51 | VAL |
| 3 | Q | 183 | PRO |
| 3 | Q | 203 | THR |
| 5 | S | 217 | LYS |
| 4 | D | 118 | GLY |
| 4 | R | 118 | GLY |
| 10 | J | 9 | VAL |
| 10 | X | 9 | VAL |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|----|
| 1 | A | 209/209 (100%) | 206 (99%) | 3 (1%) | 67 | 89 |
| 1 | O | 209/209 (100%) | 206 (99%) | 3 (1%) | 67 | 89 |
| 2 | B | 203/216 (94%) | 192 (95%) | 11 (5%) | 22 | 54 |
| 2 | P | 203/216 (94%) | 192 (95%) | 11 (5%) | 22 | 54 |
| 3 | C | 213/226 (94%) | 206 (97%) | 7 (3%) | 38 | 72 |
| 3 | Q | 213/226 (94%) | 206 (97%) | 7 (3%) | 38 | 72 |
| 4 | D | 198/215 (92%) | 190 (96%) | 8 (4%) | 31 | 65 |
| 4 | R | 198/215 (92%) | 190 (96%) | 8 (4%) | 31 | 65 |
| 5 | E | 192/193 (100%) | 181 (94%) | 11 (6%) | 20 | 51 |
| 5 | S | 192/193 (100%) | 181 (94%) | 11 (6%) | 20 | 51 |
| 6 | F | 201/239 (84%) | 190 (94%) | 11 (6%) | 21 | 53 |
| 6 | T | 201/239 (84%) | 190 (94%) | 11 (6%) | 21 | 53 |
| 7 | G | 207/210 (99%) | 199 (96%) | 8 (4%) | 32 | 66 |
| 7 | U | 207/210 (99%) | 200 (97%) | 7 (3%) | 37 | 71 |
| 8 | H | 181/190 (95%) | 177 (98%) | 4 (2%) | 52 | 81 |
| 8 | V | 181/190 (95%) | 177 (98%) | 4 (2%) | 52 | 81 |
| 9 | I | 172/173 (99%) | 169 (98%) | 3 (2%) | 60 | 86 |
| 9 | W | 172/173 (99%) | 169 (98%) | 3 (2%) | 60 | 86 |
| 10 | J | 175/175 (100%) | 173 (99%) | 2 (1%) | 73 | 92 |
| 10 | X | 175/175 (100%) | 173 (99%) | 2 (1%) | 73 | 92 |
| 11 | K | 169/169 (100%) | 161 (95%) | 8 (5%) | 26 | 59 |
| 11 | Y | 169/169 (100%) | 161 (95%) | 8 (5%) | 26 | 59 |
| 12 | L | 185/185 (100%) | 181 (98%) | 4 (2%) | 52 | 81 |
| 12 | Z | 185/185 (100%) | 181 (98%) | 4 (2%) | 52 | 81 |
| 13 | M | 199/199 (100%) | 191 (96%) | 8 (4%) | 31 | 65 |
| 13 | a | 199/199 (100%) | 192 (96%) | 7 (4%) | 36 | 70 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|-------------|----|
| 14 | N | 162/162 (100%) | 160 (99%) | 2 (1%) | 71 | 91 |
| 14 | b | 162/162 (100%) | 160 (99%) | 2 (1%) | 71 | 91 |
| All | All | 5332/5522 (97%) | 5154 (97%) | 178 (3%) | 38 | 72 |

