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

Feb 1, 2016 – 07:55 AM GMT

| | | |
|---|---|---|
| PDB ID | : | 3CMT |
| Title | : | Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures |
| Authors | : | Chen, Z.; Yang, H.; Pavletich, N.P. |
| Deposited on | : | 2008-03-24 |
| Resolution | : | 3.15 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:

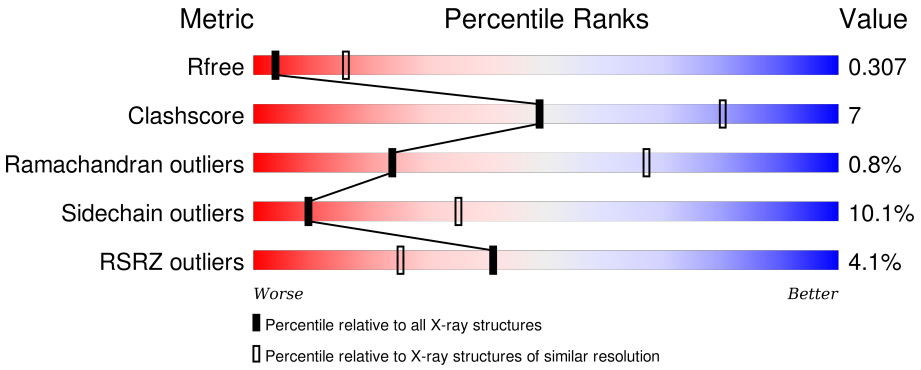
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7 (RC4), CSD as536be (2015) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20026688 |
| Percentile statistics | : | 20151230.v01 (using entries in the PDB archive December 30th 2015) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| 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 3.15 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 | 1112 (3.20-3.12) |
| Clashscore | 102246 | 1249 (3.20-3.12) |
| Ramachandran outliers | 100387 | 1222 (3.20-3.12) |
| Sidechain outliers | 100360 | 1221 (3.20-3.12) |
| RSRZ outliers | 91569 | 1117 (3.20-3.12) |

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 | B | 15 | 7% 13% 47% 20% 20% |
| 1 | E | 15 | 13% 40% 27% 20% |
| 2 | C | 6 | 67% 33% |
| 2 | F | 6 | 50% 50% |
| 3 | A | 1706 | 4% 78% 13% • 6% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | D | 1706 |   |

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 |
|---|---|---|---|---|---|---|---|
| 4 | MG | A | 500 | - | - | - | X |

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25312 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 DNA chain called DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | B | 12 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 236 | 115 | 32 | 77 | 12 | | | |
| 1 | E | 12 | Total | C | N | O | P | 0 | 0 | 0 |
| | | | 236 | 115 | 32 | 77 | 12 | | | |

- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3').

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | C | 6 | Total | C | N | O | P | 3 | 0 | 0 |
| | | | 130 | 60 | 27 | 37 | 6 | | | |
| 2 | F | 6 | Total | C | N | O | P | 3 | 0 | 0 |
| | | | 130 | 60 | 27 | 37 | 6 | | | |

- Molecule 3 is a protein called Protein recA.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | A | 1609 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 12125 | 7622 | 2100 | 2347 | 56 | | | |
| 3 | D | 1609 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 12125 | 7622 | 2101 | 2345 | 57 | | | |

