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

Aug 16, 2023 – 03:09 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 1YG6 |
| Title | : | ClpP |
| Authors | : | Bewley, M.C.; Graziano, V.; Griffin, K.; Flanagan, J.M. |
| Deposited on | : | 2005-01-04 |
| Resolution | : | 1.90 Å(reported) |

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

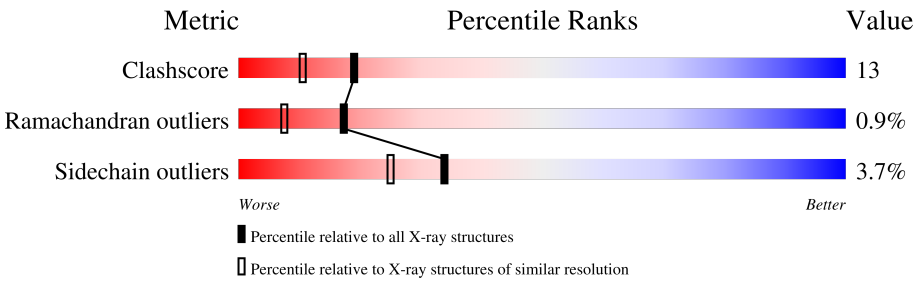
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | NOT EXECUTED |
| EDS | : | NOT EXECUTED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35 |

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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)) |
|---|---|---|
| Clashscore | 141614 | 6847 (1.90-1.90) |
| Ramachandran outliers | 138981 | 6760 (1.90-1.90) |
| Sidechain outliers | 138945 | 6760 (1.90-1.90) |

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 193 | 79% 18% • |
| 1 | B | 193 | 79% 17% • •• |
| 1 | C | 193 | 77% 20% •• |
| 1 | D | 193 | 75% 24% • |
| 1 | E | 193 | 76% 22% • |
| 1 | F | 193 | 78% 19% •• |
| 1 | G | 193 | 77% 19% ••• |
| 1 | H | 193 | 74% 19% •• • |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | I | 193 | 75% 19% • 5% |
| 1 | J | 193 | 75% 19% • 5% |
| 1 | K | 193 | 75% 15% • 8% |
| 1 | L | 193 | 81% 12% •• 6% |
| 1 | M | 193 | 79% 14% • 6% |
| 1 | N | 193 | 74% 17% • 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 |
|---|---|---|---|---|---|---|---|
| 2 | MPD | B | 194 | - | X | - | - |

# 2 Entry composition (i)

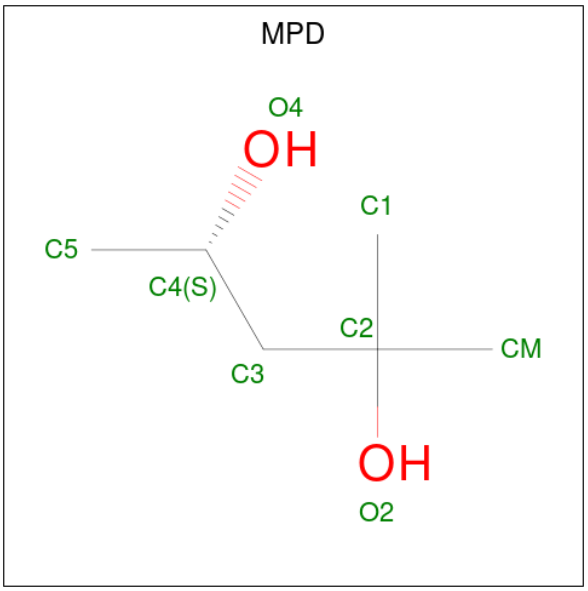
There are 3 unique types of molecules in this entry. The entry contains 21540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent Clp protease proteolytic subunit.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 193 | 1507 | 950 | 262 | 283 | 12 | 0 | 0 | 0 |
| 1 | B | 192 | 1502 | 947 | 261 | 282 | 12 | 0 | 0 | 0 |
| 1 | C | 189 | 1480 | 931 | 258 | 279 | 12 | 0 | 0 | 0 |
| 1 | D | 193 | 1507 | 950 | 262 | 283 | 12 | 0 | 0 | 0 |
| 1 | E | 193 | 1507 | 950 | 262 | 283 | 12 | 0 | 0 | 0 |
| 1 | F | 193 | 1507 | 950 | 262 | 283 | 12 | 0 | 0 | 0 |
| 1 | G | 192 | 1502 | 947 | 261 | 282 | 12 | 0 | 0 | 0 |
| 1 | H | 186 | 1457 | 915 | 255 | 276 | 11 | 0 | 0 | 0 |
| 1 | I | 184 | 1439 | 905 | 252 | 271 | 11 | 0 | 0 | 0 |
| 1 | J | 184 | 1439 | 905 | 252 | 271 | 11 | 0 | 0 | 0 |
| 1 | K | 178 | 1391 | 879 | 240 | 261 | 11 | 0 | 0 | 0 |
| 1 | L | 182 | 1426 | 898 | 250 | 267 | 11 | 0 | 0 | 0 |
| 1 | M | 182 | 1426 | 898 | 250 | 267 | 11 | 0 | 0 | 0 |
| 1 | N | 177 | 1385 | 876 | 239 | 259 | 11 | 0 | 0 | 0 |

