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

Jan 31, 2016 – 07:54 PM GMT

| | | |
|---|---|---|
| PDB ID | : | 1HL5 |
| Title | : | THE STRUCTURE OF HOLO TYPE HUMAN CU, ZN SUPEROXIDE DISMUTASE |
| Authors | : | Strange, R.W.; Antonyuk, S.; Hough, M.A.; Doucette, P.; Rodriguez, J.; Hart, P.J.; Hayward, L.J.; Valentine, J.S.; Hasnain, S.S. |
| Deposited on | : | 2003-03-13 |
| Resolution | : | 1.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

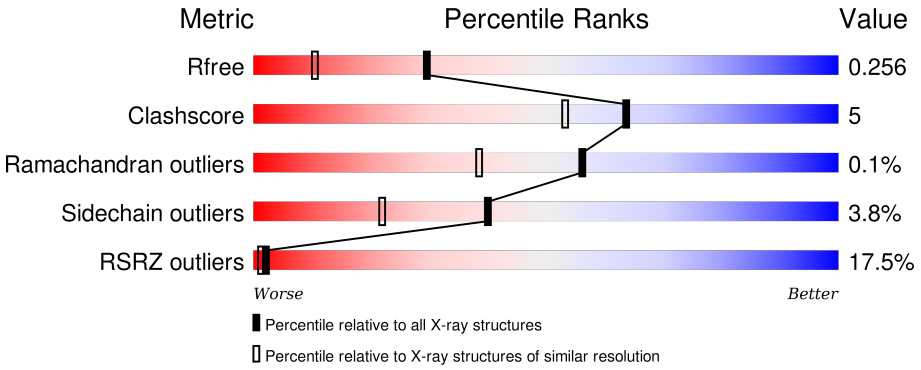
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | trunk26865 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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)) |
|---|---|---|
| $R_{free}$ | 91344 | 4533 (1.80-1.80) |
| Clashscore | 102246 | 5383 (1.80-1.80) |
| Ramachandran outliers | 100387 | 5320 (1.80-1.80) |
| Sidechain outliers | 100360 | 5319 (1.80-1.80) |
| RSRZ outliers | 91569 | 4547 (1.80-1.80) |

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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 | 153 | 7% 90% 10% |
| 1 | B | 153 | 7% 86% 12% |
| 1 | C | 153 | 8% 94% 6% |
| 1 | D | 153 | 7% 93% 6% |
| 1 | E | 153 | 5% 90% 8% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | F | 153 | 8% 84% 8% 5% |
| 1 | G | 153 | 23% 76% 22% |
| 1 | H | 153 | 7% 95% 5% |
| 1 | I | 153 | 7% 91% 8% |
| 1 | J | 153 | 5% 92% 8% |
| 1 | K | 153 | 5% 92% 7% |
| 1 | L | 153 | 7% 92% 8% |
| 1 | M | 153 | 10% 88% 11% |
| 1 | N | 153 | 14% 89% 8% |
| 1 | O | 153 | 25% 75% 20% 5% |
| 1 | P | 153 | 95% 85% 14% |
| 1 | Q | 153 | 13% 80% 16% |
| 1 | S | 153 | 63% 82% 18% |

## 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21585 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 SUPEROXIDE DISMUTASE.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | B | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | C | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1109 | 679 | 202 | 224 | 4 | | | |
| 1 | D | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1094 | 672 | 199 | 219 | 4 | | | |
| 1 | E | 151 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1082 | 669 | 195 | 214 | 4 | | | |
| 1 | F | 145 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1031 | 634 | 187 | 206 | 4 | | | |
| 1 | G | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | H | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | I | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | J | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1102 | 675 | 199 | 224 | 4 | | | |
| 1 | K | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1106 | 678 | 201 | 223 | 4 | | | |
| 1 | L | 152 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1096 | 672 | 198 | 222 | 4 | | | |
| 1 | M | 152 | Total | C | N | O | S | 0 | 0 | 1 |
| | | | 1075 | 660 | 194 | 217 | 4 | | | |
| 1 | N | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | O | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1109 | 679 | 203 | 223 | 4 | | | |
| 1 | P | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1101 | 674 | 201 | 222 | 4 | | | |

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| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Q | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1110 | 679 | 203 | 224 | 4 | | | |
| 1 | S | 153 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1108 | 678 | 202 | 224 | 4 | | | |

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 2 | P | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | G | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | J | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | Q | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | D | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | K | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | E | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | H | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | B | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | I | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | C | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | A | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | N | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | O | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | L | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | S | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |
| 2 | F | 1 | Total | Cu | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | M | 1 | Total Cu<br>1 1 | 0 | 0 |

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | P | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | G | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | J | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | Q | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | D | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | K | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | E | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | H | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | B | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | I | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | C | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | A | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | N | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | O | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | L | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | S | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | F | 1 | Total Zn<br>1 1 | 0 | 0 |
| 3 | M | 1 | Total Zn<br>1 1 | 0 | 0 |

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | O | 1 | Total Ca<br>1 1 | 0 | 0 |
| 4 | D | 1 | Total Ca<br>1 1 | 0 | 0 |
| 4 | C | 1 | Total Ca<br>1 1 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 113 | Total O<br>113 113 | 0 | 0 |
| 5 | B | 152 | Total O<br>152 152 | 0 | 0 |
| 5 | C | 144 | Total O<br>144 144 | 0 | 0 |
| 5 | D | 107 | Total O<br>107 107 | 0 | 0 |
| 5 | E | 114 | Total O<br>114 114 | 0 | 0 |
| 5 | F | 94 | Total O<br>94 94 | 0 | 0 |
| 5 | G | 43 | Total O<br>43 43 | 0 | 0 |
| 5 | H | 118 | Total O<br>118 118 | 0 | 0 |
| 5 | I | 141 | Total O<br>141 141 | 0 | 0 |
| 5 | J | 133 | Total O<br>133 133 | 0 | 0 |
| 5 | K | 148 | Total O<br>148 148 | 0 | 0 |
| 5 | L | 115 | Total O<br>115 115 | 0 | 0 |
| 5 | M | 99 | Total O<br>99 99 | 0 | 0 |
| 5 | N | 90 | Total O<br>90 90 | 0 | 0 |
| 5 | O | 50 | Total O<br>50 50 | 0 | 0 |
| 5 | P | 2 | Total O<br>2 2 | 0 | 0 |

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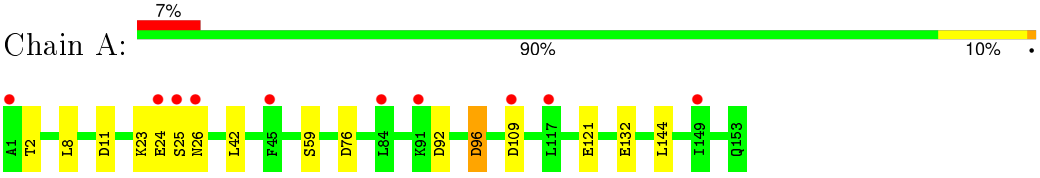
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | Q | 83 | Total O<br>83 83 | 0 | 0 |
| 5 | S | 17 | Total O<br>17 17 | 0 | 0 |

# 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 errors 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.

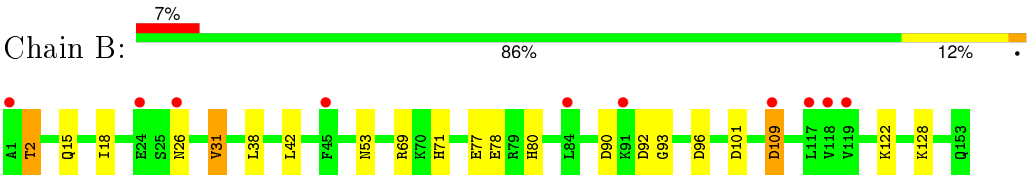
- Molecule 1: SUPEROXIDE DISMUTASE

Chain A:



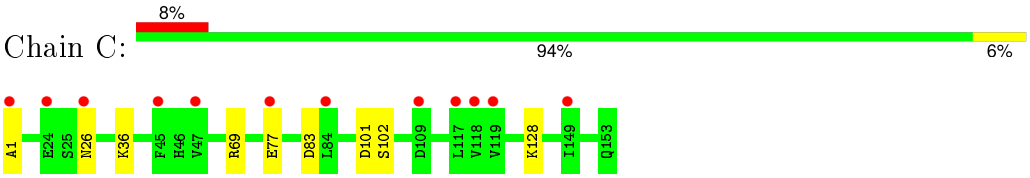

- Molecule 1: SUPEROXIDE DISMUTASE

Chain B:



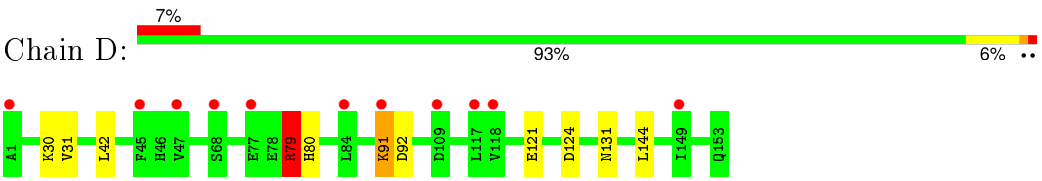

- Molecule 1: SUPEROXIDE DISMUTASE

Chain C:



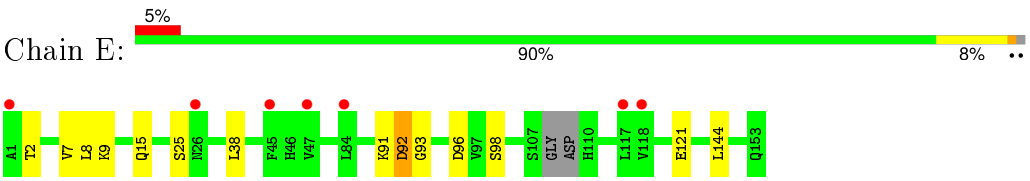

- Molecule 1: SUPEROXIDE DISMUTASE

Chain D:



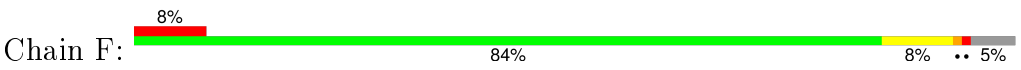

- Molecule 1: SUPEROXIDE DISMUTASE

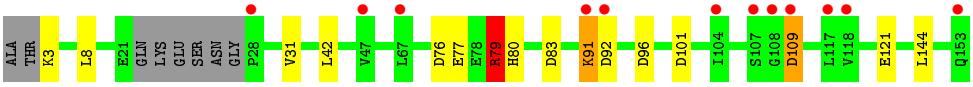
Chain E:




- Molecule 1: SUPEROXIDE DISMUTASE

Chain F:

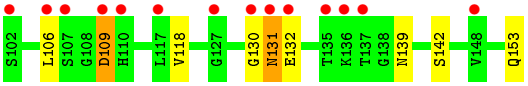





• Molecule 1: SUPEROXIDE DISMUTASE

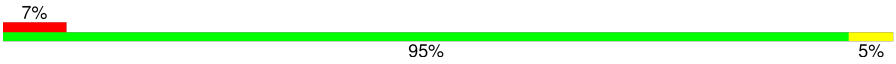
Chain G:

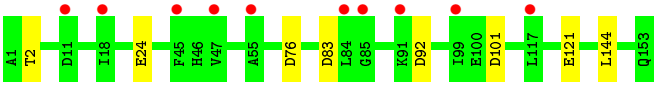





• Molecule 1: SUPEROXIDE DISMUTASE

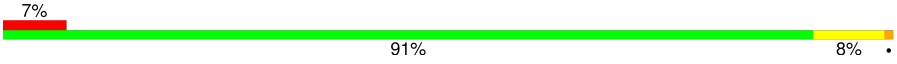
Chain H:

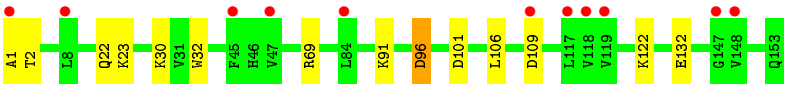



• Molecule 1: SUPEROXIDE DISMUTASE

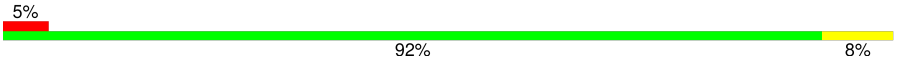
Chain I:

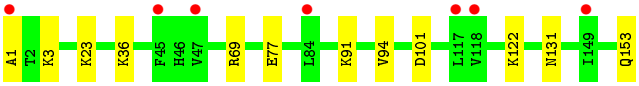



• Molecule 1: SUPEROXIDE DISMUTASE

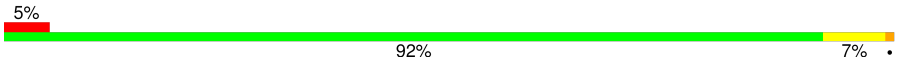
Chain J:

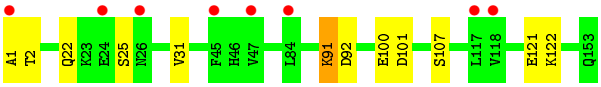



• Molecule 1: SUPEROXIDE DISMUTASE

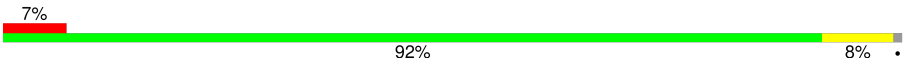
Chain K:

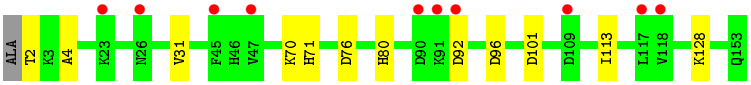



• Molecule 1: SUPEROXIDE DISMUTASE

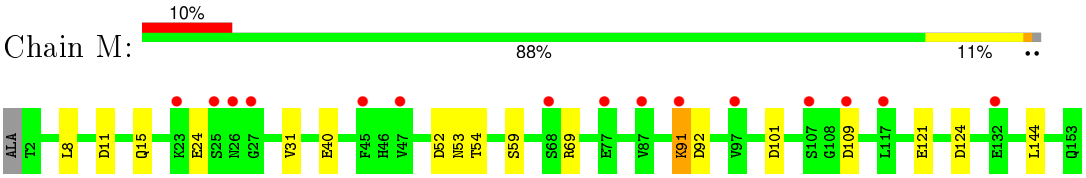
Chain L:



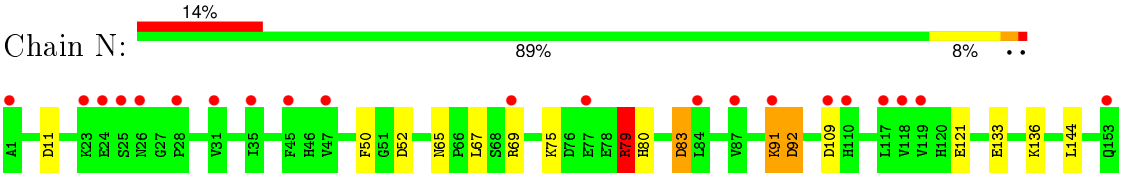

• Molecule 1: SUPEROXIDE DISMUTASE

Chain M:



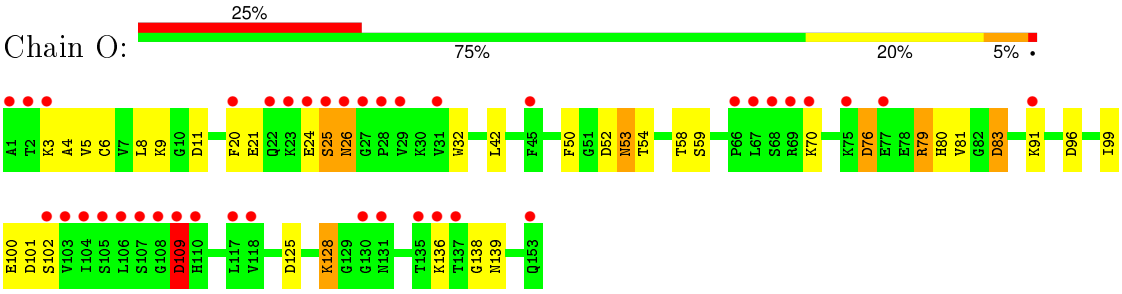

• Molecule 1: SUPEROXIDE DISMUTASE

Chain N:



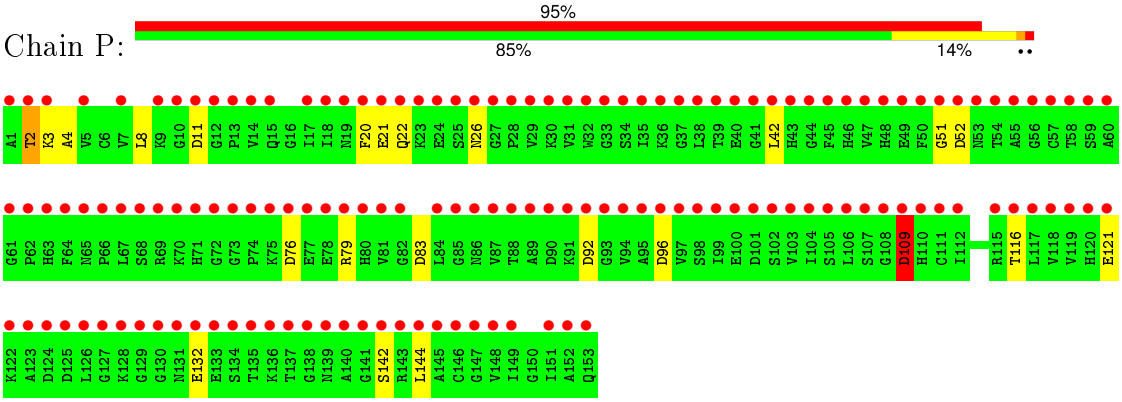

• Molecule 1: SUPEROXIDE DISMUTASE

Chain O:



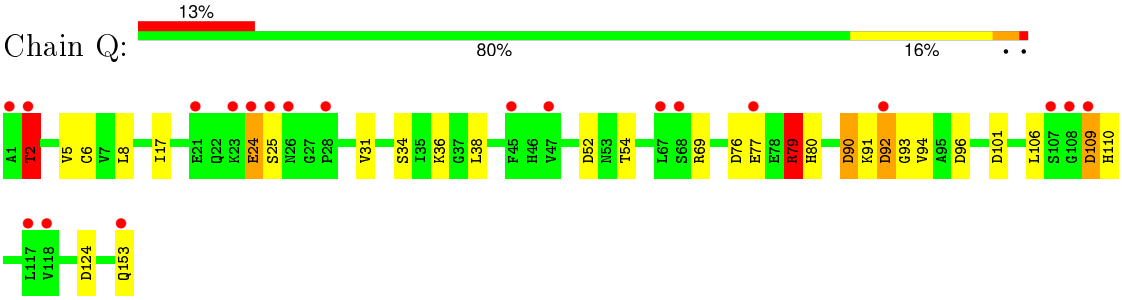

• Molecule 1: SUPEROXIDE DISMUTASE

Chain P:



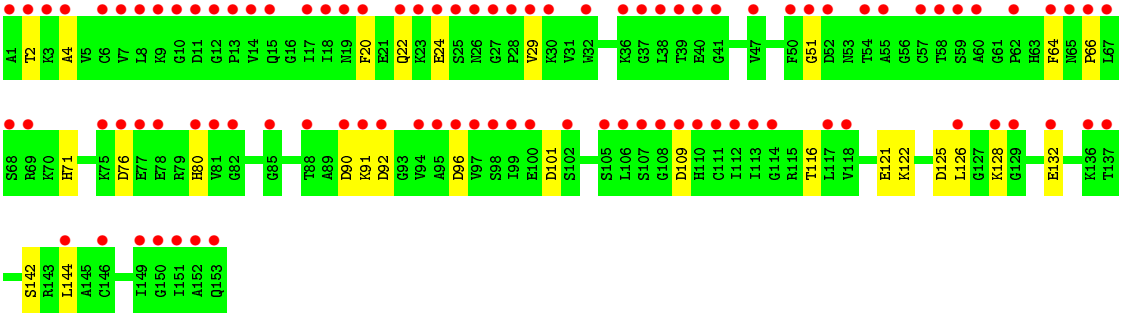

• Molecule 1: SUPEROXIDE DISMUTASE

Chain Q:




• Molecule 1: SUPEROXIDE DISMUTASE

Chain S:


A1 T2 K3 A4 V5 C6 V7 L8 K9 G10 D11 G12 P13 V14 Q15 G16 I17 I18 N19 F20 E21 Q22 K23 E24 S25 M26 G27 P28 V29 K30 V31 W32 K36 G37 I38 T39 E40 G41 V47 F50 G51 D52 N53 T54 A55 G56 C57 T58 S59 A60 G61 P62 H63 F64 N65 P66 L67
S68 R69 K70 H71 K75 D76 E77 E78 R79 H80 V81 G82 G85 T88 A89 D90 K91 D92 G93 V94 A95 D96 W97 S98 I99 E100 D101 S102 S105 L106 S107 G108 D109 H110 C111 I112 I113 G114 R115 T116 L117 V118 E121 K122 D125 L126 G127 K128 G129 E132 K136 T137
S142 R143 L144 A145 C146 I149 G150 I151 A152 Q153

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 76.87Å 172.38Å 112.45Å<br>90.00° 93.45° 90.00° | Depositor |
| Resolution (Å) | 50.00 – 1.80<br>22.00 – 1.80 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.5 (50.00-1.80)<br>98.5 (22.00-1.80) | Depositor<br>EDS |
| $R_{merge}$ | 0.05 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.68 (at 1.80Å) | Xtriage |
| Refinement program | REFMAC 5.0 | Depositor |
| R, $R_{free}$ | 0.185 , 0.222<br>0.232 , 0.256 | Depositor<br>DCC |
| $R_{free}$ test set | 13349 reflections (5.03%) | DCC |
| Wilson B-factor (Å$^2$) | 25.4 | Xtriage |
| Anisotropy | 0.068 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.42 , 58.9 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Outliers | 0 of 265949 reflections | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 21585 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 19.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, CA, CU

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 | 0.65 | 0/1128 | 0.95 | 5/1520 (0.3%) |
| 1 | B | 0.75 | 0/1128 | 0.99 | 5/1520 (0.3%) |
| 1 | C | 0.76 | 0/1127 | 0.93 | 2/1519 (0.1%) |
| 1 | D | 0.66 | 0/1112 | 1.00 | 4/1501 (0.3%) |
| 1 | E | 0.63 | 0/1099 | 0.89 | 2/1482 (0.1%) |
| 1 | F | 0.58 | 0/1048 | 1.00 | 7/1413 (0.5%) |
| 1 | G | 0.52 | 0/1128 | 0.91 | 5/1520 (0.3%) |
| 1 | H | 0.66 | 0/1128 | 0.91 | 4/1520 (0.3%) |
| 1 | I | 0.73 | 0/1128 | 0.93 | 3/1520 (0.2%) |
| 1 | J | 0.74 | 0/1120 | 0.92 | 1/1512 (0.1%) |
| 1 | K | 0.74 | 0/1124 | 0.96 | 3/1515 (0.2%) |
| 1 | L | 0.61 | 0/1114 | 0.89 | 4/1503 (0.3%) |
| 1 | M | 0.63 | 0/1092 | 0.93 | 4/1471 (0.3%) |
| 1 | N | 0.59 | 0/1128 | 0.94 | 7/1520 (0.5%) |
| 1 | O | 0.54 | 0/1127 | 0.90 | 5/1520 (0.3%) |
| 1 | P | 0.27 | 0/1118 | 0.74 | 6/1506 (0.4%) |
| 1 | Q | 0.63 | 0/1128 | 0.99 | 7/1520 (0.5%) |
| 1 | S | 0.37 | 0/1126 | 0.80 | 5/1518 (0.3%) |
| All | All | 0.63 | 0/20103 | 0.92 | 79/27100 (0.3%) |

There are no bond length outliers.