All (178) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 30 | GLN |
| 1 | A | 61 | LEU |
| 1 | A | 157 | PHE |
| 2 | B | 55 | LEU |
| 2 | B | 60 | THR |
| 2 | B | 69 | ASN |
| 2 | B | 119 | GLN |
| 2 | B | 149 | THR |
| 2 | B | 155 | ASN |
| 2 | B | 184 | LYS |
| 2 | B | 186 | ASP |
| 2 | B | 191 | LEU |
| 2 | B | 212 | PHE |
| 2 | B | 220 | ASN |
| 3 | C | 4 | ARG |
| 3 | C | 19 | GLU |
| 3 | C | 51 | LYS |
| 3 | C | 147 | GLN |
| 3 | C | 160 | GLN |
| 3 | C | 171 | GLU |
| 3 | C | 206 | LYS |
| 4 | D | 68 | CYS |
| 4 | D | 102 | GLU |
| 4 | D | 124 | ARG |
| 4 | D | 176 | LEU |
| 4 | D | 190 | LEU |
| 4 | D | 193 | LEU |
| 4 | D | 214 | ILE |
| 4 | D | 235 | LEU |
| 5 | E | 9 | THR |
| 5 | E | 29 | LYS |
| 5 | E | 54 | GLU |
| 5 | E | 71 | LEU |
| 5 | E | 92 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 116 | GLN |
| 5 | E | 184 | ASN |
| 5 | E | 188 | LEU |
| 5 | E | 198 | GLN |
| 5 | E | 227 | GLU |
| 5 | E | 231 | LYS |
| 6 | F | 7 | SER |
| 6 | F | 31 | THR |
| 6 | F | 39 | ASN |
| 6 | F | 117 | GLN |
| 6 | F | 123 | ASN |
| 6 | F | 181 | GLU |
| 6 | F | 186 | ARG |
| 6 | F | 201 | GLU |
| 6 | F | 202 | ASP |
| 6 | F | 203 | ASN |
| 6 | F | 214 | TRP |
| 7 | G | 68 | ARG |
| 7 | G | 83 | ASN |
| 7 | G | 115 | LEU |
| 7 | G | 117 | GLN |
| 7 | G | 166 | GLN |
| 7 | G | 186 | ASN |
| 7 | G | 221 | LYS |
| 7 | G | 235 | ARG |
| 8 | H | 30 | ASN |
| 8 | H | 34 | LEU |
| 8 | H | 68 | LEU |
| 8 | H | 196 | ARG |
| 9 | I | 37 | ASN |
| 9 | I | 171 | LEU |
| 9 | I | 182 | TRP |
| 10 | J | 71 | GLU |
| 10 | J | 127 | GLU |
| 11 | K | 4 | LEU |
| 11 | K | 9 | GLN |
| 11 | K | 35 | ILE |
| 11 | K | 65 | LEU |
| 11 | K | 87 | VAL |
| 11 | K | 100 | MET |
| 11 | K | 104 | TYR |
| 11 | K | 107 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 23 | LEU |
| 12 | L | 49 | ASN |
| 12 | L | 106 | TYR |
| 12 | L | 109 | THR |
| 13 | M | 48 | ASN |
| 13 | M | 69 | ASP |
| 13 | M | 70 | LEU |
| 13 | M | 104 | ARG |
| 13 | M | 146 | PHE |
| 13 | M | 159 | VAL |
| 13 | M | 161 | ARG |
| 13 | M | 226 | LYS |
| 14 | N | 119 | VAL |
| 14 | N | 149 | GLU |
| 1 | O | 30 | GLN |
| 1 | O | 61 | LEU |
| 1 | O | 157 | PHE |
| 2 | P | 55 | LEU |
| 2 | P | 60 | THR |
| 2 | P | 69 | ASN |
| 2 | P | 119 | GLN |
| 2 | P | 149 | THR |
| 2 | P | 155 | ASN |
| 2 | P | 184 | LYS |
| 2 | P | 186 | ASP |
| 2 | P | 191 | LEU |
| 2 | P | 212 | PHE |
| 2 | P | 220 | ASN |
| 3 | Q | 4 | ARG |
| 3 | Q | 19 | GLU |
| 3 | Q | 51 | LYS |
| 3 | Q | 147 | GLN |
| 3 | Q | 160 | GLN |
| 3 | Q | 171 | GLU |
| 3 | Q | 206 | LYS |
| 4 | R | 68 | CYS |
| 4 | R | 102 | GLU |
| 4 | R | 124 | ARG |
| 4 | R | 176 | LEU |
| 4 | R | 190 | LEU |
| 4 | R | 193 | LEU |
| 4 | R | 214 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 4 | R | 235 | LEU |
| 5 | S | 9 | THR |
| 5 | S | 29 | LYS |
| 5 | S | 54 | GLU |
| 5 | S | 71 | LEU |
| 5 | S | 92 | ASN |
| 5 | S | 116 | GLN |
| 5 | S | 184 | ASN |
| 5 | S | 188 | LEU |
| 5 | S | 198 | GLN |
| 5 | S | 227 | GLU |
| 5 | S | 231 | LYS |
| 6 | T | 7 | SER |
| 6 | T | 31 | THR |
| 6 | T | 39 | ASN |
| 6 | T | 117 | GLN |
| 6 | T | 123 | ASN |
| 6 | T | 181 | GLU |
| 6 | T | 186 | ARG |
| 6 | T | 201 | GLU |
| 6 | T | 202 | ASP |
| 6 | T | 203 | ASN |
| 6 | T | 214 | TRP |
| 7 | U | 68 | ARG |
| 7 | U | 83 | ASN |
| 7 | U | 115 | LEU |
| 7 | U | 117 | GLN |
| 7 | U | 166 | GLN |
| 7 | U | 221 | LYS |
| 7 | U | 235 | ARG |
| 8 | V | 30 | ASN |
| 8 | V | 34 | LEU |
| 8 | V | 68 | LEU |
| 8 | V | 196 | ARG |
| 9 | W | 37 | ASN |
| 9 | W | 171 | LEU |
| 9 | W | 182 | TRP |
| 10 | X | 71 | GLU |
| 10 | X | 127 | GLU |
| 11 | Y | 4 | LEU |
| 11 | Y | 9 | GLN |
| 11 | Y | 35 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 11 | Y | 65 | LEU |
| 11 | Y | 87 | VAL |
| 11 | Y | 100 | MET |
| 11 | Y | 104 | TYR |
| 11 | Y | 107 | LYS |
| 12 | Z | 23 | LEU |
| 12 | Z | 49 | ASN |
| 12 | Z | 106 | TYR |
| 12 | Z | 109 | THR |
| 13 | a | 48 | ASN |
| 13 | a | 69 | ASP |
| 13 | a | 70 | LEU |
| 13 | a | 104 | ARG |
| 13 | a | 146 | PHE |
| 13 | a | 161 | ARG |
| 13 | a | 226 | LYS |
| 14 | b | 119 | VAL |
| 14 | b | 149 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 30 | GLN |
| 1 | A | 94 | HIS |
| 2 | B | 20 | GLN |
| 2 | B | 69 | ASN |
| 2 | B | 95 | GLN |
| 2 | B | 119 | GLN |
| 2 | B | 123 | GLN |
| 2 | B | 155 | ASN |
| 2 | B | 176 | GLN |
| 2 | B | 220 | ASN |
| 3 | C | 17 | GLN |
| 3 | C | 77 | ASN |
| 3 | C | 147 | GLN |
| 3 | C | 160 | GLN |
| 3 | C | 236 | GLN |
| 3 | C | 241 | GLN |
| 4 | D | 15 | GLN |
| 4 | D | 100 | ASN |
| 4 | D | 210 | GLN |
| 4 | D | 225 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | E | 68 | HIS |
| 5 | E | 99 | ASN |
| 5 | E | 116 | GLN |
| 5 | E | 120 | GLN |
| 5 | E | 151 | ASN |
| 5 | E | 184 | ASN |
| 5 | E | 198 | GLN |
| 5 | E | 209 | ASN |
| 6 | F | 19 | GLN |
| 6 | F | 39 | ASN |
| 6 | F | 86 | ASN |
| 6 | F | 117 | GLN |
| 6 | F | 123 | ASN |
| 7 | G | 30 | ASN |
| 7 | G | 83 | ASN |
| 7 | G | 114 | ASN |
| 7 | G | 117 | GLN |
| 7 | G | 121 | GLN |
| 7 | G | 166 | GLN |
| 7 | G | 167 | GLN |
| 7 | G | 175 | ASN |
| 7 | G | 186 | ASN |
| 8 | H | 22 | GLN |
| 8 | H | 30 | ASN |
| 8 | H | 66 | HIS |
| 8 | H | 144 | GLN |
| 8 | H | 165 | ASN |
| 8 | H | 172 | ASN |
| 8 | H | 189 | ASN |
| 9 | I | 37 | ASN |
| 10 | J | 55 | GLN |
| 10 | J | 118 | GLN |
| 10 | J | 191 | GLN |
| 10 | J | 198 | GLN |
| 11 | K | 9 | GLN |
| 11 | K | 85 | ASN |
| 11 | K | 176 | ASN |
| 11 | K | 208 | ASN |
| 12 | L | 1 | GLN |
| 12 | L | 3 | ASN |
| 12 | L | 49 | ASN |
| 12 | L | 70 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | L | 80 | ASN |
| 12 | L | 92 | ASN |
| 12 | L | 135 | GLN |
| 12 | L | 158 | ASN |
| 12 | L | 165 | ASN |
| 12 | L | 195 | HIS |
| 13 | M | 2 | GLN |
| 13 | M | 18 | ASN |
| 13 | M | 48 | ASN |
| 13 | M | 102 | GLN |
| 13 | M | 108 | ASN |
| 13 | M | 171 | GLN |
| 13 | M | 179 | ASN |
| 13 | M | 213 | GLN |
| 14 | N | 161 | GLN |
| 1 | O | 30 | GLN |
| 1 | O | 94 | HIS |
| 2 | P | 20 | GLN |
| 2 | P | 69 | ASN |
| 2 | P | 95 | GLN |
| 2 | P | 119 | GLN |
| 2 | P | 123 | GLN |
| 2 | P | 155 | ASN |
| 2 | P | 176 | GLN |
| 2 | P | 220 | ASN |
| 3 | Q | 17 | GLN |
| 3 | Q | 77 | ASN |
| 3 | Q | 147 | GLN |
| 3 | Q | 160 | GLN |
| 3 | Q | 236 | GLN |
| 3 | Q | 241 | GLN |
| 4 | R | 15 | GLN |
| 4 | R | 100 | ASN |
| 4 | R | 210 | GLN |
| 4 | R | 225 | ASN |
| 5 | S | 68 | HIS |
| 5 | S | 99 | ASN |
| 5 | S | 116 | GLN |
| 5 | S | 120 | GLN |
| 5 | S | 151 | ASN |
| 5 | S | 184 | ASN |
| 5 | S | 198 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5 | S | 209 | ASN |
| 6 | T | 19 | GLN |
| 6 | T | 39 | ASN |
| 6 | T | 86 | ASN |
| 6 | T | 117 | GLN |
| 6 | T | 123 | ASN |
| 7 | U | 30 | ASN |
| 7 | U | 83 | ASN |
| 7 | U | 114 | ASN |
| 7 | U | 117 | GLN |
| 7 | U | 121 | GLN |
| 7 | U | 166 | GLN |
| 7 | U | 167 | GLN |
| 7 | U | 175 | ASN |
| 7 | U | 186 | ASN |
| 7 | U | 231 | ASN |
| 8 | V | 22 | GLN |
| 8 | V | 30 | ASN |
| 8 | V | 66 | HIS |
| 8 | V | 144 | GLN |
| 8 | V | 165 | ASN |
| 8 | V | 172 | ASN |
| 8 | V | 189 | ASN |
| 9 | W | 37 | ASN |
| 9 | W | 88 | GLN |
| 10 | X | 55 | GLN |
| 10 | X | 86 | GLN |
| 10 | X | 118 | GLN |
| 10 | X | 191 | GLN |
| 10 | X | 198 | GLN |
| 11 | Y | 9 | GLN |
| 11 | Y | 85 | ASN |
| 11 | Y | 176 | ASN |
| 11 | Y | 208 | ASN |
| 12 | Z | 1 | GLN |
| 12 | Z | 3 | ASN |
| 12 | Z | 49 | ASN |
| 12 | Z | 70 | ASN |
| 12 | Z | 80 | ASN |
| 12 | Z | 92 | ASN |
| 12 | Z | 135 | GLN |
| 12 | Z | 158 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 12 | Z | 165 | ASN |
| 12 | Z | 195 | HIS |
| 13 | a | 2 | GLN |
| 13 | a | 18 | ASN |
| 13 | a | 48 | ASN |
| 13 | a | 102 | GLN |
| 13 | a | 108 | ASN |
| 13 | a | 171 | GLN |
| 13 | a | 179 | ASN |
| 13 | a | 213 | GLN |
| 14 | b | 161 | GLN |