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).




| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | | |
| 2 | A | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | B | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | C | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | D | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | E | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | F | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | G | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | H | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | I | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | J | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | K | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | L | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | M | 1 | 8 | 6 | 2 | 0 | 0 |
| 2 | N | 1 | 8 | 6 | 2 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 75 | Total O<br>75 75 | 0 | 0 |
| 3 | B | 62 | Total O<br>62 62 | 0 | 0 |
| 3 | C | 53 | Total O<br>53 53 | 0 | 0 |
| 3 | D | 33 | Total O<br>33 33 | 0 | 0 |
| 3 | E | 65 | Total O<br>65 65 | 0 | 0 |
| 3 | F | 69 | Total O<br>69 69 | 0 | 0 |
| 3 | G | 89 | Total O<br>89 89 | 0 | 0 |
| 3 | H | 60 | Total O<br>60 60 | 0 | 0 |
| 3 | I | 61 | Total O<br>61 61 | 0 | 0 |
| 3 | J | 52 | Total O<br>52 52 | 0 | 0 |
| 3 | K | 61 | Total O<br>61 61 | 0 | 0 |
| 3 | L | 102 | Total O<br>102 102 | 0 | 0 |
| 3 | M | 104 | Total O<br>104 104 | 0 | 0 |
| 3 | N | 67 | Total O<br>67 67 | 0 | 0 |

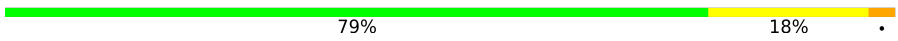
# 3 Residue-property plots (i)

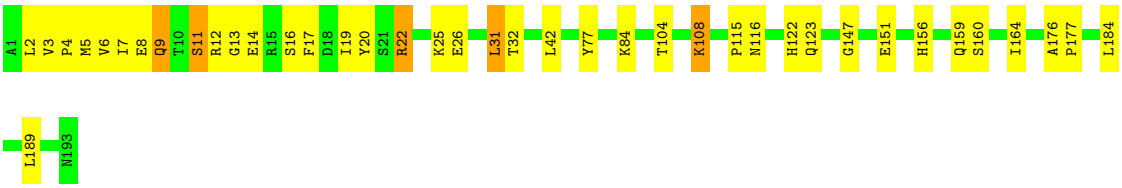
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