All (79) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 79 | ARG | NE-CZ-NH2 | -11.85 | 114.37 | 120.30 |
| 1 | Q | 79 | ARG | NE-CZ-NH2 | -10.69 | 114.96 | 120.30 |
| 1 | F | 79 | ARG | NE-CZ-NH2 | -9.37 | 115.62 | 120.30 |
| 1 | F | 101 | ASP | CB-CG-OD2 | 7.52 | 125.07 | 118.30 |
| 1 | D | 31 | VAL | CG1-CB-CG2 | 6.99 | 122.08 | 110.90 |
| 1 | I | 96 | ASP | CB-CG-OD2 | 6.98 | 124.58 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 109 | ASP | CB-CG-OD2 | 6.93 | 124.54 | 118.30 |
| 1 | D | 79 | ARG | NE-CZ-NH1 | 6.85 | 123.73 | 120.30 |
| 1 | L | 76 | ASP | CB-CG-OD2 | 6.82 | 124.44 | 118.30 |
| 1 | C | 101 | ASP | CB-CG-OD2 | 6.77 | 124.40 | 118.30 |
| 1 | N | 79 | ARG | NE-CZ-NH2 | -6.75 | 116.93 | 120.30 |
| 1 | A | 96 | ASP | CB-CG-OD2 | 6.68 | 124.31 | 118.30 |
| 1 | B | 31 | VAL | CG1-CB-CG2 | 6.67 | 121.57 | 110.90 |
| 1 | I | 101 | ASP | CB-CG-OD2 | 6.53 | 124.18 | 118.30 |
| 1 | Q | 101 | ASP | CB-CG-OD2 | 6.40 | 124.06 | 118.30 |
| 1 | F | 79 | ARG | NE-CZ-NH1 | 6.37 | 123.49 | 120.30 |
| 1 | M | 124 | ASP | CB-CG-OD1 | 6.28 | 123.95 | 118.30 |
| 1 | I | 109 | ASP | CB-CG-OD2 | 6.27 | 123.94 | 118.30 |
| 1 | Q | 79 | ARG | NE-CZ-NH1 | 6.27 | 123.44 | 120.30 |
| 1 | B | 109 | ASP | CB-CG-OD2 | 6.23 | 123.91 | 118.30 |
| 1 | M | 109 | ASP | CB-CG-OD2 | 6.19 | 123.87 | 118.30 |
| 1 | O | 83 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | L | 92 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | G | 83 | ASP | CB-CG-OD2 | 6.04 | 123.73 | 118.30 |
| 1 | P | 109 | ASP | CB-CG-OD2 | 5.95 | 123.66 | 118.30 |
| 1 | K | 31 | VAL | CG1-CB-CG2 | 5.88 | 120.31 | 110.90 |
| 1 | P | 96 | ASP | CB-CG-OD2 | 5.88 | 123.59 | 118.30 |
| 1 | F | 96 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | G | 11 | ASP | CB-CG-OD2 | 5.87 | 123.58 | 118.30 |
| 1 | S | 109 | ASP | CB-CG-OD2 | 5.79 | 123.51 | 118.30 |
| 1 | L | 101 | ASP | CB-CG-OD2 | 5.76 | 123.49 | 118.30 |
| 1 | Q | 96 | ASP | CB-CG-OD2 | 5.75 | 123.48 | 118.30 |
| 1 | Q | 124 | ASP | CB-CG-OD1 | 5.75 | 123.47 | 118.30 |
| 1 | A | 76 | ASP | CB-CG-OD2 | 5.74 | 123.46 | 118.30 |
| 1 | H | 101 | ASP | CB-CG-OD2 | 5.71 | 123.44 | 118.30 |
| 1 | G | 109 | ASP | CB-CG-OD2 | 5.69 | 123.42 | 118.30 |
| 1 | G | 96 | ASP | CB-CG-OD2 | 5.61 | 123.35 | 118.30 |
| 1 | Q | 109 | ASP | CB-CG-OD2 | 5.60 | 123.34 | 118.30 |
| 1 | K | 31 | VAL | CA-CB-CG2 | 5.59 | 119.29 | 110.90 |
| 1 | B | 96 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 1 | N | 79 | ARG | NE-CZ-NH1 | 5.56 | 123.08 | 120.30 |
| 1 | N | 109 | ASP | CB-CG-OD2 | 5.53 | 123.27 | 118.30 |
| 1 | S | 76 | ASP | CB-CG-OD2 | 5.50 | 123.25 | 118.30 |
| 1 | S | 90 | ASP | CB-CG-OD2 | 5.47 | 123.22 | 118.30 |
| 1 | S | 101 | ASP | CB-CG-OD2 | 5.45 | 123.20 | 118.30 |
| 1 | P | 83 | ASP | CB-CG-OD2 | 5.43 | 123.18 | 118.30 |
| 1 | P | 92 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |
| 1 | P | 11 | ASP | CB-CG-OD2 | 5.39 | 123.15 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | N | 11 | ASP | CB-CG-OD2 | 5.36 | 123.12 | 118.30 |
| 1 | Q | 76 | ASP | CB-CG-OD2 | 5.36 | 123.12 | 118.30 |
| 1 | A | 11 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | D | 124 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | S | 96 | ASP | CB-CG-OD2 | 5.35 | 123.11 | 118.30 |
| 1 | N | 83 | ASP | CB-CG-OD2 | 5.34 | 123.11 | 118.30 |
| 1 | G | 101 | ASP | CB-CG-OD2 | 5.32 | 123.09 | 118.30 |
| 1 | K | 101 | ASP | CB-CG-OD2 | 5.31 | 123.08 | 118.30 |
| 1 | F | 83 | ASP | CB-CG-OD2 | 5.29 | 123.06 | 118.30 |
| 1 | M | 11 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | E | 92 | ASP | CB-CG-OD2 | 5.28 | 123.05 | 118.30 |
| 1 | F | 109 | ASP | CB-CG-OD2 | 5.27 | 123.05 | 118.30 |
| 1 | F | 76 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 1 | J | 101 | ASP | CB-CG-OD2 | 5.26 | 123.03 | 118.30 |
| 1 | B | 92 | ASP | CB-CG-OD2 | 5.24 | 123.02 | 118.30 |
| 1 | N | 92 | ASP | CB-CG-OD2 | 5.23 | 123.01 | 118.30 |
| 1 | H | 76 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | B | 101 | ASP | CB-CG-OD2 | 5.21 | 122.99 | 118.30 |
| 1 | H | 92 | ASP | CB-CG-OD2 | 5.20 | 122.98 | 118.30 |
| 1 | A | 92 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | O | 96 | ASP | CB-CG-OD2 | 5.18 | 122.96 | 118.30 |
| 1 | L | 96 | ASP | CB-CG-OD2 | 5.17 | 122.95 | 118.30 |
| 1 | E | 96 | ASP | CB-CG-OD2 | 5.16 | 122.95 | 118.30 |
| 1 | P | 52 | ASP | CB-CG-OD2 | 5.13 | 122.92 | 118.30 |
| 1 | C | 83 | ASP | CB-CG-OD2 | 5.12 | 122.91 | 118.30 |
| 1 | M | 101 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | H | 83 | ASP | CB-CG-OD2 | 5.05 | 122.85 | 118.30 |
| 1 | O | 109 | ASP | CB-CG-OD2 | 5.05 | 122.85 | 118.30 |
| 1 | O | 11 | ASP | CB-CG-OD2 | 5.03 | 122.83 | 118.30 |
| 1 | N | 52 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 1 | O | 76 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1110 | 0 | 1077 | 6 | 0 |
| 1 | B | 1110 | 0 | 1077 | 11 | 1 |
| 1 | C | 1109 | 0 | 1072 | 7 | 0 |
| 1 | D | 1094 | 0 | 1041 | 7 | 0 |
| 1 | E | 1082 | 0 | 1031 | 10 | 0 |
| 1 | F | 1031 | 0 | 982 | 8 | 0 |
| 1 | G | 1110 | 0 | 1077 | 20 | 0 |
| 1 | H | 1110 | 0 | 1077 | 1 | 0 |
| 1 | I | 1110 | 0 | 1077 | 9 | 0 |
| 1 | J | 1102 | 0 | 1049 | 18 | 0 |
| 1 | K | 1106 | 0 | 1068 | 7 | 0 |
| 1 | L | 1096 | 0 | 1044 | 6 | 0 |
| 1 | M | 1075 | 0 | 1009 | 11 | 2 |
| 1 | N | 1110 | 0 | 1077 | 13 | 0 |
| 1 | O | 1109 | 0 | 1077 | 32 | 0 |
| 1 | P | 1101 | 0 | 1059 | 9 | 0 |
| 1 | Q | 1110 | 0 | 1077 | 22 | 0 |
| 1 | S | 1108 | 0 | 1070 | 24 | 1 |
| 2 | A | 1 | 0 | 0 | 0 | 0 |
| 2 | B | 1 | 0 | 0 | 0 | 0 |
| 2 | C | 1 | 0 | 0 | 0 | 0 |
| 2 | D | 1 | 0 | 0 | 0 | 0 |
| 2 | E | 1 | 0 | 0 | 0 | 0 |
| 2 | F | 1 | 0 | 0 | 0 | 0 |
| 2 | G | 1 | 0 | 0 | 0 | 0 |
| 2 | H | 1 | 0 | 0 | 0 | 0 |
| 2 | I | 1 | 0 | 0 | 0 | 0 |
| 2 | J | 1 | 0 | 0 | 0 | 0 |
| 2 | K | 1 | 0 | 0 | 0 | 0 |
| 2 | L | 1 | 0 | 0 | 0 | 0 |
| 2 | M | 1 | 0 | 0 | 0 | 0 |
| 2 | N | 1 | 0 | 0 | 0 | 0 |
| 2 | O | 1 | 0 | 0 | 0 | 0 |
| 2 | P | 1 | 0 | 0 | 0 | 0 |
| 2 | Q | 1 | 0 | 0 | 0 | 0 |
| 2 | S | 1 | 0 | 0 | 0 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 3 | C | 1 | 0 | 0 | 0 | 0 |
| 3 | D | 1 | 0 | 0 | 0 | 0 |
| 3 | E | 1 | 0 | 0 | 0 | 0 |
| 3 | F | 1 | 0 | 0 | 0 | 0 |
| 3 | G | 1 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | H | 1 | 0 | 0 | 0 | 0 |
| 3 | I | 1 | 0 | 0 | 0 | 0 |
| 3 | J | 1 | 0 | 0 | 0 | 0 |
| 3 | K | 1 | 0 | 0 | 0 | 0 |
| 3 | L | 1 | 0 | 0 | 0 | 0 |
| 3 | M | 1 | 0 | 0 | 0 | 0 |
| 3 | N | 1 | 0 | 0 | 0 | 0 |
| 3 | O | 1 | 0 | 0 | 0 | 0 |
| 3 | P | 1 | 0 | 0 | 0 | 0 |
| 3 | Q | 1 | 0 | 0 | 0 | 0 |
| 3 | S | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | D | 1 | 0 | 0 | 0 | 0 |
| 4 | O | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 113 | 0 | 0 | 2 | 0 |
| 5 | B | 152 | 0 | 0 | 4 | 0 |
| 5 | C | 144 | 0 | 0 | 5 | 1 |
| 5 | D | 107 | 0 | 0 | 1 | 0 |
| 5 | E | 114 | 0 | 0 | 0 | 0 |
| 5 | F | 94 | 0 | 0 | 1 | 0 |
| 5 | G | 43 | 0 | 0 | 4 | 0 |
| 5 | H | 118 | 0 | 0 | 0 | 1 |
| 5 | I | 141 | 0 | 0 | 1 | 0 |
| 5 | J | 133 | 0 | 0 | 3 | 0 |
| 5 | K | 148 | 0 | 0 | 2 | 0 |
| 5 | L | 115 | 0 | 0 | 5 | 0 |
| 5 | M | 99 | 0 | 0 | 3 | 0 |
| 5 | N | 90 | 0 | 0 | 6 | 0 |
| 5 | O | 50 | 0 | 0 | 10 | 0 |
| 5 | P | 2 | 0 | 0 | 0 | 0 |
| 5 | Q | 83 | 0 | 0 | 4 | 0 |
| 5 | S | 17 | 0 | 0 | 3 | 0 |
| All | All | 21585 | 0 | 19041 | 203 | 3 |