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | $\# Z > 2$ | Counts | RMSZ | $\# Z > 2$ |
| 15 | TY5 | d | 5 | 15 | 19,20,21 | 1.06 | 0 | 22,25,27 | 0.83 | 0 |
| 15 | ACA | f | 4 | 15 | 7,7,8 | 0.72 | 0 | 6,6,8 | 0.81 | 0 |
| 15 | ACA | e | 4 | 15 | 7,7,8 | 0.72 | 0 | 6,6,8 | 0.81 | 0 |
| 15 | ACA | d | 4 | 15 | 7,7,8 | 0.72 | 0 | 6,6,8 | 0.80 | 0 |
| 15 | ACA | c | 4 | 15 | 7,7,8 | 0.72 | 0 | 6,6,8 | 0.81 | 0 |
| 15 | RE0 | c | 7 | 15 | 15,17,18 | 1.20 | 2 (13%) | 19,25,27 | 2.01 | 5 (26%) |
| 15 | TY5 | e | 5 | 15 | 19,20,21 | 1.06 | 0 | 22,25,27 | 0.63 | 0 |
| 15 | TY5 | c | 5 | 15 | 19,20,21 | 1.06 | 0 | 22,25,27 | 0.85 | 0 |
| 15 | RE0 | e | 7 | 15 | 15,17,18 | 1.25 | 2 (13%) | 19,25,27 | 1.87 | 5 (26%) |
| 15 | RE0 | f | 7 | 15 | 15,17,18 | 1.25 | 2 (13%) | 19,25,27 | 1.89 | 5 (26%) |
| 15 | RE0 | d | 7 | 15 | 15,17,18 | 1.21 | 2 (13%) | 19,25,27 | 1.97 | 5 (26%) |
| 15 | TY5 | f | 5 | 15 | 19,20,21 | 1.05 | 0 | 22,25,27 | 0.67 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 15 | TY5 | d | 5 | 15 | - | 5/10/11/13 | 0/2/2/2 |
| 15 | ACA | f | 4 | 15 | - | 1/4/5/6 | - |
| 15 | ACA | e | 4 | 15 | - | 1/4/5/6 | - |
| 15 | ACA | d | 4 | 15 | - | 1/4/5/6 | - |
| 15 | ACA | c | 4 | 15 | - | 2/4/5/6 | - |
| 15 | RE0 | c | 7 | 15 | - | 0/6/23/25 | 0/2/2/2 |
| 15 | TY5 | e | 5 | 15 | - | 2/10/11/13 | 0/2/2/2 |
| 15 | TY5 | c | 5 | 15 | - | 5/10/11/13 | 0/2/2/2 |
| 15 | RE0 | e | 7 | 15 | - | 2/6/23/25 | 0/2/2/2 |
| 15 | RE0 | f | 7 | 15 | - | 2/6/23/25 | 0/2/2/2 |
| 15 | RE0 | d | 7 | 15 | - | 0/6/23/25 | 0/2/2/2 |
| 15 | TY5 | f | 5 | 15 | - | 2/10/11/13 | 0/2/2/2 |