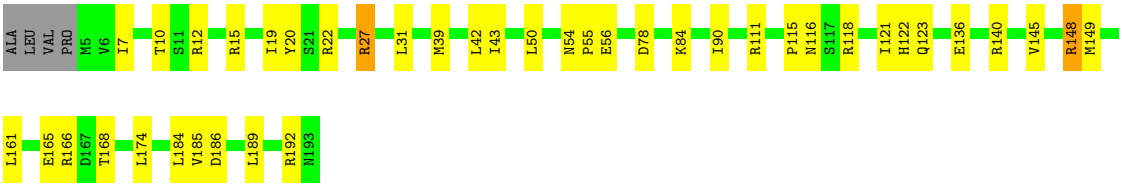




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:

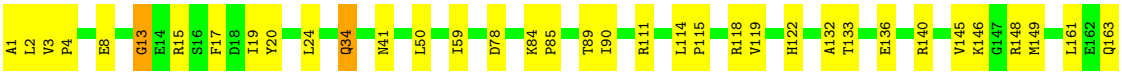
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain C:




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain D:



I164 E165 R166 E169 R170 S175 A176 P177 E178 E181 L184 V185 D186 L189 R192 N193

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E: 76% 22% •

A1 L2 V3 V6 I7 E8 R12 G13 E14 R15 S16 I19 Y20 S21 R22 L23 L24 L31 T32 G33 Q34 V35 E36 L42 A45 E53 N54 G68 Y77 C91 L114 P115 H122 Q123 A132 T133 E136 I137 R140 V145 K146 G147 R148 M149

N150 E151 H156 S175 E178 L184 L189 R192 N193

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F: 78% 19% • •

A1 L2 V3 P4 M5 V6 I7 E8 Q9 G13 E14 R15 S16 F17 D18 I19 Y20 S21 R27 L31 V35 N41 L50 G67 G68 Y77 D78 F101 R111 P115 N116 I121 H122 Q123 P124 L125 H138 I142 L143 K144 V145 M149 H156

L161 E165 R166 R170 V185 D186 L189 N193

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G: 77% 19% • • •

ALA L2 V3 P4 M5 V6 I7 E8 Q9 T10 S11 R12 G13 E14 R15 S16 F17 D18 I19 Y20 S21 K25 E26 R27 L31 T32 N41 L42 I43 L50 I59 Y77 R111 L114 P115 H122 Q129 E136 G147 R148 E151 H156 R172 A176

P177 E181 L184 V185 L189 N193

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain H: 74% 19% • • •

ALA LEU VAL PRO MET VAL ILE E8 Q9 T10 S11 R12 G13 E14 R15 S16 F17 D18 R22 K25 E26 R27 L31 M39 L42 I43 Q46 E53 Y77 D78 F82 I83 K84 C91 F101 T104 L114 P115 H122 A132 R140 K144 V145

R148 M149 H156 L161 E162 Q163 I164 E165 R170 A176 P177 L189 T190 H191 R192 N193

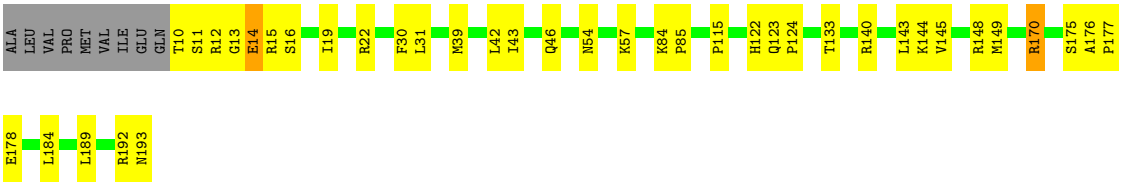
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain I: 75% 19% • 5%

ALA LEU VAL PRO MET VAL ILE GLU GLN T10 S11 R12 G13 E14 R15 S16 F17 D18 I19 Y20 S21 K25 I29 F30 L31 M39 I43 Q46 Y77 K108 P115 N116 H122 Q129 A132 T133 D134 V145 R148 M149 H156 L161 E165