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

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:96:ASP:HB3 | 5:I:2092:HOH:O | 1.27 | 1.25 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:96:ASP:HB3 | 5:A:2072:HOH:O | 1.42 | 1.16 |
| 1:O:125:ASP:O | 1:O:128:LYS:HE2 | 1.47 | 1.14 |
| 1:J:153:GLN:O | 1:S:92:ASP:OD1 | 1.68 | 1.10 |
| 1:B:53:ASN:OD1 | 5:B:2071:HOH:O | 1.76 | 1.04 |
| 1:J:3:LYS:NZ | 1:S:92:ASP:OD2 | 1.97 | 0.97 |
| 1:N:91:LYS:HG3 | 5:N:2051:HOH:O | 1.68 | 0.93 |
| 1:B:69:ARG:NH1 | 1:B:78:GLU:OE1 | 2.06 | 0.88 |
| 1:L:70:LYS:HE2 | 5:L:2056:HOH:O | 1.74 | 0.87 |
| 1:B:69:ARG:NH2 | 1:B:77:GLU:OE2 | 2.07 | 0.86 |
| 1:O:3:LYS:HG2 | 1:O:21:GLU:HG2 | 1.57 | 0.84 |
| 5:J:2132:HOH:O | 1:S:91:LYS:HG3 | 1.76 | 0.83 |
| 1:M:53:ASN:HB2 | 5:M:2036:HOH:O | 1.78 | 0.82 |
| 1:D:79:ARG:HD3 | 1:D:80:HIS:O | 1.80 | 0.81 |
| 1:K:91:LYS:HD2 | 1:K:92:ASP:OD1 | 1.81 | 0.81 |
| 1:G:46:HIS:HB2 | 5:G:2010:HOH:O | 1.81 | 0.80 |
| 1:C:102:SER:HB3 | 5:C:2035:HOH:O | 1.81 | 0.80 |
| 1:F:3:LYS:C | 5:F:2001:HOH:O | 2.20 | 0.80 |
| 1:O:79:ARG:NH2 | 1:O:101:ASP:OD1 | 2.17 | 0.77 |
| 1:D:79:ARG:CD | 1:D:80:HIS:O | 2.32 | 0.77 |
| 1:J:3:LYS:CD | 1:S:92:ASP:OD2 | 2.33 | 0.76 |
| 1:J:1:ALA:N | 1:J:23:LYS:HA | 2.01 | 0.76 |
| 1:J:153:GLN:C | 1:S:92:ASP:OD1 | 2.25 | 0.75 |
| 1:O:128:LYS:CG | 5:O:2044:HOH:O | 2.35 | 0.75 |
| 1:O:24:GLU:O | 1:O:26:ASN:N | 2.18 | 0.74 |
| 1:O:128:LYS:HG2 | 5:O:2044:HOH:O | 1.87 | 0.74 |
| 1:F:79:ARG:HD3 | 1:F:80:HIS:O | 1.88 | 0.74 |
| 1:B:69:ARG:HH22 | 1:B:77:GLU:CD | 1.90 | 0.73 |
| 1:O:109:ASP:HB2 | 5:O:2038:HOH:O | 1.89 | 0.72 |
| 1:N:133:GLU:OE2 | 5:N:2076:HOH:O | 2.08 | 0.71 |
| 1:N:136:LYS:HE3 | 5:N:2076:HOH:O | 1.91 | 0.71 |
| 1:O:128:LYS:HB3 | 5:O:2044:HOH:O | 1.89 | 0.70 |
| 1:F:91:LYS:HE2 | 1:F:92:ASP:OD2 | 1.92 | 0.70 |
| 1:J:36:LYS:HG3 | 1:J:94:VAL:HG22 | 1.73 | 0.70 |
| 1:D:91:LYS:HE2 | 1:D:92:ASP:OD1 | 1.91 | 0.70 |
| 1:G:130:GLY:O | 1:G:131:ASN:O | 2.10 | 0.70 |
| 1:I:1:ALA:HB3 | 1:I:22:GLN:O | 1.92 | 0.69 |
| 1:M:24:GLU:C | 1:M:24:GLU:N | 2.47 | 0.69 |
| 1:P:132:GLU:C | 1:P:132:GLU:N | 2.46 | 0.69 |
| 1:M:91:LYS:HD2 | 5:M:2057:HOH:O | 1.94 | 0.67 |
| 1:O:79:ARG:HD3 | 1:O:80:HIS:O | 1.94 | 0.66 |
| 1:O:128:LYS:CB | 5:O:2044:HOH:O | 2.44 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:Q:94:VAL:HG23 | 5:Q:2049:HOH:O | 1.95 | 0.66 |
| 1:Q:2:THR:HG21 | 1:Q:106:LEU:HB2 | 1.78 | 0.65 |
| 1:J:153:GLN:OXT | 1:S:91:LYS:HG3 | 1.96 | 0.65 |
| 1:O:80:HIS:CE1 | 5:O:2030:HOH:O | 2.50 | 0.64 |
| 1:B:53:ASN:HB2 | 5:B:2075:HOH:O | 1.98 | 0.63 |
| 1:I:30:LYS:HG2 | 1:I:32:TRP:CE3 | 2.35 | 0.62 |
| 1:K:91:LYS:HD2 | 1:K:92:ASP:CG | 2.19 | 0.62 |
| 1:J:153:GLN:OXT | 1:S:91:LYS:HE3 | 1.99 | 0.62 |
| 1:Q:90:ASP:HB2 | 1:Q:92:ASP:HB2 | 1.82 | 0.61 |
| 1:O:54:THR:HG22 | 1:Q:17:ILE:HD13 | 1.83 | 0.60 |
| 1:K:91:LYS:CD | 1:K:92:ASP:OD1 | 2.50 | 0.60 |
| 1:Q:38:LEU:O | 1:Q:93:GLY:HA2 | 2.02 | 0.59 |
| 1:Q:2:THR:HG22 | 1:Q:106:LEU:HD12 | 1.85 | 0.59 |
| 1:N:79:ARG:HD2 | 1:N:80:HIS:O | 2.03 | 0.59 |
| 1:M:15:GLN:CD | 5:M:2003:HOH:O | 2.40 | 0.58 |
| 1:J:3:LYS:HD3 | 1:S:92:ASP:OD2 | 2.03 | 0.58 |
| 1:Q:79:ARG:CD | 1:Q:80:HIS:O | 2.52 | 0.58 |
| 1:J:69:ARG:NH1 | 1:J:77:GLU:OE2 | 2.37 | 0.58 |
| 1:M:91:LYS:H | 1:M:91:LYS:HD2 | 1.68 | 0.58 |
| 1:N:79:ARG:CD | 1:N:80:HIS:O | 2.52 | 0.58 |
| 1:K:1:ALA:HB3 | 1:K:22:GLN:O | 2.04 | 0.58 |
| 1:F:91:LYS:HE2 | 1:F:92:ASP:CG | 2.23 | 0.57 |
| 1:C:36:LYS:HE3 | 5:C:2015:HOH:O | 2.04 | 0.57 |
| 1:S:4:ALA:HB3 | 1:S:20:PHE:HB2 | 1.84 | 0.57 |
| 1:D:79:ARG:HD2 | 1:D:80:HIS:O | 2.04 | 0.56 |
| 1:O:80:HIS:HB2 | 1:O:83:ASP:CG | 2.26 | 0.56 |
| 1:J:3:LYS:CE | 1:S:92:ASP:OD2 | 2.53 | 0.56 |
| 1:F:121:GLU:HA | 1:F:144:LEU:HD11 | 1.87 | 0.56 |
| 1:G:131:ASN:HD21 | 1:G:139:ASN:HD21 | 1.54 | 0.56 |
| 1:E:7:VAL:CG1 | 1:E:9:LYS:HE2 | 2.36 | 0.55 |
| 1:Q:79:ARG:HD3 | 1:Q:80:HIS:O | 2.05 | 0.55 |
| 1:O:79:ARG:HH22 | 1:O:101:ASP:CG | 2.09 | 0.55 |
| 1:S:121:GLU:HA | 1:S:144:LEU:HD11 | 1.88 | 0.55 |
| 1:J:153:GLN:OXT | 1:S:91:LYS:CD | 2.56 | 0.54 |
| 1:J:153:GLN:OXT | 1:S:91:LYS:CE | 2.56 | 0.54 |
| 1:C:1:ALA:C | 5:C:2001:HOH:O | 2.45 | 0.54 |
| 1:E:7:VAL:HG12 | 1:E:9:LYS:HE2 | 1.89 | 0.53 |
| 1:O:53:ASN:CG | 5:O:2021:HOH:O | 2.47 | 0.53 |
| 1:O:50:PHE:CZ | 1:Q:153:GLN:HB2 | 2.44 | 0.53 |
| 1:P:4:ALA:HB3 | 1:P:20:PHE:HB2 | 1.89 | 0.53 |
| 1:A:23:LYS:HG3 | 5:A:2015:HOH:O | 2.09 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:71:HIS:HB2 | 1:G:80:HIS:CE1 | 2.44 | 0.53 |
| 1:G:118:VAL:HB | 5:G:2010:HOH:O | 2.08 | 0.52 |
| 1:S:122:LYS:HE2 | 5:S:2017:HOH:O | 2.09 | 0.52 |
| 1:A:96:ASP:O | 1:J:131:ASN:HB3 | 2.10 | 0.52 |
| 1:E:91:LYS:HD2 | 1:E:92:ASP:N | 2.24 | 0.51 |
| 1:O:52:ASP:O | 1:O:59:SER:HB2 | 2.10 | 0.51 |
| 1:S:71:HIS:HB2 | 1:S:80:HIS:CE1 | 2.46 | 0.51 |
| 1:O:25:SER:O | 1:O:26:ASN:HB3 | 2.11 | 0.51 |
| 1:O:21:GLU:HG3 | 1:O:32:TRP:HH2 | 1.77 | 0.50 |
| 1:O:99:ILE:HG22 | 1:O:100:GLU:N | 2.25 | 0.50 |
| 1:S:51:GLY:HA2 | 1:S:116:THR:OG1 | 2.12 | 0.50 |
| 1:Q:2:THR:CG2 | 1:Q:106:LEU:HD12 | 2.41 | 0.50 |
| 1:O:9:LYS:HD2 | 5:Q:2035:HOH:O | 2.11 | 0.50 |
| 1:Q:52:ASP:OD1 | 1:Q:54:THR:HG23 | 2.12 | 0.49 |
| 1:K:100:GLU:OE1 | 5:K:2100:HOH:O | 2.19 | 0.49 |
| 1:G:65:ASN:HD21 | 1:G:69:ARG:N | 2.10 | 0.49 |
| 1:P:51:GLY:HA2 | 1:P:116:THR:OG1 | 2.12 | 0.49 |
| 1:P:76:ASP:O | 1:P:79:ARG:HG2 | 2.13 | 0.49 |
| 1:C:26:ASN:ND2 | 5:C:2034:HOH:O | 2.45 | 0.49 |
| 1:E:9:LYS:NZ | 1:E:15:GLN:HB2 | 2.28 | 0.48 |
| 1:N:121:GLU:HA | 1:N:144:LEU:HD11 | 1.95 | 0.48 |
| 1:Q:36:LYS:HB3 | 5:Q:2016:HOH:O | 2.14 | 0.48 |
| 1:L:4:ALA:HB2 | 1:L:113:ILE:HD11 | 1.94 | 0.48 |
| 1:O:70:LYS:HD3 | 1:O:70:LYS:HA | 1.66 | 0.48 |
| 1:M:91:LYS:H | 1:M:91:LYS:CD | 2.27 | 0.48 |
| 1:J:153:GLN:OXT | 1:S:91:LYS:CG | 2.61 | 0.48 |
| 1:B:90:ASP:OD1 | 1:B:90:ASP:C | 2.53 | 0.48 |
| 1:M:91:LYS:HD3 | 1:M:92:ASP:N | 2.29 | 0.47 |
| 1:Q:24:GLU:HB3 | 1:Q:25:SER:H | 1.56 | 0.47 |
| 1:N:92:ASP:HB3 | 5:N:2053:HOH:O | 2.14 | 0.47 |
| 1:M:91:LYS:N | 1:M:91:LYS:CD | 2.78 | 0.47 |
| 1:E:91:LYS:C | 1:E:91:LYS:HD2 | 2.35 | 0.47 |
| 1:Q:109:ASP:O | 1:Q:109:ASP:OD2 | 2.33 | 0.47 |
| 1:J:3:LYS:HE3 | 5:J:2023:HOH:O | 2.15 | 0.47 |
| 1:A:132:GLU:HG2 | 1:E:98:SER:HB2 | 1.97 | 0.47 |
| 1:G:65:ASN:HD21 | 1:G:69:ARG:H | 1.63 | 0.47 |
| 1:G:64:PHE:CZ | 1:G:66:PRO:HG3 | 2.50 | 0.47 |
| 1:F:91:LYS:HE2 | 1:F:92:ASP:OD1 | 2.16 | 0.46 |
| 1:S:125:ASP:HA | 5:S:2010:HOH:O | 2.15 | 0.46 |
| 1:D:30:LYS:HD2 | 5:D:2020:HOH:O | 2.14 | 0.46 |
| 1:N:79:ARG:HD3 | 1:N:83:ASP:HB2 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:153:GLN:HG3 | 1:N:50:PHE:CZ | 2.51 | 0.46 |
| 1:O:80:HIS:HE1 | 5:O:2030:HOH:O | 1.93 | 0.46 |
| 1:J:1:ALA:H1 | 1:J:23:LYS:HA | 1.77 | 0.46 |
| 1:O:5:VAL:HG22 | 1:O:6:CYS:N | 2.31 | 0.46 |
| 1:B:128:LYS:NZ | 5:B:2131:HOH:O | 2.35 | 0.46 |
| 1:S:132:GLU:HG2 | 5:S:2013:HOH:O | 2.16 | 0.46 |
| 1:D:131:ASN:HB3 | 1:I:96:ASP:O | 2.16 | 0.46 |
| 1:G:48:HIS:CD2 | 5:G:2010:HOH:O | 2.68 | 0.46 |
| 1:G:40:GLU:OE2 | 1:G:91:LYS:HG2 | 2.15 | 0.46 |
| 1:E:8:LEU:O | 1:E:9:LYS:HD3 | 2.15 | 0.46 |
| 1:G:74:PRO:HD2 | 5:G:2023:HOH:O | 2.16 | 0.46 |
| 1:K:107:SER:OG | 5:K:2106:HOH:O | 2.21 | 0.46 |
| 1:F:79:ARG:CD | 1:F:80:HIS:O | 2.63 | 0.46 |
| 1:O:79:ARG:CD | 1:O:80:HIS:O | 2.62 | 0.46 |
| 1:A:121:GLU:HA | 1:A:144:LEU:HD11 | 1.99 | 0.45 |
| 1:O:26:ASN:OD1 | 1:O:26:ASN:N | 2.49 | 0.45 |
| 1:O:99:ILE:CG2 | 1:O:100:GLU:N | 2.79 | 0.45 |
| 1:Q:8:LEU:HD22 | 1:Q:8:LEU:N | 2.32 | 0.45 |
| 1:O:128:LYS:NZ | 5:O:2043:HOH:O | 2.50 | 0.45 |
| 1:G:131:ASN:ND2 | 1:G:139:ASN:HD21 | 2.15 | 0.45 |
| 1:I:1:ALA:CB | 1:I:23:LYS:HA | 2.47 | 0.45 |
| 1:Q:91:LYS:HG3 | 1:Q:91:LYS:O | 2.16 | 0.45 |
| 1:O:4:ALA:HB3 | 1:O:20:PHE:HB2 | 1.99 | 0.45 |
| 1:Q:79:ARG:HD2 | 1:Q:80:HIS:O | 2.17 | 0.44 |
| 1:S:126:LEU:HB2 | 1:S:128:LYS:HE3 | 1.99 | 0.44 |
| 1:N:92:ASP:OD2 | 5:N:2053:HOH:O | 2.21 | 0.44 |
| 5:J:2132:HOH:O | 1:S:91:LYS:CG | 2.52 | 0.43 |
| 1:G:4:ALA:HB3 | 1:G:20:PHE:HB2 | 2.00 | 0.43 |
| 1:N:79:ARG:HD3 | 1:N:80:HIS:O | 2.17 | 0.43 |
| 1:E:8:LEU:HD12 | 1:E:8:LEU:N | 2.33 | 0.43 |
| 1:B:2:THR:CG2 | 5:B:2032:HOH:O | 2.65 | 0.43 |
| 1:S:64:PHE:CE1 | 1:S:66:PRO:HD3 | 2.53 | 0.43 |
| 1:H:121:GLU:HA | 1:H:144:LEU:HD11 | 2.00 | 0.43 |
| 1:D:121:GLU:HA | 1:D:144:LEU:HD11 | 1.99 | 0.43 |
| 1:Q:94:VAL:CG2 | 5:Q:2049:HOH:O | 2.61 | 0.43 |
| 1:O:81:VAL:HG23 | 5:O:2025:HOH:O | 2.18 | 0.43 |
| 1:G:2:THR:HG21 | 1:G:106:LEU:HB2 | 2.00 | 0.43 |
| 1:J:3:LYS:NZ | 1:S:92:ASP:CG | 2.70 | 0.43 |
| 1:A:24:GLU:OE1 | 1:A:24:GLU:HA | 2.18 | 0.43 |
| 1:I:2:THR:HG21 | 1:I:106:LEU:HB2 | 2.00 | 0.43 |
| 1:C:69:ARG:NH1 | 1:C:77:GLU:OE2 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:I:122:LYS:NZ | 5:N:2022:HOH:O | 2.48 | 0.43 |
| 1:G:2:THR:CG2 | 1:G:106:LEU:HB2 | 2.49 | 0.42 |
| 1:M:121:GLU:HA | 1:M:144:LEU:HD11 | 2.00 | 0.42 |
| 1:E:121:GLU:HA | 1:E:144:LEU:HD11 | 2.01 | 0.42 |
| 1:N:65:ASN:CG | 1:N:80:HIS:CD2 | 2.92 | 0.42 |
| 1:G:22:GLN:HB2 | 1:G:29:VAL:HG22 | 2.01 | 0.42 |
| 1:Q:92:ASP:HB3 | 1:Q:94:VAL:H | 1.85 | 0.42 |
| 1:E:38:LEU:O | 1:E:93:GLY:HA2 | 2.19 | 0.42 |
| 1:G:36:LYS:HE3 | 5:L:2006:HOH:O | 2.20 | 0.42 |
| 1:M:8:LEU:N | 1:M:8:LEU:HD12 | 2.35 | 0.42 |
| 1:L:70:LYS:CD | 5:L:2056:HOH:O | 2.67 | 0.42 |
| 1:G:8:LEU:N | 1:G:8:LEU:HD22 | 2.35 | 0.42 |
| 1:O:138:GLY:O | 1:O:139:ASN:HB2 | 2.20 | 0.42 |
| 1:B:38:LEU:O | 1:B:93:GLY:HA2 | 2.20 | 0.42 |
| 1:O:21:GLU:HG3 | 1:O:32:TRP:CH2 | 2.54 | 0.41 |
| 1:P:2:THR:HG23 | 1:P:22:GLN:HB3 | 2.02 | 0.41 |
| 1:M:52:ASP:O | 1:M:59:SER:HB2 | 2.20 | 0.41 |
| 1:L:70:LYS:HD3 | 5:L:2056:HOH:O | 2.18 | 0.41 |
| 1:I:2:THR:CG2 | 1:I:106:LEU:HB2 | 2.50 | 0.41 |
| 1:S:22:GLN:HB2 | 1:S:29:VAL:HG22 | 2.03 | 0.41 |
| 1:C:77:GLU:HA | 1:C:77:GLU:OE1 | 2.21 | 0.41 |
| 1:Q:5:VAL:HG22 | 1:Q:6:CYS:N | 2.36 | 0.41 |
| 1:B:18:ILE:CG2 | 1:B:31:VAL:HG23 | 2.50 | 0.41 |
| 1:P:109:ASP:N | 1:P:109:ASP:OD2 | 2.54 | 0.41 |
| 1:L:71:HIS:HB2 | 1:L:80:HIS:CE1 | 2.55 | 0.41 |
| 1:L:128:LYS:HE3 | 5:L:2091:HOH:O | 2.20 | 0.41 |
| 1:P:3:LYS:HG2 | 1:P:21:GLU:HG3 | 2.03 | 0.40 |
| 1:F:77:GLU:OE1 | 1:F:77:GLU:C | 2.59 | 0.40 |
| 1:B:71:HIS:HB2 | 1:B:80:HIS:CE1 | 2.55 | 0.40 |
| 1:P:121:GLU:HA | 1:P:144:LEU:HD11 | 2.03 | 0.40 |
| 1:P:121:GLU:HB2 | 1:P:142:SER:OG | 2.21 | 0.40 |
| 1:C:128:LYS:HE3 | 5:C:2081:HOH:O | 2.21 | 0.40 |
| 1:I:2:THR:HG23 | 1:I:106:LEU:HD12 | 2.03 | 0.40 |
| 1:K:121:GLU:HG2 | 1:K:122:LYS:HG3 | 2.04 | 0.40 |
| 1:Q:109:ASP:C | 1:Q:109:ASP:OD2 | 2.59 | 0.40 |
| 1:N:67:LEU:N | 1:N:67:LEU:HD23 | 2.36 | 0.40 |
| 1:Q:109:ASP:OD2 | 1:Q:110:HIS:HD2 | 2.04 | 0.40 |
| 1:G:64:PHE:CE1 | 1:G:66:PRO:HG3 | 2.56 | 0.40 |