All (8) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 15 | e | 7 | RE0 | CG-CD2 | 2.76 | 1.54 | 1.51 |
| 15 | f | 7 | RE0 | CG-CD2 | 2.71 | 1.54 | 1.51 |
| 15 | d | 7 | RE0 | CG-CD2 | 2.70 | 1.54 | 1.51 |
| 15 | c | 7 | RE0 | CG-CD2 | 2.65 | 1.54 | 1.51 |
| 15 | f | 7 | RE0 | CB-CA | 2.51 | 1.57 | 1.54 |
| 15 | e | 7 | RE0 | CB-CA | 2.42 | 1.57 | 1.54 |
| 15 | d | 7 | RE0 | CB-CA | 2.38 | 1.57 | 1.54 |
| 15 | c | 7 | RE0 | CB-CA | 2.34 | 1.57 | 1.54 |

All (20) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15 | c | 7 | RE0 | CG-CD2-CE2 | -5.52 | 106.64 | 108.86 |
| 15 | d | 7 | RE0 | CG-CD2-CE2 | -5.41 | 106.69 | 108.86 |
| 15 | f | 7 | RE0 | CG-CD2-CE2 | -4.96 | 106.87 | 108.86 |
| 15 | e | 7 | RE0 | CG-CD2-CE2 | -4.85 | 106.91 | 108.86 |
| 15 | c | 7 | RE0 | CD2-CE2-NE1 | 3.65 | 112.04 | 109.59 |
| 15 | d | 7 | RE0 | CD2-CE2-NE1 | 3.61 | 112.01 | 109.59 |
| 15 | f | 7 | RE0 | CD2-CE2-NE1 | 3.46 | 111.91 | 109.59 |
| 15 | e | 7 | RE0 | CD2-CE2-NE1 | 3.40 | 111.87 | 109.59 |
| 15 | c | 7 | RE0 | CE2-NE1-CD1 | -3.34 | 109.85 | 111.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 15 | d | 7 | RE0 | CE2-NE1-CD1 | -3.30 | 109.88 | 111.86 |
| 15 | f | 7 | RE0 | CE2-NE1-CD1 | -3.25 | 109.91 | 111.86 |
| 15 | e | 7 | RE0 | CE2-NE1-CD1 | -3.19 | 109.95 | 111.86 |
| 15 | c | 7 | RE0 | CZ2-CE2-NE1 | -2.65 | 125.47 | 130.87 |
| 15 | d | 7 | RE0 | CZ2-CE2-NE1 | -2.63 | 125.52 | 130.87 |
| 15 | e | 7 | RE0 | CZ2-CE2-NE1 | -2.59 | 125.61 | 130.87 |
| 15 | f | 7 | RE0 | CZ2-CE2-NE1 | -2.58 | 125.62 | 130.87 |
| 15 | e | 7 | RE0 | CG-CD1-NE1 | 2.37 | 109.85 | 108.41 |
| 15 | f | 7 | RE0 | CG-CD1-NE1 | 2.30 | 109.81 | 108.41 |
| 15 | c | 7 | RE0 | CG-CD1-NE1 | 2.14 | 109.71 | 108.41 |
| 15 | d | 7 | RE0 | CG-CD1-NE1 | 2.11 | 109.70 | 108.41 |

There are no chirality outliers.