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain J:

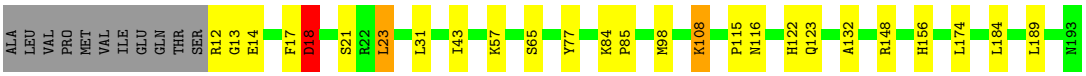



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain K:

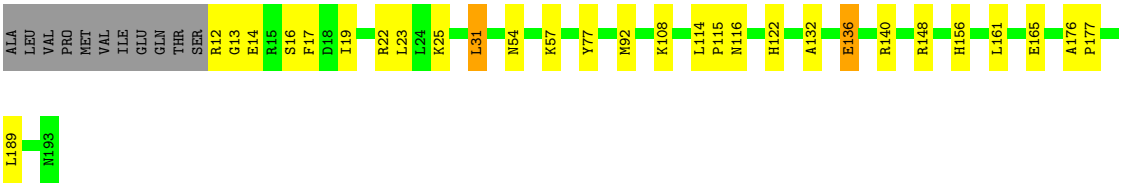
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain L:



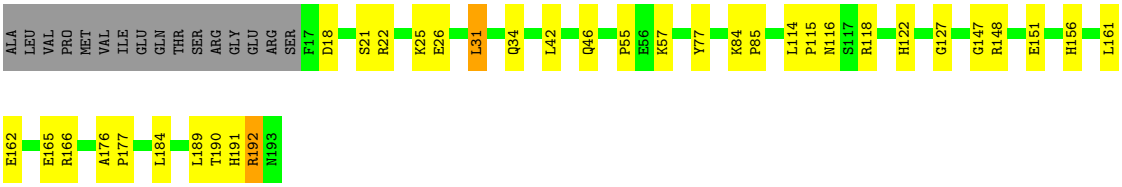

• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain M:




• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain N:



# 4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 192.50Å 103.30Å 159.00Å<br>90.00° 98.40° 90.00° | Depositor |
| Resolution (Å) | 30.00 – 1.90 | Depositor |
| % Data completeness<br>(in resolution range) | (Not available) (30.00-1.90) | Depositor |
| $R_{merge}$ | 0.09 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| Refinement program | CNS | Depositor |
| R, $R_{free}$ | 0.221 , 0.251 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 21540 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 34.0 | wwPDB-VP |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD