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:M:54:THR:O | 1:S:132:GLU:OE2[1_456] | 1.86 | 0.34 |
| 1:B:122:LYS:NZ | 1:M:40:GLU:OE2[2_546] | 1.92 | 0.28 |
| 5:C:2120:HOH:O | 5:H:2064:HOH:O[1_554] | 2.06 | 0.14 |

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | A | 151/153 (99%) | 150 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | B | 151/153 (99%) | 150 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | C | 151/153 (99%) | 150 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | D | 151/153 (99%) | 149 (99%) | 2 (1%) | 0 | 100 100 |
| 1 | E | 147/153 (96%) | 146 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | F | 141/153 (92%) | 140 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | G | 151/153 (99%) | 146 (97%) | 4 (3%) | 1 (1%) | 26 11 |
| 1 | H | 151/153 (99%) | 149 (99%) | 2 (1%) | 0 | 100 100 |
| 1 | I | 151/153 (99%) | 148 (98%) | 3 (2%) | 0 | 100 100 |
| 1 | J | 151/153 (99%) | 150 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | K | 151/153 (99%) | 146 (97%) | 5 (3%) | 0 | 100 100 |
| 1 | L | 150/153 (98%) | 149 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | M | 149/153 (97%) | 148 (99%) | 1 (1%) | 0 | 100 100 |
| 1 | N | 151/153 (99%) | 151 (100%) | 0 | 0 | 100 100 |
| 1 | O | 151/153 (99%) | 146 (97%) | 3 (2%) | 2 (1%) | 15 4 |
| 1 | P | 150/153 (98%) | 147 (98%) | 3 (2%) | 0 | 100 100 |
| 1 | Q | 151/153 (99%) | 146 (97%) | 4 (3%) | 1 (1%) | 26 11 |
| 1 | S | 151/153 (99%) | 145 (96%) | 6 (4%) | 0 | 100 100 |
| All | All | 2700/2754 (98%) | 2656 (98%) | 40 (2%) | 4 (0%) | 56 38 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 131 | ASN |
| 1 | O | 25 | SER |
| 1 | O | 26 | ASN |
| 1 | Q | 2 | THR |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | A | 118/118 (100%) | 112 (95%) | 6 (5%) | 29 12 |
| 1 | B | 118/118 (100%) | 113 (96%) | 5 (4%) | 36 18 |
| 1 | C | 117/118 (99%) | 117 (100%) | 0 | 100 100 |
| 1 | D | 111/118 (94%) | 108 (97%) | 3 (3%) | 52 36 |
| 1 | E | 108/118 (92%) | 106 (98%) | 2 (2%) | 65 52 |
| 1 | F | 107/118 (91%) | 101 (94%) | 6 (6%) | 26 10 |
| 1 | G | 118/118 (100%) | 109 (92%) | 9 (8%) | 16 5 |
| 1 | H | 118/118 (100%) | 116 (98%) | 2 (2%) | 68 57 |
| 1 | I | 118/118 (100%) | 115 (98%) | 3 (2%) | 55 39 |
| 1 | J | 114/118 (97%) | 112 (98%) | 2 (2%) | 66 54 |
| 1 | K | 116/118 (98%) | 113 (97%) | 3 (3%) | 54 37 |
| 1 | L | 114/118 (97%) | 112 (98%) | 2 (2%) | 66 54 |
| 1 | M | 108/118 (92%) | 105 (97%) | 3 (3%) | 51 35 |
| 1 | N | 118/118 (100%) | 114 (97%) | 4 (3%) | 44 26 |
| 1 | O | 118/118 (100%) | 107 (91%) | 11 (9%) | 11 3 |
| 1 | P | 115/118 (98%) | 110 (96%) | 5 (4%) | 35 17 |
| 1 | Q | 118/118 (100%) | 109 (92%) | 9 (8%) | 16 5 |
| 1 | S | 117/118 (99%) | 114 (97%) | 3 (3%) | 54 37 |
| All | All | 2071/2124 (98%) | 1993 (96%) | 78 (4%) | 40 22 |