All (23) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 15 | e | 4 | ACA | C1-C2-C3-C4 |
| 15 | e | 7 | RE0 | N-CA-CB-CG |
| 15 | e | 7 | RE0 | C-CA-CB-CG |
| 15 | f | 7 | RE0 | N-CA-CB-CG |
| 15 | f | 7 | RE0 | C-CA-CB-CG |
| 15 | e | 5 | TY5 | CE2-CZ-OH-C49 |
| 15 | e | 5 | TY5 | CE1-CZ-OH-C49 |
| 15 | f | 5 | TY5 | CE1-CZ-OH-C49 |
| 15 | f | 5 | TY5 | CE2-CZ-OH-C49 |
| 15 | d | 5 | TY5 | CE2-CZ-OH-C49 |
| 15 | d | 5 | TY5 | CE1-CZ-OH-C49 |
| 15 | c | 5 | TY5 | CE2-CZ-OH-C49 |
| 15 | c | 5 | TY5 | CE1-CZ-OH-C49 |
| 15 | d | 4 | ACA | C2-C3-C4-C5 |
| 15 | d | 5 | TY5 | N-CA-CB-CG |
| 15 | c | 4 | ACA | C2-C3-C4-C5 |
| 15 | f | 4 | ACA | C1-C2-C3-C4 |
| 15 | c | 4 | ACA | C1-C2-C3-C4 |
| 15 | c | 5 | TY5 | N-CA-CB-CG |
| 15 | d | 5 | TY5 | CA-CB-CG-CD2 |
| 15 | d | 5 | TY5 | CA-CB-CG-CD1 |
| 15 | c | 5 | TY5 | CA-CB-CG-CD2 |
| 15 | c | 5 | TY5 | CA-CB-CG-CD1 |

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 16 | MES | Y | 301 | - | 12,12,12 | 1.32 | 1 (8%) | 14,16,16 | 1.77 | 4 (28%) |
| 16 | MES | K | 301 | - | 12,12,12 | 1.33 | 2 (16%) | 14,16,16 | 1.74 | 3 (21%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 16 | MES | Y | 301 | - | - | 2/6/14/14 | 0/1/1/1 |
| 16 | MES | K | 301 | - | - | 2/6/14/14 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 16 | K | 301 | MES | C8-S | 2.85 | 1.81 | 1.77 |
| 16 | Y | 301 | MES | C8-S | 2.84 | 1.81 | 1.77 |
| 16 | K | 301 | MES | O2S-S | 2.01 | 1.51 | 1.45 |

All (7) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 16 | K | 301 | MES | O2S-S-C8 | -3.81 | 102.33 | 106.92 |
| 16 | Y | 301 | MES | O2S-S-C8 | -3.68 | 102.48 | 106.92 |
| 16 | Y | 301 | MES | O3S-S-O1S | 3.25 | 119.21 | 111.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 16 | K | 301 | MES | O3S-S-O1S | 2.94 | 118.45 | 111.27 |
| 16 | K | 301 | MES | C7-N4-C5 | 2.46 | 117.52 | 111.23 |
| 16 | Y | 301 | MES | C7-N4-C5 | 2.41 | 117.41 | 111.23 |
| 16 | Y | 301 | MES | O3S-S-C8 | 2.01 | 109.02 | 105.77 |

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 16 | Y | 301 | MES | C8-C7-N4-C5 |
| 16 | K | 301 | MES | C8-C7-N4-C5 |
| 16 | Y | 301 | MES | C8-C7-N4-C3 |
| 16 | K | 301 | MES | C8-C7-N4-C3 |