There are 130 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 26 | GLY | - | linker | UNP P0A7G6 |
| A | 27 | ALA | - | linker | UNP P0A7G6 |
| A | 28 | MET | - | linker | UNP P0A7G6 |
| A | 29 | HIS | - | linker | UNP P0A7G6 |
| A | 986 | THR | - | linker | UNP P0A7G6 |
| A | 987 | GLY | - | linker | UNP P0A7G6 |
| A | 988 | SER | - | linker | UNP P0A7G6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 989 | THR | - | linker | UNP P0A7G6 |
| A | 990 | GLY | - | linker | UNP P0A7G6 |
| A | 991 | SER | - | linker | UNP P0A7G6 |
| A | 992 | GLY | - | linker | UNP P0A7G6 |
| A | 993 | THR | - | linker | UNP P0A7G6 |
| A | 994 | THR | - | linker | UNP P0A7G6 |
| A | 995 | GLY | - | linker | UNP P0A7G6 |
| A | 996 | SER | - | linker | UNP P0A7G6 |
| A | 997 | THR | - | linker | UNP P0A7G6 |
| A | 998 | GLY | - | linker | UNP P0A7G6 |
| A | 999 | SER | - | linker | UNP P0A7G6 |
| A | 1000 | MET | - | linker | UNP P0A7G6 |
| A | 1986 | THR | - | linker | UNP P0A7G6 |
| A | 1987 | GLY | - | linker | UNP P0A7G6 |
| A | 1988 | SER | - | linker | UNP P0A7G6 |
| A | 1989 | THR | - | linker | UNP P0A7G6 |
| A | 1990 | GLY | - | linker | UNP P0A7G6 |
| A | 1991 | SER | - | linker | UNP P0A7G6 |
| A | 1992 | MET | - | linker | UNP P0A7G6 |
| A | 1993 | GLY | - | linker | UNP P0A7G6 |
| A | 1994 | HIS | - | linker | UNP P0A7G6 |
| A | 1995 | THR | - | linker | UNP P0A7G6 |
| A | 1996 | THR | - | linker | UNP P0A7G6 |
| A | 1997 | GLY | - | linker | UNP P0A7G6 |
| A | 1998 | SER | - | linker | UNP P0A7G6 |
| A | 1999 | MET | - | linker | UNP P0A7G6 |
| A | 2000 | SER | - | linker | UNP P0A7G6 |
| A | 2985 | THR | - | linker | UNP P0A7G6 |
| A | 2986 | GLY | - | linker | UNP P0A7G6 |
| A | 2987 | SER | - | linker | UNP P0A7G6 |
| A | 2988 | THR | - | linker | UNP P0A7G6 |
| A | 2989 | GLY | - | linker | UNP P0A7G6 |
| A | 2990 | SER | - | linker | UNP P0A7G6 |
| A | 2991 | ALA | - | linker | UNP P0A7G6 |
| A | 2992 | SER | - | linker | UNP P0A7G6 |
| A | 2993 | GLY | - | linker | UNP P0A7G6 |
| A | 2994 | SER | - | linker | UNP P0A7G6 |
| A | 2995 | SER | - | linker | UNP P0A7G6 |
| A | 2996 | THR | - | linker | UNP P0A7G6 |
| A | 2997 | GLY | - | linker | UNP P0A7G6 |
| A | 2998 | SER | - | linker | UNP P0A7G6 |
| A | 2999 | MET | - | linker | UNP P0A7G6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 3000 | SER | - | linker | UNP P0A7G6 |
| A | 3986 | THR | - | linker | UNP P0A7G6 |
| A | 3987 | GLY | - | linker | UNP P0A7G6 |
| A | 3988 | SER | - | linker | UNP P0A7G6 |
| A | 3989 | THR | - | linker | UNP P0A7G6 |
| A | 3990 | GLY | - | linker | UNP P0A7G6 |
| A | 3991 | SER | - | linker | UNP P0A7G6 |
| A | 3992 | MET | - | linker | UNP P0A7G6 |
| A | 3993 | SER | - | linker | UNP P0A7G6 |
| A | 3994 | GLY | - | linker | UNP P0A7G6 |
| A | 3995 | ARG | - | linker | UNP P0A7G6 |
| A | 3996 | THR | - | linker | UNP P0A7G6 |
| A | 3997 | GLY | - | linker | UNP P0A7G6 |
| A | 3998 | SER | - | linker | UNP P0A7G6 |
| A | 3999 | MET | - | linker | UNP P0A7G6 |
| A | 4000 | SER | - | linker | UNP P0A7G6 |
| D | 26 | GLY | - | linker | UNP P0A7G6 |
| D | 27 | ALA | - | linker | UNP P0A7G6 |
| D | 28 | MET | - | linker | UNP P0A7G6 |
| D | 29 | HIS | - | linker | UNP P0A7G6 |
| D | 986 | THR | - | linker | UNP P0A7G6 |
| D | 987 | GLY | - | linker | UNP P0A7G6 |
| D | 988 | SER | - | linker | UNP P0A7G6 |
| D | 989 | THR | - | linker | UNP P0A7G6 |
| D | 990 | GLY | - | linker | UNP P0A7G6 |
| D | 991 | SER | - | linker | UNP P0A7G6 |
| D | 992 | GLY | - | linker | UNP P0A7G6 |
| D | 993 | THR | - | linker | UNP P0A7G6 |
| D | 994 | THR | - | linker | UNP P0A7G6 |
| D | 995 | GLY | - | linker | UNP P0A7G6 |
| D | 996 | SER | - | linker | UNP P0A7G6 |
| D | 997 | THR | - | linker | UNP P0A7G6 |
| D | 998 | GLY | - | linker | UNP P0A7G6 |
| D | 999 | SER | - | linker | UNP P0A7G6 |
| D | 1000 | MET | - | linker | UNP P0A7G6 |
| D | 1986 | THR | - | linker | UNP P0A7G6 |
| D | 1987 | GLY | - | linker | UNP P0A7G6 |
| D | 1988 | SER | - | linker | UNP P0A7G6 |
| D | 1989 | THR | - | linker | UNP P0A7G6 |
| D | 1990 | GLY | - | linker | UNP P0A7G6 |
| D | 1991 | SER | - | linker | UNP P0A7G6 |
| D | 1992 | MET | - | linker | UNP P0A7G6 |