All (78) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 2 | THR |
| 1 | A | 8 | LEU |
| 1 | A | 25 | SER |
| 1 | A | 26 | ASN |
| 1 | A | 42 | LEU |
| 1 | A | 59 | SER |
| 1 | B | 2 | THR |
| 1 | B | 15 | GLN |
| 1 | B | 26 | ASN |
| 1 | B | 42 | LEU |
| 1 | B | 109 | ASP |
| 1 | D | 42 | LEU |
| 1 | D | 79 | ARG |
| 1 | D | 91 | LYS |
| 1 | E | 2 | THR |
| 1 | E | 25 | SER |
| 1 | F | 8 | LEU |
| 1 | F | 31 | VAL |
| 1 | F | 42 | LEU |
| 1 | F | 79 | ARG |
| 1 | F | 91 | LYS |
| 1 | F | 109 | ASP |
| 1 | G | 2 | THR |
| 1 | G | 26 | ASN |
| 1 | G | 31 | VAL |
| 1 | G | 42 | LEU |
| 1 | G | 59 | SER |
| 1 | G | 100 | GLU |
| 1 | G | 109 | ASP |
| 1 | G | 132 | GLU |
| 1 | G | 142 | SER |
| 1 | H | 2 | THR |
| 1 | H | 24 | GLU |
| 1 | I | 69 | ARG |
| 1 | I | 91 | LYS |
| 1 | I | 132 | GLU |
| 1 | J | 91 | LYS |
| 1 | J | 122 | LYS |
| 1 | K | 2 | THR |
| 1 | K | 25 | SER |
| 1 | K | 91 | LYS |
| 1 | L | 2 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | L | 31 | VAL |
| 1 | M | 31 | VAL |
| 1 | M | 69 | ARG |
| 1 | M | 91 | LYS |
| 1 | N | 69 | ARG |
| 1 | N | 75 | LYS |
| 1 | N | 79 | ARG |
| 1 | N | 91 | LYS |
| 1 | O | 8 | LEU |
| 1 | O | 42 | LEU |
| 1 | O | 53 | ASN |
| 1 | O | 58 | THR |
| 1 | O | 76 | ASP |
| 1 | O | 79 | ARG |
| 1 | O | 91 | LYS |
| 1 | O | 102 | SER |
| 1 | O | 109 | ASP |
| 1 | O | 128 | LYS |
| 1 | O | 136 | LYS |
| 1 | P | 2 | THR |
| 1 | P | 8 | LEU |
| 1 | P | 26 | ASN |
| 1 | P | 42 | LEU |
| 1 | P | 109 | ASP |
| 1 | Q | 2 | THR |
| 1 | Q | 24 | GLU |
| 1 | Q | 31 | VAL |
| 1 | Q | 34 | SER |
| 1 | Q | 69 | ARG |
| 1 | Q | 77 | GLU |
| 1 | Q | 79 | ARG |
| 1 | Q | 90 | ASP |
| 1 | Q | 92 | ASP |
| 1 | S | 2 | THR |
| 1 | S | 24 | GLU |
| 1 | S | 142 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 26 | ASN |
| 1 | G | 15 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 65 | ASN |
| 1 | G | 139 | ASN |
| 1 | H | 15 | GLN |
| 1 | J | 15 | GLN |
| 1 | J | 53 | ASN |
| 1 | M | 53 | ASN |
| 1 | O | 15 | GLN |
| 1 | Q | 53 | ASN |
| 1 | Q | 110 | HIS |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates

There are no carbohydrates in this entry.

### 5.6 Ligand geometry

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

# 6 Fit of model and data

## 6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, $95^{th}$ 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 | 153/153 (100%) | 0.40 | 10 (6%) 22 18 | 6, 11, 22, 33 | 0 |
| 1 | B | 153/153 (100%) | 0.33 | 10 (6%) 22 18 | 5, 7, 19, 29 | 0 |
| 1 | C | 153/153 (100%) | 0.25 | 12 (7%) 16 12 | 5, 6, 19, 25 | 0 |
| 1 | D | 153/153 (100%) | 0.34 | 11 (7%) 18 14 | 5, 12, 20, 26 | 0 |
| 1 | E | 151/153 (98%) | 0.24 | 7 (4%) 36 30 | 6, 11, 19, 29 | 0 |
| 1 | F | 145/153 (94%) | 0.38 | 12 (8%) 14 11 | 10, 15, 24, 33 | 0 |
| 1 | G | 153/153 (100%) | 1.29 | 35 (22%) 1 1 | 15, 21, 35, 42 | 0 |
| 1 | H | 153/153 (100%) | 0.36 | 10 (6%) 22 18 | 7, 11, 21, 28 | 0 |
| 1 | I | 153/153 (100%) | 0.28 | 11 (7%) 18 14 | 5, 8, 18, 22 | 0 |
| 1 | J | 153/153 (100%) | 0.22 | 7 (4%) 36 30 | 5, 7, 16, 24 | 0 |
| 1 | K | 153/153 (100%) | 0.21 | 8 (5%) 31 25 | 5, 7, 16, 26 | 0 |
| 1 | L | 152/153 (99%) | 0.32 | 10 (6%) 22 17 | 8, 13, 22, 29 | 0 |
| 1 | M | 152/153 (99%) | 0.42 | 15 (9%) 9 7 | 5, 11, 22, 32 | 0 |
| 1 | N | 153/153 (100%) | 0.68 | 21 (13%) 4 3 | 6, 14, 25, 31 | 1 (0%) |
| 1 | O | 153/153 (100%) | 1.33 | 39 (25%) 1 0 | 15, 21, 34, 40 | 0 |
| 1 | P | 153/153 (100%) | 5.28 | 145 (94%) 0 0 | 50, 62, 66, 69 | 0 |
| 1 | Q | 153/153 (100%) | 0.75 | 20 (13%) 5 3 | 5, 14, 26, 36 | 0 |
| 1 | S | 153/153 (100%) | 2.81 | 96 (62%) 0 0 | 25, 35, 47, 52 | 0 |
| All | All | 2742/2754 (99%) | 0.89 | 479 (17%) 2 1 | 5, 13, 54, 69 | 1 (0%) |