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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 ²) | Q<0.9 |
|-----|-------|----------------|--------|---------------|-----------------------|-------|
| 1 | A | 250/250 (100%) | -0.22 | 5 (2%) 65 63 | 50, 63, 82, 94 | 0 |
| 1 | O | 250/250 (100%) | -0.14 | 9 (3%) 42 37 | 55, 71, 92, 105 | 0 |
| 2 | B | 244/258 (94%) | 0.04 | 13 (5%) 26 22 | 53, 68, 98, 108 | 0 |
| 2 | P | 244/258 (94%) | 0.16 | 15 (6%) 21 17 | 59, 72, 101, 117 | 0 |
| 3 | C | 241/254 (94%) | 0.07 | 15 (6%) 20 16 | 51, 69, 105, 142 | 0 |
| 3 | Q | 241/254 (94%) | 0.24 | 17 (7%) 16 12 | 61, 85, 125, 158 | 0 |
| 4 | D | 242/260 (93%) | 0.01 | 12 (4%) 28 25 | 55, 69, 97, 108 | 0 |
| 4 | R | 242/260 (93%) | 0.10 | 14 (5%) 23 19 | 60, 76, 105, 118 | 0 |
| 5 | E | 233/234 (99%) | -0.04 | 10 (4%) 35 31 | 57, 73, 91, 101 | 0 |
| 5 | S | 233/234 (99%) | 0.02 | 10 (4%) 35 31 | 62, 81, 103, 115 | 0 |
| 6 | F | 244/288 (84%) | -0.16 | 10 (4%) 37 32 | 54, 67, 92, 108 | 0 |
| 6 | T | 244/288 (84%) | -0.08 | 10 (4%) 37 32 | 58, 74, 101, 123 | 0 |
| 7 | G | 243/252 (96%) | -0.13 | 7 (2%) 51 47 | 49, 64, 86, 120 | 0 |
| 7 | U | 243/252 (96%) | -0.14 | 5 (2%) 63 61 | 57, 66, 83, 114 | 0 |
| 8 | H | 222/232 (95%) | -0.34 | 4 (1%) 68 67 | 50, 60, 74, 88 | 0 |
| 8 | V | 222/232 (95%) | -0.30 | 3 (1%) 75 75 | 52, 61, 74, 99 | 0 |
| 9 | I | 204/205 (99%) | -0.47 | 2 (0%) 82 82 | 48, 57, 71, 78 | 0 |
| 9 | W | 204/205 (99%) | -0.40 | 2 (0%) 82 82 | 51, 59, 73, 83 | 0 |
| 10 | J | 198/198 (100%) | -0.20 | 6 (3%) 50 45 | 49, 59, 74, 116 | 0 |
| 10 | X | 198/198 (100%) | -0.16 | 7 (3%) 44 38 | 55, 62, 75, 117 | 0 |
| 11 | K | 212/212 (100%) | -0.18 | 8 (3%) 40 36 | 48, 60, 78, 84 | 0 |
| 11 | Y | 212/212 (100%) | -0.18 | 9 (4%) 36 32 | 53, 63, 82, 88 | 0 |
| 12 | L | 222/222 (100%) | -0.30 | 6 (2%) 54 50 | 50, 60, 84, 89 | 0 |
| 12 | Z | 222/222 (100%) | -0.29 | 5 (2%) 60 58 | 53, 61, 83, 90 | 0 |

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| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|----------------|-----------------------|-------|
| 13 | M | 233/233 (100%) | -0.39 | 2 (0%) 84 84 | 49, 60, 71, 74 | 0 |
| 13 | a | 233/233 (100%) | -0.37 | 1 (0%) 92 93 | 51, 60, 69, 72 | 0 |
| 14 | N | 196/196 (100%) | -0.44 | 1 (0%) 91 91 | 50, 56, 71, 78 | 0 |
| 14 | b | 196/196 (100%) | -0.36 | 1 (0%) 91 91 | 51, 57, 72, 81 | 0 |
| 15 | c | 1/8 (12%) | 0.40 | 0 100 100 | 55, 55, 55, 55 | 0 |
| 15 | d | 1/8 (12%) | 0.16 | 0 100 100 | 54, 54, 54, 54 | 0 |
| 15 | e | 1/8 (12%) | 0.65 | 0 100 100 | 77, 77, 77, 77 | 0 |
| 15 | f | 1/8 (12%) | 0.31 | 0 100 100 | 81, 81, 81, 81 | 0 |
| All | All | 6372/6620 (96%) | -0.16 | 209 (3%) 46 41 | 48, 65, 96, 158 | 0 |