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 | 0.51 | 0/1531 | 0.66 | 1/2064 (0.0%) |
| 1 | B | 0.46 | 0/1526 | 0.65 | 1/2057 (0.0%) |
| 1 | C | 0.43 | 0/1503 | 0.62 | 0/2024 |
| 1 | D | 0.43 | 0/1531 | 0.61 | 0/2064 |
| 1 | E | 0.49 | 0/1531 | 0.65 | 0/2064 |
| 1 | F | 0.55 | 0/1531 | 0.67 | 1/2064 (0.0%) |
| 1 | G | 0.58 | 0/1526 | 0.70 | 1/2057 (0.0%) |
| 1 | H | 0.51 | 1/1480 (0.1%) | 0.87 | 3/1993 (0.2%) |
| 1 | I | 0.47 | 0/1462 | 0.69 | 1/1969 (0.1%) |
| 1 | J | 0.44 | 0/1462 | 0.62 | 0/1969 |
| 1 | K | 0.48 | 0/1414 | 0.66 | 1/1906 (0.1%) |
| 1 | L | 0.59 | 0/1449 | 0.71 | 1/1951 (0.1%) |
| 1 | M | 0.61 | 1/1449 (0.1%) | 0.70 | 1/1951 (0.1%) |
| 1 | N | 0.51 | 0/1408 | 0.66 | 1/1898 (0.1%) |
| All | All | 0.51 | 2/20803 (0.0%) | 0.68 | 12/28031 (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 |
|---|---|---|---|
| 1 | H | 0 | 1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | H | 14 | GLU | CD-OE2 | 6.89 | 1.33 | 1.25 |
| 1 | M | 14 | GLU | CD-OE2 | 6.86 | 1.33 | 1.25 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | H | 22 | ARG | CG-CD-NE | 23.98 | 162.17 | 111.80 |
| 1 | H | 22 | ARG | CB-CG-CD | 7.88 | 132.09 | 111.60 |
| 1 | L | 12 | ARG | NE-CZ-NH2 | 7.41 | 124.00 | 120.30 |
| 1 | I | 15 | ARG | NE-CZ-NH2 | 7.29 | 123.94 | 120.30 |
| 1 | A | 31 | LEU | CA-CB-CG | 6.37 | 129.95 | 115.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | H | 22 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 1507 | 0 | 1521 | 50 | 0 |
| 1 | B | 1502 | 0 | 1513 | 55 | 0 |
| 1 | C | 1480 | 0 | 1486 | 37 | 0 |
| 1 | D | 1507 | 0 | 1521 | 50 | 0 |
| 1 | E | 1507 | 0 | 1521 | 38 | 0 |
| 1 | F | 1507 | 0 | 1521 | 44 | 0 |
| 1 | G | 1502 | 0 | 1513 | 39 | 0 |
| 1 | H | 1457 | 0 | 1455 | 70 | 0 |
| 1 | I | 1439 | 0 | 1441 | 98 | 0 |
| 1 | J | 1439 | 0 | 1443 | 67 | 0 |
| 1 | K | 1391 | 0 | 1396 | 38 | 0 |
| 1 | L | 1426 | 0 | 1431 | 24 | 0 |
| 1 | M | 1426 | 0 | 1431 | 31 | 0 |
| 1 | N | 1385 | 0 | 1391 | 34 | 0 |
| 2 | A | 8 | 0 | 14 | 1 | 0 |
| 2 | B | 8 | 0 | 13 | 1 | 0 |
| 2 | C | 8 | 0 | 14 | 1 | 0 |
| 2 | D | 8 | 0 | 14 | 1 | 0 |
| 2 | E | 8 | 0 | 14 | 2 | 0 |
| 2 | F | 8 | 0 | 14 | 3 | 0 |
| 2 | G | 8 | 0 | 14 | 1 | 0 |
| 2 | H | 8 | 0 | 14 | 1 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 2 | I | 8 | 0 | 14 | 1 | 0 |
| 2 | J | 8 | 0 | 14 | 0 | 0 |
| 2 | K | 8 | 0 | 14 | 2 | 0 |
| 2 | L | 8 | 0 | 14 | 1 | 0 |
| 2 | M | 8 | 0 | 14 | 2 | 0 |
| 2 | N | 8 | 0 | 14 | 1 | 0 |
| 3 | A | 75 | 0 | 0 | 2 | 0 |
| 3 | B | 62 | 0 | 0 | 0 | 0 |
| 3 | C | 53 | 0 | 0 | 0 | 0 |
| 3 | D | 33 | 0 | 0 | 0 | 0 |
| 3 | E | 65 | 0 | 0 | 0 | 0 |
| 3 | F | 69 | 0 | 0 | 1 | 0 |
| 3 | G | 89 | 0 | 0 | 3 | 0 |
| 3 | H | 60 | 0 | 0 | 11 | 0 |
| 3 | I | 61 | 0 | 0 | 0 | 0 |
| 3 | J | 52 | 0 | 0 | 0 | 0 |
| 3 | K | 61 | 0 | 0 | 1 | 0 |
| 3 | L | 102 | 0 | 0 | 3 | 0 |
| 3 | M | 104 | 0 | 0 | 1 | 0 |
| 3 | N | 67 | 0 | 0 | 0 | 0 |
| All | All | 21540 | 0 | 20779 | 538 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 538 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:15:ARG:CZ | 1:I:20:TYR:HE2 | 1.34 | 1.37 |
| 1:I:15:ARG:HG3 | 1:J:42:LEU:CD1 | 1.58 | 1.33 |
| 1:I:15:ARG:CG | 1:J:42:LEU:HD11 | 1.59 | 1.32 |
| 1:H:8:GLU:CD | 1:I:29:ILE:HG22 | 1.52 | 1.29 |
| 1:I:13:GLY:O | 1:I:14:GLU:HG3 | 1.35 | 1.20 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 191/193 (99%) | 178 (93%) | 9 (5%) | 4 (2%) | 7 | 1 |
| 1 | B | 190/193 (98%) | 177 (93%) | 10 (5%) | 3 (2%) | 9 | 2 |
| 1 | C | 187/193 (97%) | 177 (95%) | 9 (5%) | 1 (0%) | 29 | 18 |
| 1 | D | 191/193 (99%) | 179 (94%) | 10 (5%) | 2 (1%) | 15 | 6 |
| 1 | E | 191/193 (99%) | 181 (95%) | 7 (4%) | 3 (2%) | 9 | 2 |
| 1 | F | 191/193 (99%) | 181 (95%) | 9 (5%) | 1 (0%) | 29 | 18 |
| 1 | G | 190/193 (98%) | 179 (94%) | 8 (4%) | 3 (2%) | 9 | 2 |
| 1 | H | 184/193 (95%) | 176 (96%) | 6 (3%) | 2 (1%) | 14 | 5 |
| 1 | I | 182/193 (94%) | 170 (93%) | 10 (6%) | 2 (1%) | 14 | 5 |
| 1 | J | 182/193 (94%) | 170 (93%) | 10 (6%) | 2 (1%) | 14 | 5 |
| 1 | K | 176/193 (91%) | 172 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | L | 180/193 (93%) | 172 (96%) | 7 (4%) | 1 (1%) | 25 | 15 |
| 1 | M | 180/193 (93%) | 172 (96%) | 8 (4%) | 0 | 100 | 100 |
| 1 | N | 175/193 (91%) | 171 (98%) | 4 (2%) | 0 | 100 | 100 |
| All | All | 2590/2702 (96%) | 2455 (95%) | 111 (4%) | 24 (1%) | 17 | 7 |