All (479) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | S | 1 | ALA | 11.5 |
| 1 | G | 1 | ALA | 11.5 |
| 1 | P | 42 | LEU | 10.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 76 | ASP | 10.2 |
| 1 | P | 67 | LEU | 10.0 |
| 1 | P | 50 | PHE | 9.9 |
| 1 | P | 92 | ASP | 9.8 |
| 1 | P | 135 | THR | 9.8 |
| 1 | P | 12 | GLY | 9.6 |
| 1 | P | 55 | ALA | 9.4 |
| 1 | P | 129 | GLY | 9.3 |
| 1 | P | 75 | LYS | 9.0 |
| 1 | P | 110 | HIS | 8.9 |
| 1 | P | 26 | ASN | 8.9 |
| 1 | P | 89 | ALA | 8.9 |
| 1 | P | 122 | LYS | 8.8 |
| 1 | P | 25 | SER | 8.8 |
| 1 | P | 123 | ALA | 8.8 |
| 1 | P | 108 | GLY | 8.5 |
| 1 | K | 1 | ALA | 8.4 |
| 1 | P | 87 | VAL | 8.3 |
| 1 | P | 130 | GLY | 8.1 |
| 1 | P | 45 | PHE | 7.8 |
| 1 | P | 13 | PRO | 7.7 |
| 1 | P | 140 | ALA | 7.7 |
| 1 | I | 1 | ALA | 7.6 |
| 1 | P | 134 | SER | 7.6 |
| 1 | P | 57 | CYS | 7.6 |
| 1 | P | 88 | THR | 7.5 |
| 1 | P | 58 | THR | 7.4 |
| 1 | P | 94 | VAL | 7.4 |
| 1 | P | 80 | HIS | 7.4 |
| 1 | P | 93 | GLY | 7.4 |
| 1 | P | 84 | LEU | 7.3 |
| 1 | P | 31 | VAL | 7.3 |
| 1 | P | 139 | ASN | 7.2 |
| 1 | P | 143 | ARG | 7.0 |
| 1 | N | 1 | ALA | 7.0 |
| 1 | P | 133 | GLU | 6.8 |
| 1 | P | 90 | ASP | 6.8 |
| 1 | P | 107 | SER | 6.8 |
| 1 | P | 35 | ILE | 6.7 |
| 1 | P | 29 | VAL | 6.7 |
| 1 | P | 101 | ASP | 6.7 |
| 1 | G | 27 | GLY | 6.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 126 | LEU | 6.6 |
| 1 | P | 118 | VAL | 6.6 |
| 1 | P | 128 | LYS | 6.5 |
| 1 | P | 71 | HIS | 6.5 |
| 1 | P | 23 | LYS | 6.5 |
| 1 | S | 54 | THR | 6.5 |
| 1 | P | 74 | PRO | 6.5 |
| 1 | P | 131 | ASN | 6.4 |
| 1 | P | 24 | GLU | 6.4 |
| 1 | P | 68 | SER | 6.4 |
| 1 | S | 25 | SER | 6.4 |
| 1 | P | 79 | ARG | 6.4 |
| 1 | S | 27 | GLY | 6.3 |
| 1 | P | 116 | THR | 6.3 |
| 1 | P | 77 | GLU | 6.3 |
| 1 | P | 1 | ALA | 6.3 |
| 1 | P | 144 | LEU | 6.2 |
| 1 | P | 78 | GLU | 6.2 |
| 1 | P | 70 | LYS | 6.2 |
| 1 | P | 119 | VAL | 6.2 |
| 1 | P | 91 | LYS | 6.1 |
| 1 | P | 142 | SER | 6.1 |
| 1 | S | 50 | PHE | 6.1 |
| 1 | O | 109 | ASP | 6.1 |
| 1 | P | 103 | VAL | 6.1 |
| 1 | S | 109 | ASP | 6.1 |
| 1 | P | 14 | VAL | 6.0 |
| 1 | P | 38 | LEU | 6.0 |
| 1 | S | 24 | GLU | 5.9 |
| 1 | G | 26 | ASN | 5.9 |
| 1 | Q | 1 | ALA | 5.9 |
| 1 | P | 99 | ILE | 5.8 |
| 1 | P | 109 | ASP | 5.8 |
| 1 | S | 77 | GLU | 5.7 |
| 1 | P | 11 | ASP | 5.7 |
| 1 | P | 5 | VAL | 5.7 |
| 1 | P | 125 | ASP | 5.7 |
| 1 | P | 39 | THR | 5.7 |
| 1 | S | 107 | SER | 5.7 |
| 1 | B | 1 | ALA | 5.6 |
| 1 | P | 43 | HIS | 5.6 |
| 1 | P | 81 | VAL | 5.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 127 | GLY | 5.6 |
| 1 | P | 36 | LYS | 5.6 |
| 1 | P | 72 | GLY | 5.6 |
| 1 | P | 151 | ILE | 5.5 |
| 1 | O | 1 | ALA | 5.5 |
| 1 | P | 73 | GLY | 5.5 |
| 1 | P | 2 | THR | 5.5 |
| 1 | Q | 24 | GLU | 5.4 |
| 1 | S | 15 | GLN | 5.4 |
| 1 | S | 150 | GLY | 5.3 |
| 1 | P | 86 | ASN | 5.3 |
| 1 | P | 82 | GLY | 5.3 |
| 1 | G | 23 | LYS | 5.3 |
| 1 | P | 59 | SER | 5.3 |
| 1 | O | 25 | SER | 5.3 |
| 1 | S | 106 | LEU | 5.3 |
| 1 | S | 91 | LYS | 5.2 |
| 1 | S | 152 | ALA | 5.2 |
| 1 | P | 132 | GLU | 5.2 |
| 1 | P | 17 | ILE | 5.2 |
| 1 | S | 68 | SER | 5.2 |
| 1 | S | 90 | ASP | 5.2 |
| 1 | P | 32 | TRP | 5.2 |
| 1 | O | 2 | THR | 5.1 |
| 1 | C | 109 | ASP | 5.1 |
| 1 | P | 61 | GLY | 5.1 |
| 1 | S | 2 | THR | 5.1 |
| 1 | P | 136 | LYS | 5.0 |
| 1 | P | 65 | ASN | 5.0 |
| 1 | S | 26 | ASN | 5.0 |
| 1 | S | 7 | VAL | 5.0 |
| 1 | G | 28 | PRO | 5.0 |
| 1 | P | 41 | GLY | 4.9 |
| 1 | P | 54 | THR | 4.9 |
| 1 | P | 40 | GLU | 4.9 |
| 1 | P | 62 | PRO | 4.9 |
| 1 | A | 1 | ALA | 4.8 |
| 1 | S | 66 | PRO | 4.8 |
| 1 | P | 137 | THR | 4.8 |
| 1 | S | 117 | LEU | 4.7 |
| 1 | P | 121 | GLU | 4.7 |
| 1 | P | 152 | ALA | 4.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | S | 36 | LYS | 4.7 |
| 1 | P | 141 | GLY | 4.7 |
| 1 | S | 151 | ILE | 4.7 |
| 1 | S | 11 | ASP | 4.7 |
| 1 | C | 1 | ALA | 4.6 |
| 1 | D | 1 | ALA | 4.6 |
| 1 | G | 130 | GLY | 4.6 |
| 1 | S | 9 | LYS | 4.6 |
| 1 | P | 64 | PHE | 4.5 |
| 1 | S | 108 | GLY | 4.5 |
| 1 | P | 117 | LEU | 4.5 |
| 1 | P | 96 | ASP | 4.5 |
| 1 | J | 1 | ALA | 4.5 |
| 1 | P | 104 | ILE | 4.5 |
| 1 | P | 49 | GLU | 4.4 |
| 1 | S | 10 | GLY | 4.4 |
| 1 | Q | 109 | ASP | 4.4 |
| 1 | O | 108 | GLY | 4.4 |
| 1 | S | 58 | THR | 4.4 |
| 1 | S | 29 | VAL | 4.4 |
| 1 | P | 85 | GLY | 4.4 |
| 1 | S | 105 | SER | 4.3 |
| 1 | G | 131 | ASN | 4.3 |
| 1 | S | 18 | ILE | 4.3 |
| 1 | P | 111 | CYS | 4.2 |
| 1 | P | 146 | CYS | 4.2 |
| 1 | S | 13 | PRO | 4.2 |
| 1 | O | 31 | VAL | 4.2 |
| 1 | O | 26 | ASN | 4.2 |
| 1 | P | 153 | GLN | 4.2 |
| 1 | N | 117 | LEU | 4.2 |
| 1 | S | 75 | LYS | 4.2 |
| 1 | S | 37 | GLY | 4.2 |
| 1 | P | 47 | VAL | 4.1 |
| 1 | G | 75 | LYS | 4.1 |
| 1 | S | 17 | ILE | 4.1 |
| 1 | J | 117 | LEU | 4.1 |
| 1 | P | 3 | LYS | 4.1 |
| 1 | Q | 25 | SER | 4.1 |
| 1 | P | 53 | ASN | 4.0 |
| 1 | N | 45 | PHE | 4.0 |
| 1 | N | 26 | ASN | 4.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | Q | 26 | ASN | 4.0 |
| 1 | P | 124 | ASP | 4.0 |
| 1 | P | 15 | GLN | 4.0 |
| 1 | S | 12 | GLY | 4.0 |
| 1 | M | 26 | ASN | 4.0 |
| 1 | S | 98 | SER | 4.0 |
| 1 | P | 100 | GLU | 4.0 |
| 1 | Q | 108 | GLY | 3.9 |
| 1 | P | 28 | PRO | 3.9 |
| 1 | S | 23 | LYS | 3.9 |
| 1 | O | 27 | GLY | 3.9 |
| 1 | G | 67 | LEU | 3.8 |
| 1 | M | 117 | LEU | 3.8 |
| 1 | S | 126 | LEU | 3.8 |
| 1 | O | 110 | HIS | 3.8 |
| 1 | P | 20 | PHE | 3.8 |
| 1 | S | 81 | VAL | 3.8 |
| 1 | P | 9 | LYS | 3.8 |
| 1 | G | 77 | GLU | 3.8 |
| 1 | S | 96 | ASP | 3.7 |
| 1 | O | 69 | ARG | 3.7 |
| 1 | S | 69 | ARG | 3.7 |
| 1 | I | 109 | ASP | 3.7 |
| 1 | S | 153 | GLN | 3.7 |
| 1 | O | 107 | SER | 3.7 |
| 1 | S | 40 | GLU | 3.7 |
| 1 | S | 28 | PRO | 3.7 |
| 1 | I | 117 | LEU | 3.7 |
| 1 | M | 45 | PHE | 3.6 |
| 1 | S | 30 | LYS | 3.6 |
| 1 | F | 67 | LEU | 3.6 |
| 1 | P | 21 | GLU | 3.6 |
| 1 | S | 94 | VAL | 3.6 |
| 1 | S | 32 | TRP | 3.6 |
| 1 | G | 127 | GLY | 3.6 |
| 1 | S | 146 | CYS | 3.6 |
| 1 | F | 91 | LYS | 3.6 |
| 1 | O | 70 | LYS | 3.6 |
| 1 | P | 149 | ILE | 3.6 |
| 1 | F | 109 | ASP | 3.6 |
| 1 | H | 117 | LEU | 3.5 |
| 1 | Q | 77 | GLU | 3.5 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 66 | PRO | 3.5 |
| 1 | S | 55 | ALA | 3.5 |
| 1 | H | 84 | LEU | 3.5 |
| 1 | K | 26 | ASN | 3.5 |
| 1 | A | 24 | GLU | 3.5 |
| 1 | P | 27 | GLY | 3.5 |
| 1 | P | 34 | SER | 3.5 |
| 1 | J | 47 | VAL | 3.4 |
| 1 | O | 102 | SER | 3.4 |
| 1 | G | 135 | THR | 3.4 |
| 1 | O | 66 | PRO | 3.4 |
| 1 | E | 1 | ALA | 3.4 |
| 1 | G | 72 | GLY | 3.4 |
| 1 | S | 144 | LEU | 3.4 |
| 1 | G | 24 | GLU | 3.4 |
| 1 | O | 23 | LYS | 3.4 |
| 1 | S | 39 | THR | 3.4 |
| 1 | P | 69 | ARG | 3.4 |
| 1 | C | 117 | LEU | 3.4 |
| 1 | P | 44 | GLY | 3.4 |
| 1 | P | 52 | ASP | 3.4 |
| 1 | L | 117 | LEU | 3.3 |
| 1 | Q | 47 | VAL | 3.3 |
| 1 | S | 14 | VAL | 3.3 |
| 1 | O | 28 | PRO | 3.3 |
| 1 | E | 45 | PHE | 3.3 |
| 1 | S | 113 | ILE | 3.3 |
| 1 | P | 145 | ALA | 3.3 |
| 1 | I | 45 | PHE | 3.3 |
| 1 | K | 117 | LEU | 3.3 |
| 1 | P | 60 | ALA | 3.3 |
| 1 | N | 25 | SER | 3.3 |
| 1 | P | 95 | ALA | 3.2 |
| 1 | S | 41 | GLY | 3.2 |
| 1 | P | 106 | LEU | 3.2 |
| 1 | N | 77 | GLU | 3.2 |
| 1 | G | 25 | SER | 3.2 |
| 1 | B | 109 | ASP | 3.2 |
| 1 | S | 129 | GLY | 3.2 |
| 1 | G | 29 | VAL | 3.2 |
| 1 | P | 97 | VAL | 3.2 |
| 1 | D | 45 | PHE | 3.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | N | 24 | GLU | 3.2 |
| 1 | A | 45 | PHE | 3.1 |
| 1 | S | 149 | ILE | 3.1 |
| 1 | N | 109 | ASP | 3.1 |
| 1 | S | 19 | ASN | 3.1 |
| 1 | E | 117 | LEU | 3.1 |
| 1 | Q | 117 | LEU | 3.1 |
| 1 | S | 128 | LYS | 3.1 |
| 1 | S | 57 | CYS | 3.1 |
| 1 | B | 24 | GLU | 3.1 |
| 1 | I | 47 | VAL | 3.1 |
| 1 | S | 100 | GLU | 3.0 |
| 1 | O | 131 | ASN | 3.0 |
| 1 | A | 25 | SER | 3.0 |
| 1 | A | 84 | LEU | 3.0 |
| 1 | B | 45 | PHE | 3.0 |
| 1 | P | 51 | GLY | 3.0 |
| 1 | O | 137 | THR | 3.0 |
| 1 | S | 92 | ASP | 3.0 |
| 1 | G | 132 | GLU | 3.0 |
| 1 | D | 117 | LEU | 3.0 |
| 1 | D | 47 | VAL | 2.9 |
| 1 | O | 77 | GLU | 2.9 |
| 1 | A | 109 | ASP | 2.9 |
| 1 | G | 102 | SER | 2.9 |
| 1 | P | 120 | HIS | 2.9 |
| 1 | S | 137 | THR | 2.9 |
| 1 | G | 78 | GLU | 2.9 |
| 1 | M | 23 | LYS | 2.9 |
| 1 | S | 76 | ASP | 2.9 |
| 1 | D | 77 | GLU | 2.9 |
| 1 | P | 105 | SER | 2.9 |
| 1 | H | 45 | PHE | 2.9 |
| 1 | L | 45 | PHE | 2.9 |
| 1 | P | 19 | ASN | 2.9 |
| 1 | B | 84 | LEU | 2.9 |
| 1 | L | 47 | VAL | 2.9 |
| 1 | M | 47 | VAL | 2.9 |
| 1 | S | 132 | GLU | 2.8 |
| 1 | A | 91 | LYS | 2.8 |
| 1 | S | 110 | HIS | 2.8 |
| 1 | L | 26 | ASN | 2.8 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 37 | GLY | 2.8 |
| 1 | S | 22 | GLN | 2.8 |
| 1 | S | 78 | GLU | 2.8 |
| 1 | G | 109 | ASP | 2.8 |
| 1 | Q | 153 | GLN | 2.8 |
| 1 | S | 51 | GLY | 2.8 |
| 1 | G | 66 | PRO | 2.8 |
| 1 | O | 24 | GLU | 2.8 |
| 1 | G | 148 | VAL | 2.8 |
| 1 | O | 118 | VAL | 2.8 |
| 1 | Q | 118 | VAL | 2.8 |
| 1 | M | 109 | ASP | 2.8 |
| 1 | S | 52 | ASP | 2.7 |
| 1 | P | 22 | GLN | 2.7 |
| 1 | O | 68 | SER | 2.7 |
| 1 | S | 65 | ASN | 2.7 |
| 1 | P | 63 | HIS | 2.7 |
| 1 | S | 136 | LYS | 2.7 |
| 1 | I | 118 | VAL | 2.7 |
| 1 | D | 68 | SER | 2.7 |
| 1 | G | 21 | GLU | 2.7 |
| 1 | G | 71 | HIS | 2.7 |
| 1 | G | 110 | HIS | 2.7 |
| 1 | N | 23 | LYS | 2.7 |
| 1 | Q | 2 | THR | 2.7 |
| 1 | C | 26 | ASN | 2.7 |
| 1 | B | 119 | VAL | 2.7 |
| 1 | N | 119 | VAL | 2.7 |
| 1 | O | 135 | THR | 2.7 |
| 1 | S | 64 | PHE | 2.7 |
| 1 | E | 84 | LEU | 2.7 |
| 1 | M | 25 | SER | 2.7 |
| 1 | P | 98 | SER | 2.7 |
| 1 | C | 118 | VAL | 2.7 |
| 1 | I | 148 | VAL | 2.7 |
| 1 | O | 103 | VAL | 2.7 |
| 1 | P | 148 | VAL | 2.7 |
| 1 | P | 115 | ARG | 2.7 |
| 1 | K | 45 | PHE | 2.7 |
| 1 | H | 47 | VAL | 2.6 |
| 1 | S | 47 | VAL | 2.6 |
| 1 | G | 117 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | P | 30 | LYS | 2.6 |
| 1 | S | 20 | PHE | 2.6 |
| 1 | K | 118 | VAL | 2.6 |
| 1 | N | 118 | VAL | 2.6 |
| 1 | F | 92 | ASP | 2.6 |
| 1 | S | 95 | ALA | 2.6 |
| 1 | D | 118 | VAL | 2.6 |
| 1 | S | 3 | LYS | 2.6 |
| 1 | Q | 107 | SER | 2.6 |
| 1 | D | 109 | ASP | 2.6 |
| 1 | C | 119 | VAL | 2.6 |
| 1 | N | 47 | VAL | 2.6 |
| 1 | P | 7 | VAL | 2.6 |
| 1 | M | 68 | SER | 2.6 |
| 1 | S | 80 | HIS | 2.6 |
| 1 | G | 137 | THR | 2.6 |
| 1 | E | 26 | ASN | 2.5 |
| 1 | Q | 67 | LEU | 2.5 |
| 1 | G | 136 | LYS | 2.5 |
| 1 | P | 10 | GLY | 2.5 |
| 1 | J | 45 | PHE | 2.5 |
| 1 | G | 107 | SER | 2.5 |
| 1 | P | 18 | ILE | 2.5 |
| 1 | S | 62 | PRO | 2.5 |
| 1 | N | 110 | HIS | 2.5 |
| 1 | O | 117 | LEU | 2.5 |
| 1 | P | 48 | HIS | 2.5 |
| 1 | S | 111 | CYS | 2.5 |
| 1 | F | 104 | ILE | 2.5 |
| 1 | O | 104 | ILE | 2.5 |
| 1 | M | 107 | SER | 2.5 |
| 1 | S | 59 | SER | 2.5 |
| 1 | N | 84 | LEU | 2.5 |
| 1 | N | 91 | LYS | 2.5 |
| 1 | P | 138 | GLY | 2.5 |
| 1 | F | 117 | LEU | 2.5 |
| 1 | S | 38 | LEU | 2.5 |
| 1 | L | 118 | VAL | 2.4 |
| 1 | G | 30 | LYS | 2.4 |
| 1 | S | 60 | ALA | 2.4 |
| 1 | S | 114 | GLY | 2.4 |
| 1 | G | 69 | ARG | 2.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | Q | 28 | PRO | 2.4 |
| 1 | G | 68 | SER | 2.4 |
| 1 | O | 20 | PHE | 2.4 |
| 1 | K | 47 | VAL | 2.4 |
| 1 | Q | 23 | LYS | 2.4 |
| 1 | P | 102 | SER | 2.4 |
| 1 | L | 92 | ASP | 2.4 |
| 1 | P | 56 | GLY | 2.4 |
| 1 | C | 77 | GLU | 2.4 |
| 1 | A | 117 | LEU | 2.4 |
| 1 | O | 136 | LYS | 2.4 |
| 1 | P | 112 | ILE | 2.4 |
| 1 | O | 75 | LYS | 2.4 |
| 1 | C | 47 | VAL | 2.4 |
| 1 | I | 119 | VAL | 2.4 |
| 1 | S | 88 | THR | 2.4 |
| 1 | O | 22 | GLN | 2.3 |
| 1 | M | 132 | GLU | 2.3 |
| 1 | J | 84 | LEU | 2.3 |
| 1 | K | 84 | LEU | 2.3 |
| 1 | S | 4 | ALA | 2.3 |
| 1 | D | 91 | LYS | 2.3 |
| 1 | S | 118 | VAL | 2.3 |
| 1 | H | 11 | ASP | 2.3 |
| 1 | H | 55 | ALA | 2.3 |
| 1 | C | 24 | GLU | 2.3 |
| 1 | M | 77 | GLU | 2.3 |
| 1 | A | 26 | ASN | 2.3 |
| 1 | B | 26 | ASN | 2.3 |
| 1 | O | 45 | PHE | 2.3 |
| 1 | J | 149 | ILE | 2.3 |
| 1 | S | 99 | ILE | 2.3 |
| 1 | I | 84 | LEU | 2.3 |
| 1 | H | 91 | LYS | 2.3 |
| 1 | O | 105 | SER | 2.3 |
| 1 | O | 91 | LYS | 2.3 |
| 1 | O | 130 | GLY | 2.3 |
| 1 | Q | 21 | GLU | 2.2 |
| 1 | F | 118 | VAL | 2.2 |
| 1 | G | 2 | THR | 2.2 |
| 1 | B | 117 | LEU | 2.2 |
| 1 | S | 82 | GLY | 2.2 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 45 | PHE | 2.2 |
| 1 | L | 91 | LYS | 2.2 |
| 1 | O | 153 | GLN | 2.2 |
| 1 | O | 67 | LEU | 2.2 |
| 1 | E | 47 | VAL | 2.2 |
| 1 | M | 87 | VAL | 2.2 |
| 1 | S | 85 | GLY | 2.2 |
| 1 | L | 23 | LYS | 2.2 |
| 1 | S | 8 | LEU | 2.2 |
| 1 | K | 24 | GLU | 2.2 |
| 1 | N | 153 | GLN | 2.2 |
| 1 | N | 87 | VAL | 2.2 |
| 1 | M | 27 | GLY | 2.2 |
| 1 | L | 109 | ASP | 2.2 |
| 1 | Q | 68 | SER | 2.2 |
| 1 | F | 108 | GLY | 2.1 |
| 1 | I | 147 | GLY | 2.1 |
| 1 | D | 149 | ILE | 2.1 |
| 1 | N | 69 | ARG | 2.1 |
| 1 | C | 84 | LEU | 2.1 |
| 1 | G | 106 | LEU | 2.1 |
| 1 | I | 8 | LEU | 2.1 |
| 1 | B | 118 | VAL | 2.1 |
| 1 | J | 118 | VAL | 2.1 |
| 1 | P | 46 | HIS | 2.1 |
| 1 | M | 91 | LYS | 2.1 |
| 1 | F | 107 | SER | 2.1 |
| 1 | H | 99 | ILE | 2.1 |
| 1 | S | 102 | SER | 2.1 |
| 1 | S | 112 | ILE | 2.1 |
| 1 | Q | 92 | ASP | 2.1 |
| 1 | D | 84 | LEU | 2.1 |
| 1 | E | 118 | VAL | 2.1 |
| 1 | B | 91 | LYS | 2.1 |
| 1 | M | 97 | VAL | 2.1 |
| 1 | A | 149 | ILE | 2.1 |
| 1 | S | 67 | LEU | 2.1 |
| 1 | F | 47 | VAL | 2.1 |
| 1 | S | 97 | VAL | 2.1 |
| 1 | F | 28 | PRO | 2.1 |
| 1 | C | 149 | ILE | 2.0 |
| 1 | N | 35 | ILE | 2.0 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | Q | 45 | PHE | 2.0 |
| 1 | S | 6 | CYS | 2.0 |
| 1 | O | 29 | VAL | 2.0 |
| 1 | N | 28 | PRO | 2.0 |
| 1 | H | 18 | ILE | 2.0 |
| 1 | G | 3 | LYS | 2.0 |
| 1 | O | 3 | LYS | 2.0 |
| 1 | O | 106 | LEU | 2.0 |
| 1 | P | 147 | GLY | 2.0 |
| 1 | F | 153 | GLN | 2.0 |
| 1 | N | 31 | VAL | 2.0 |
| 1 | H | 85 | GLY | 2.0 |
| 1 | L | 90 | ASP | 2.0 |
| 1 | P | 33 | GLY | 2.0 |