All (209) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 4 | R | 119 | ALA | 10.7 |
| 4 | R | 118 | GLY | 9.7 |
| 4 | D | 120 | SER | 9.7 |
| 4 | R | 120 | SER | 9.4 |
| 4 | D | 118 | GLY | 8.9 |
| 2 | P | 220 | ASN | 8.3 |
| 10 | J | 197 | ALA | 8.0 |
| 10 | X | 198 | GLN | 7.9 |
| 3 | C | 49 | THR | 7.9 |
| 4 | D | 119 | ALA | 7.9 |
| 2 | B | 220 | ASN | 7.6 |
| 7 | U | 243 | ASP | 7.6 |
| 3 | C | 50 | LEU | 7.5 |
| 4 | R | 121 | GLY | 7.3 |
| 2 | P | 219 | ALA | 7.3 |
| 2 | B | 219 | ALA | 7.1 |
| 7 | G | 1 | ALA | 6.3 |
| 7 | G | 243 | ASP | 6.1 |
| 10 | X | 197 | ALA | 6.0 |
| 12 | L | 174 | TYR | 6.0 |
| 7 | U | 1 | ALA | 6.0 |
| 6 | F | 1 | GLY | 5.9 |
| 10 | J | 198 | GLN | 5.9 |
| 3 | Q | 240 | GLU | 5.7 |
| 12 | Z | 174 | TYR | 5.6 |
| 11 | K | 104 | TYR | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 51 | VAL | 5.5 |
| 4 | D | 121 | GLY | 5.4 |
| 3 | Q | 49 | THR | 5.3 |
| 3 | Q | 239 | GLN | 5.3 |
| 8 | V | 222 | ASP | 5.2 |
| 10 | J | 196 | GLN | 5.2 |
| 11 | Y | 104 | TYR | 5.1 |
| 2 | P | 61 | SER | 5.0 |
| 9 | W | 1 | SER | 4.9 |
| 3 | Q | 48 | SER | 4.9 |
| 5 | S | 202 | ASP | 4.9 |
| 1 | O | 1 | MET | 4.7 |
| 11 | Y | 182 | GLU | 4.6 |
| 3 | Q | 50 | LEU | 4.5 |
| 3 | C | 239 | GLN | 4.5 |
| 1 | A | 1 | MET | 4.4 |
| 3 | Q | 203 | THR | 4.4 |
| 4 | R | 125 | LEU | 4.4 |
| 3 | C | 241 | GLN | 4.3 |
| 3 | Q | 241 | GLN | 4.3 |
| 4 | D | 122 | GLU | 4.3 |
| 7 | G | 242 | GLN | 4.3 |
| 3 | C | 203 | THR | 4.3 |
| 5 | E | 202 | ASP | 4.2 |
| 2 | B | 218 | GLY | 4.2 |
| 2 | P | 51 | VAL | 4.2 |
| 10 | J | 1 | MET | 4.1 |
| 2 | P | 60 | THR | 4.0 |
| 11 | K | 208 | ASN | 4.0 |
| 5 | S | 2 | ARG | 4.0 |
| 4 | R | 124 | ARG | 4.0 |
| 2 | P | 59 | ASP | 3.9 |
| 4 | D | 124 | ARG | 3.9 |
| 10 | X | 194 | ASP | 3.9 |
| 2 | B | 223 | GLU | 3.8 |
| 2 | P | 221 | ASP | 3.8 |
| 12 | Z | 173 | LYS | 3.7 |
| 8 | V | 221 | CYS | 3.7 |
| 2 | P | 218 | GLY | 3.7 |
| 1 | A | 2 | THR | 3.7 |
| 1 | O | 2 | THR | 3.7 |
| 10 | X | 196 | GLN | 3.6 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | A | 201 | GLU | 3.6 |
| 8 | H | 221 | CYS | 3.6 |
| 6 | T | 1 | GLY | 3.6 |
| 10 | X | 1 | MET | 3.6 |
| 5 | S | 1 | PHE | 3.6 |
| 8 | H | 198 | GLU | 3.6 |
| 2 | P | 50 | LYS | 3.5 |
| 13 | a | 1 | THR | 3.5 |
| 5 | E | 1 | PHE | 3.5 |
| 2 | P | 223 | GLU | 3.5 |
| 7 | U | 242 | GLN | 3.5 |
| 1 | O | 201 | GLU | 3.5 |
| 6 | T | 244 | ASN | 3.5 |
| 3 | C | 202 | GLN | 3.5 |
| 11 | K | 183 | ASP | 3.5 |
| 7 | G | 2 | GLY | 3.5 |
| 8 | H | 222 | ASP | 3.4 |
| 4 | D | 125 | LEU | 3.4 |
| 5 | E | 3 | ASN | 3.3 |
| 4 | R | 1 | ASP | 3.3 |
| 6 | F | 2 | THR | 3.3 |
| 13 | M | 1 | THR | 3.3 |
| 2 | P | 225 | TYR | 3.3 |
| 6 | F | 202 | ASP | 3.3 |
| 4 | R | 177 | ASN | 3.3 |
| 11 | Y | 209 | ASN | 3.2 |
| 12 | L | 173 | LYS | 3.2 |
| 2 | B | 61 | SER | 3.2 |
| 2 | B | 221 | ASP | 3.2 |
| 6 | T | 2 | THR | 3.2 |
| 11 | Y | 212 | GLY | 3.2 |
| 4 | R | 122 | GLU | 3.1 |
| 10 | J | 139 | TYR | 3.1 |
| 11 | K | 182 | GLU | 3.1 |
| 11 | K | 209 | ASN | 3.1 |
| 5 | S | 30 | GLN | 3.1 |
| 1 | O | 52 | SER | 3.0 |
| 6 | T | 241 | LYS | 3.0 |
| 1 | A | 250 | LEU | 3.0 |
| 5 | S | 173 | ARG | 3.0 |
| 2 | B | 60 | THR | 3.0 |
| 12 | L | 165 | ASN | 3.0 |