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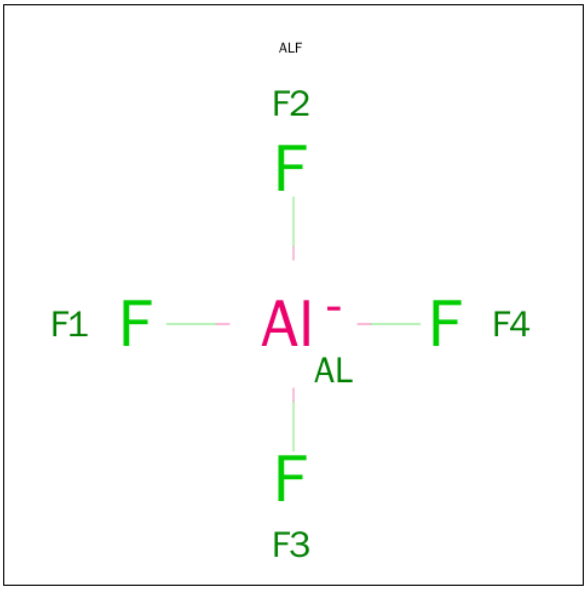
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 1993 | GLY | - | linker | UNP P0A7G6 |
| D | 1994 | HIS | - | linker | UNP P0A7G6 |
| D | 1995 | THR | - | linker | UNP P0A7G6 |
| D | 1996 | THR | - | linker | UNP P0A7G6 |
| D | 1997 | GLY | - | linker | UNP P0A7G6 |
| D | 1998 | SER | - | linker | UNP P0A7G6 |
| D | 1999 | MET | - | linker | UNP P0A7G6 |
| D | 2000 | SER | - | linker | UNP P0A7G6 |
| D | 2985 | THR | - | linker | UNP P0A7G6 |
| D | 2986 | GLY | - | linker | UNP P0A7G6 |
| D | 2987 | SER | - | linker | UNP P0A7G6 |
| D | 2988 | THR | - | linker | UNP P0A7G6 |
| D | 2989 | GLY | - | linker | UNP P0A7G6 |
| D | 2990 | SER | - | linker | UNP P0A7G6 |
| D | 2991 | ALA | - | linker | UNP P0A7G6 |
| D | 2992 | SER | - | linker | UNP P0A7G6 |
| D | 2993 | GLY | - | linker | UNP P0A7G6 |
| D | 2994 | SER | - | linker | UNP P0A7G6 |
| D | 2995 | SER | - | linker | UNP P0A7G6 |
| D | 2996 | THR | - | linker | UNP P0A7G6 |
| D | 2997 | GLY | - | linker | UNP P0A7G6 |
| D | 2998 | SER | - | linker | UNP P0A7G6 |
| D | 2999 | MET | - | linker | UNP P0A7G6 |
| D | 3000 | SER | - | linker | UNP P0A7G6 |
| D | 3986 | THR | - | linker | UNP P0A7G6 |
| D | 3987 | GLY | - | linker | UNP P0A7G6 |
| D | 3988 | SER | - | linker | UNP P0A7G6 |
| D | 3989 | THR | - | linker | UNP P0A7G6 |
| D | 3990 | GLY | - | linker | UNP P0A7G6 |
| D | 3991 | SER | - | linker | UNP P0A7G6 |
| D | 3992 | MET | - | linker | UNP P0A7G6 |
| D | 3993 | SER | - | linker | UNP P0A7G6 |
| D | 3994 | GLY | - | linker | UNP P0A7G6 |
| D | 3995 | ARG | - | linker | UNP P0A7G6 |
| D | 3996 | THR | - | linker | UNP P0A7G6 |
| D | 3997 | GLY | - | linker | UNP P0A7G6 |
| D | 3998 | SER | - | linker | UNP P0A7G6 |
| D | 3999 | MET | - | linker | UNP P0A7G6 |
| D | 4000 | SER | - | linker | UNP P0A7G6 |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