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

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

## 6.3 Carbohydrates (i)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, $95^{th}$ 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 | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 4 | CA | D | 156 | 1/1 | 0.95 | 0.14 | -0.01 | 47,47,47,47 | 0 |
| 3 | ZN | K | 155 | 1/1 | 1.00 | 0.10 | -0.21 | 5,5,5,5 | 0 |
| 3 | ZN | A | 155 | 1/1 | 0.99 | 0.09 | -0.56 | 8,8,8,8 | 0 |
| 3 | ZN | E | 155 | 1/1 | 0.99 | 0.08 | -0.87 | 8,8,8,8 | 0 |
| 3 | ZN | Q | 155 | 1/1 | 0.99 | 0.09 | -0.89 | 12,12,12,12 | 0 |
| 3 | ZN | B | 155 | 1/1 | 1.00 | 0.09 | -1.10 | 5,5,5,5 | 0 |
| 3 | ZN | C | 155 | 1/1 | 0.99 | 0.07 | -1.12 | 5,5,5,5 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 3 | ZN | H | 155 | 1/1 | 0.96 | 0.05 | -1.29 | 10,10,10,10 | 0 |
| 3 | ZN | I | 155 | 1/1 | 0.99 | 0.07 | -1.51 | 7,7,7,7 | 0 |
| 3 | ZN | P | 155 | 1/1 | 0.46 | 0.14 | -1.78 | 61,61,61,61 | 0 |
| 3 | ZN | J | 155 | 1/1 | 0.99 | 0.07 | -1.99 | 6,6,6,6 | 0 |
| 3 | ZN | D | 155 | 1/1 | 0.99 | 0.07 | -2.00 | 10,10,10,10 | 0 |
| 3 | ZN | M | 155 | 1/1 | 0.99 | 0.05 | -2.00 | 9,9,9,9 | 0 |
| 3 | ZN | S | 155 | 1/1 | 0.99 | 0.06 | -2.06 | 27,27,27,27 | 0 |
| 3 | ZN | N | 155 | 1/1 | 0.93 | 0.06 | -2.22 | 11,11,11,11 | 0 |
| 3 | ZN | F | 155 | 1/1 | 0.97 | 0.06 | -2.30 | 12,12,12,12 | 0 |
| 3 | ZN | G | 155 | 1/1 | 0.90 | 0.07 | -2.34 | 20,20,20,20 | 0 |
| 3 | ZN | O | 155 | 1/1 | 0.98 | 0.04 | -2.35 | 18,18,18,18 | 0 |
| 3 | ZN | L | 155 | 1/1 | 0.99 | 0.09 | -2.58 | 9,9,9,9 | 0 |
| 2 | CU | F | 154 | 1/1 | 0.97 | 0.09 | - | 22,22,22,22 | 0 |
| 2 | CU | Q | 154 | 1/1 | 0.92 | 0.14 | - | 22,22,22,22 | 0 |
| 2 | CU | C | 154 | 1/1 | 0.97 | 0.09 | - | 16,16,16,16 | 0 |
| 2 | CU | O | 154 | 1/1 | 0.96 | 0.04 | - | 29,29,29,29 | 0 |
| 2 | CU | I | 154 | 1/1 | 0.98 | 0.11 | - | 17,17,17,17 | 0 |
| 4 | CA | O | 156 | 1/1 | 0.97 | 0.15 | - | 44,44,44,44 | 0 |
| 4 | CA | C | 156 | 1/1 | 0.95 | 0.23 | - | 37,37,37,37 | 1 |
| 2 | CU | G | 154 | 1/1 | 0.91 | 0.09 | - | 27,27,27,27 | 0 |
| 2 | CU | A | 154 | 1/1 | 0.97 | 0.10 | - | 17,17,17,17 | 0 |
| 2 | CU | L | 154 | 1/1 | 0.98 | 0.15 | - | 22,22,22,22 | 0 |
| 2 | CU | E | 154 | 1/1 | 0.98 | 0.12 | - | 20,20,20,20 | 0 |
| 2 | CU | N | 154 | 1/1 | 0.97 | 0.09 | - | 22,22,22,22 | 0 |
| 2 | CU | H | 154 | 1/1 | 0.94 | 0.07 | - | 22,22,22,22 | 0 |
| 2 | CU | B | 154 | 1/1 | 0.99 | 0.09 | - | 15,15,15,15 | 0 |
| 2 | CU | M | 154 | 1/1 | 0.98 | 0.09 | - | 23,23,23,23 | 0 |
| 2 | CU | S | 154 | 1/1 | 0.93 | 0.05 | - | 46,46,46,46 | 0 |
| 2 | CU | J | 154 | 1/1 | 0.98 | 0.12 | - | 15,15,15,15 | 0 |
| 2 | CU | K | 154 | 1/1 | 0.98 | 0.11 | - | 13,13,13,13 | 0 |
| 2 | CU | D | 154 | 1/1 | 0.97 | 0.08 | - | 21,21,21,21 | 0 |
| 2 | CU | P | 154 | 1/1 | 0.79 | 0.12 | - | 69,69,69,69 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.