5 of 24 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | H | 14 | GLU |
| 1 | D | 8 | GLU |
| 1 | H | 15 | ARG |
| 1 | I | 14 | GLU |
| 1 | I | 16 | SER |

### 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 | 163/163 (100%) | 158 (97%) | 5 (3%) | 40 | 32 |
| 1 | B | 163/163 (100%) | 155 (95%) | 8 (5%) | 25 | 15 |
| 1 | C | 160/163 (98%) | 154 (96%) | 6 (4%) | 33 | 24 |
| 1 | D | 163/163 (100%) | 157 (96%) | 6 (4%) | 34 | 25 |
| 1 | E | 163/163 (100%) | 157 (96%) | 6 (4%) | 34 | 25 |
| 1 | F | 163/163 (100%) | 156 (96%) | 7 (4%) | 29 | 19 |
| 1 | G | 163/163 (100%) | 156 (96%) | 7 (4%) | 29 | 19 |
| 1 | H | 157/163 (96%) | 151 (96%) | 6 (4%) | 33 | 24 |
| 1 | I | 155/163 (95%) | 151 (97%) | 4 (3%) | 46 | 39 |
| 1 | J | 155/163 (95%) | 151 (97%) | 4 (3%) | 46 | 39 |
| 1 | K | 150/163 (92%) | 142 (95%) | 8 (5%) | 22 | 13 |
| 1 | L | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 39 |
| 1 | M | 153/163 (94%) | 149 (97%) | 4 (3%) | 46 | 39 |
| 1 | N | 149/163 (91%) | 142 (95%) | 7 (5%) | 26 | 16 |
| All | All | 2210/2282 (97%) | 2128 (96%) | 82 (4%) | 34 | 25 |