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| Mol | Chain | Res | Type | RSRZ |
|------------|--------------|------------|-------------|-------------|
| 8 | H | 219 | ASN | 2.9 |
| 1 | O | 231 | LYS | 2.9 |
| 11 | Y | 106 | ARG | 2.9 |
| 2 | P | 52 | THR | 2.9 |
| 11 | Y | 183 | ASP | 2.9 |
| 11 | Y | 211 | ILE | 2.9 |
| 13 | M | 47 | ASP | 2.9 |
| 1 | O | 250 | LEU | 2.9 |
| 4 | D | 123 | GLU | 2.9 |
| 1 | O | 249 | ALA | 2.9 |
| 3 | C | 235 | GLU | 2.9 |
| 10 | X | 139 | TYR | 2.9 |
| 5 | S | 3 | ASN | 2.9 |
| 5 | S | 52 | ALA | 2.8 |
| 3 | Q | 202 | GLN | 2.8 |
| 3 | C | 1 | GLY | 2.8 |
| 6 | F | 205 | GLU | 2.8 |
| 8 | V | 219 | ASN | 2.8 |
| 6 | F | 243 | ILE | 2.7 |
| 9 | I | 1 | SER | 2.7 |
| 10 | J | 194 | ASP | 2.7 |
| 6 | F | 203 | ASN | 2.7 |
| 6 | F | 181 | GLU | 2.7 |
| 3 | C | 206 | LYS | 2.7 |
| 3 | Q | 47 | ARG | 2.7 |
| 3 | C | 240 | GLU | 2.7 |
| 7 | U | 222 | ASP | 2.7 |
| 11 | Y | 40 | PHE | 2.7 |
| 7 | G | 181 | LYS | 2.7 |
| 12 | Z | 168 | VAL | 2.7 |
| 11 | Y | 208 | ASN | 2.7 |
| 2 | P | 241 | THR | 2.6 |
| 3 | Q | 181 | GLU | 2.6 |
| 6 | F | 204 | LYS | 2.6 |
| 4 | R | 117 | GLU | 2.6 |
| 1 | O | 53 | SER | 2.6 |
| 5 | E | 2 | ARG | 2.6 |
| 4 | D | 1 | ASP | 2.6 |
| 5 | S | 201 | ARG | 2.6 |
| 2 | B | 240 | LYS | 2.6 |
| 3 | Q | 60 | SER | 2.6 |
| 14 | b | 105 | LYS | 2.5 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 5 | S | 163 | ARG | 2.5 |
| 10 | X | 174 | MET | 2.5 |
| 2 | P | 203 | SER | 2.5 |
| 4 | R | 242 | GLU | 2.5 |
| 6 | T | 205 | GLU | 2.5 |
| 5 | E | 180 | LYS | 2.4 |
| 3 | Q | 58 | THR | 2.4 |
| 3 | C | 238 | LYS | 2.4 |
| 11 | K | 40 | PHE | 2.4 |
| 14 | N | 195 | GLN | 2.4 |
| 4 | D | 2 | ARG | 2.4 |
| 5 | E | 203 | GLU | 2.4 |
| 11 | K | 212 | GLY | 2.4 |
| 5 | E | 30 | GLN | 2.4 |
| 3 | C | 46 | ARG | 2.4 |
| 5 | E | 218 | ASP | 2.4 |
| 4 | R | 123 | GLU | 2.3 |
| 11 | K | 147 | ASP | 2.3 |
| 4 | R | 113 | LEU | 2.3 |
| 3 | Q | 171 | GLU | 2.3 |
| 6 | T | 240 | GLN | 2.3 |
| 12 | Z | 163 | GLY | 2.3 |
| 2 | P | 240 | LYS | 2.3 |
| 1 | A | 202 | GLY | 2.3 |
| 7 | U | 2 | GLY | 2.3 |
| 3 | Q | 206 | LYS | 2.3 |
| 3 | C | 175 | LYS | 2.2 |
| 2 | B | 217 | LYS | 2.2 |
| 1 | O | 228 | PRO | 2.2 |
| 2 | B | 50 | LYS | 2.2 |
| 7 | G | 240 | ALA | 2.2 |
| 4 | D | 238 | LYS | 2.2 |
| 3 | C | 27 | ARG | 2.1 |
| 4 | D | 242 | GLU | 2.1 |
| 6 | T | 166 | GLN | 2.1 |
| 6 | T | 243 | ILE | 2.1 |
| 4 | R | 2 | ARG | 2.1 |
| 6 | F | 229 | GLY | 2.1 |
| 12 | L | 168 | VAL | 2.1 |
| 3 | C | 180 | LYS | 2.1 |
| 12 | L | 80 | ASN | 2.1 |
| 3 | Q | 46 | ARG | 2.1 |

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| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 2 | B | 230 | LYS | 2.1 |
| 5 | E | 173 | ARG | 2.1 |
| 3 | Q | 225 | GLU | 2.1 |
| 6 | T | 230 | ASP | 2.1 |
| 7 | G | 3 | TYR | 2.1 |
| 6 | T | 180 | PRO | 2.1 |
| 5 | E | 201 | ARG | 2.1 |
| 12 | Z | 171 | PRO | 2.1 |
| 9 | I | 192 | ASP | 2.0 |
| 12 | L | 171 | PRO | 2.0 |
| 3 | Q | 52 | LEU | 2.0 |
| 9 | W | 192 | ASP | 2.0 |
| 5 | S | 58 | TYR | 2.0 |
| 2 | B | 62 | THR | 2.0 |
| 6 | F | 240 | GLN | 2.0 |

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|----------------------------|-------|
| 15 | RE0 | f | 7 | 16/17 | 0.49 | 0.61 | 81,90,91,91 | 0 |
| 15 | RE0 | e | 7 | 16/17 | 0.61 | 0.43 | 79,85,86,86 | 0 |
| 15 | ACA | f | 4 | 8/9 | 0.72 | 0.37 | 76,77,79,79 | 0 |
| 15 | ACA | e | 4 | 8/9 | 0.77 | 0.34 | 72,72,73,74 | 0 |
| 15 | ACA | c | 4 | 8/9 | 0.81 | 0.34 | 59,59,60,60 | 0 |
| 15 | TY5 | f | 5 | 19/20 | 0.84 | 0.32 | 75,76,80,81 | 0 |
| 15 | TY5 | e | 5 | 19/20 | 0.86 | 0.31 | 70,71,75,76 | 0 |
| 15 | ACA | d | 4 | 8/9 | 0.88 | 0.29 | 57,58,58,58 | 0 |
| 15 | TY5 | d | 5 | 19/20 | 0.88 | 0.25 | 55,56,57,57 | 0 |
| 15 | TY5 | c | 5 | 19/20 | 0.89 | 0.27 | 57,58,58,58 | 0 |
| 15 | RE0 | d | 7 | 16/17 | 0.92 | 0.22 | 52,53,53,53 | 0 |
| 15 | RE0 | c | 7 | 16/17 | 0.92 | 0.17 | 53,54,54,54 | 0 |

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | B-factors(\AA^2) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-----------------------------|-------|
| 16 | MES | Y | 301 | 12/12 | 0.92 | 0.28 | 56,57,58,58 | 0 |
| 16 | MES | K | 301 | 12/12 | 0.94 | 0.25 | 54,55,56,56 | 0 |

6.5 Other polymers [i](#)

There are no such residues in this entry.