5 of 82 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 170 | ARG |
| 1 | M | 31 | LEU |
| 1 | K | 17 | PHE |
| 1 | K | 172 | ARG |
| 1 | N | 26 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | K | 131 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | N | 123 | GLN |
| 1 | L | 116 | ASN |
| 1 | M | 123 | GLN |
| 1 | E | 156 | HIS |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

14 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 | $\#\|Z\| > 2$ |
| 2 | MPD | B | 194 | - | 7,7,7 | 2.06 | 3 (42%) | 9,10,10 | 3.69 | 6 (66%) |
| 2 | MPD | I | 194 | - | 7,7,7 | 1.52 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | A | 194 | - | 7,7,7 | 1.52 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | E | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.65 | 6 (66%) |
| 2 | MPD | J | 194 | - | 7,7,7 | 1.21 | 1 (14%) | 9,10,10 | 0.92 | 1 (11%) |
| 2 | MPD | L | 194 | - | 7,7,7 | 1.20 | 1 (14%) | 9,10,10 | 0.92 | 1 (11%) |
| 2 | MPD | M | 194 | - | 7,7,7 | 1.49 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | N | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.65 | 6 (66%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 2 | MPD | F | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | G | 194 | - | 7,7,7 | 1.50 | 2 (28%) | 9,10,10 | 3.65 | 6 (66%) |
| 2 | MPD | K | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | C | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | D | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.66 | 6 (66%) |
| 2 | MPD | H | 194 | - | 7,7,7 | 1.51 | 2 (28%) | 9,10,10 | 3.65 | 6 (66%) |

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 |
|---|---|---|---|---|---|---|---|
| 2 | MPD | B | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | I | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | A | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | E | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | J | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | L | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | M | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | N | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | F | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | G | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | K | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | C | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | D | 194 | - | - | 0/5/5/5 | - |
| 2 | MPD | H | 194 | - | - | 0/5/5/5 | - |

The worst 5 of 27 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | B | 194 | MPD | O4-C4 | -4.03 | 1.25 | 1.43 |
| 2 | G | 194 | MPD | C3-C2 | 2.90 | 1.61 | 1.53 |
| 2 | E | 194 | MPD | C3-C2 | 2.89 | 1.61 | 1.53 |
| 2 | D | 194 | MPD | C3-C2 | 2.88 | 1.61 | 1.53 |
| 2 | C | 194 | MPD | C3-C2 | 2.87 | 1.61 | 1.53 |

The worst 5 of 74 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | C | 194 | MPD | O2-C2-C3 | -6.15 | 86.70 | 109.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 194 | MPD | O2-C2-C3 | -6.12 | 86.82 | 109.80 |
| 2 | I | 194 | MPD | O2-C2-C3 | -6.11 | 86.83 | 109.80 |
| 2 | D | 194 | MPD | O2-C2-C3 | -6.11 | 86.85 | 109.80 |
| 2 | G | 194 | MPD | O2-C2-C3 | -6.11 | 86.86 | 109.80 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 18 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | B | 194 | MPD | 1 | 0 |
| 2 | I | 194 | MPD | 1 | 0 |
| 2 | A | 194 | MPD | 1 | 0 |
| 2 | E | 194 | MPD | 2 | 0 |
| 2 | L | 194 | MPD | 1 | 0 |
| 2 | M | 194 | MPD | 2 | 0 |
| 2 | N | 194 | MPD | 1 | 0 |
| 2 | F | 194 | MPD | 3 | 0 |
| 2 | G | 194 | MPD | 1 | 0 |
| 2 | K | 194 | MPD | 2 | 0 |
| 2 | C | 194 | MPD | 1 | 0 |
| 2 | D | 194 | MPD | 1 | 0 |
| 2 | H | 194 | MPD | 1 | 0 |

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Fit of model and data (i)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

## 6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

## 6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

## 6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.