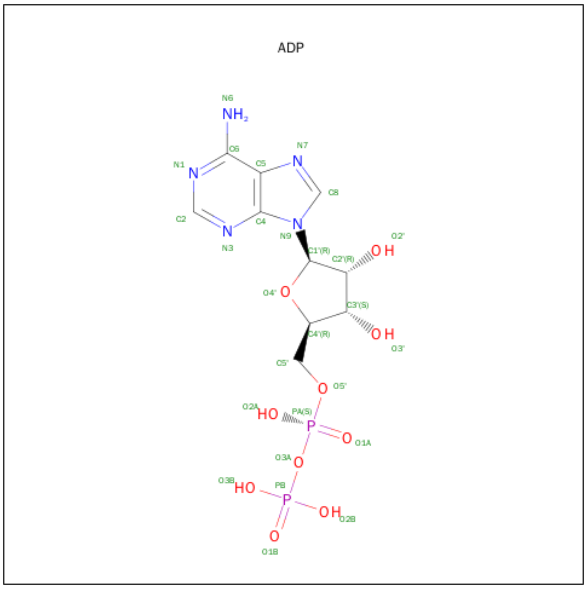
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 4 | A | 5 | Total Mg<br>5 5 | 0 | 0 |
| 4 | D | 5 | Total Mg<br>5 5 | 0 | 0 |

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: $AlF_4$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 5 | A | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | A | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | A | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | A | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | A | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | D | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | D | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | D | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | D | 1 | Total Al F<br>5 1 4 | 0 | 0 |
| 5 | D | 1 | Total Al F<br>5 1 4 | 0 | 0 |

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



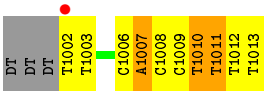

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | A | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |
| 6 | D | 1 | Total | C | N | O | P | 0 | 0 |
| | | | 27 | 10 | 5 | 10 | 2 | | |

# 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.

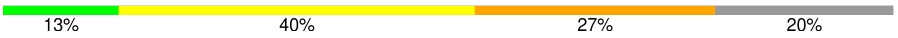
• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

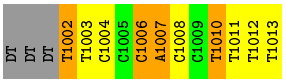
Chain B:


• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

Chain E:




• Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

Chain C:



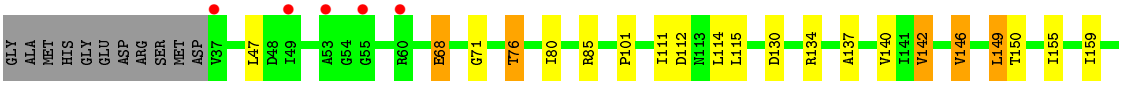
• Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

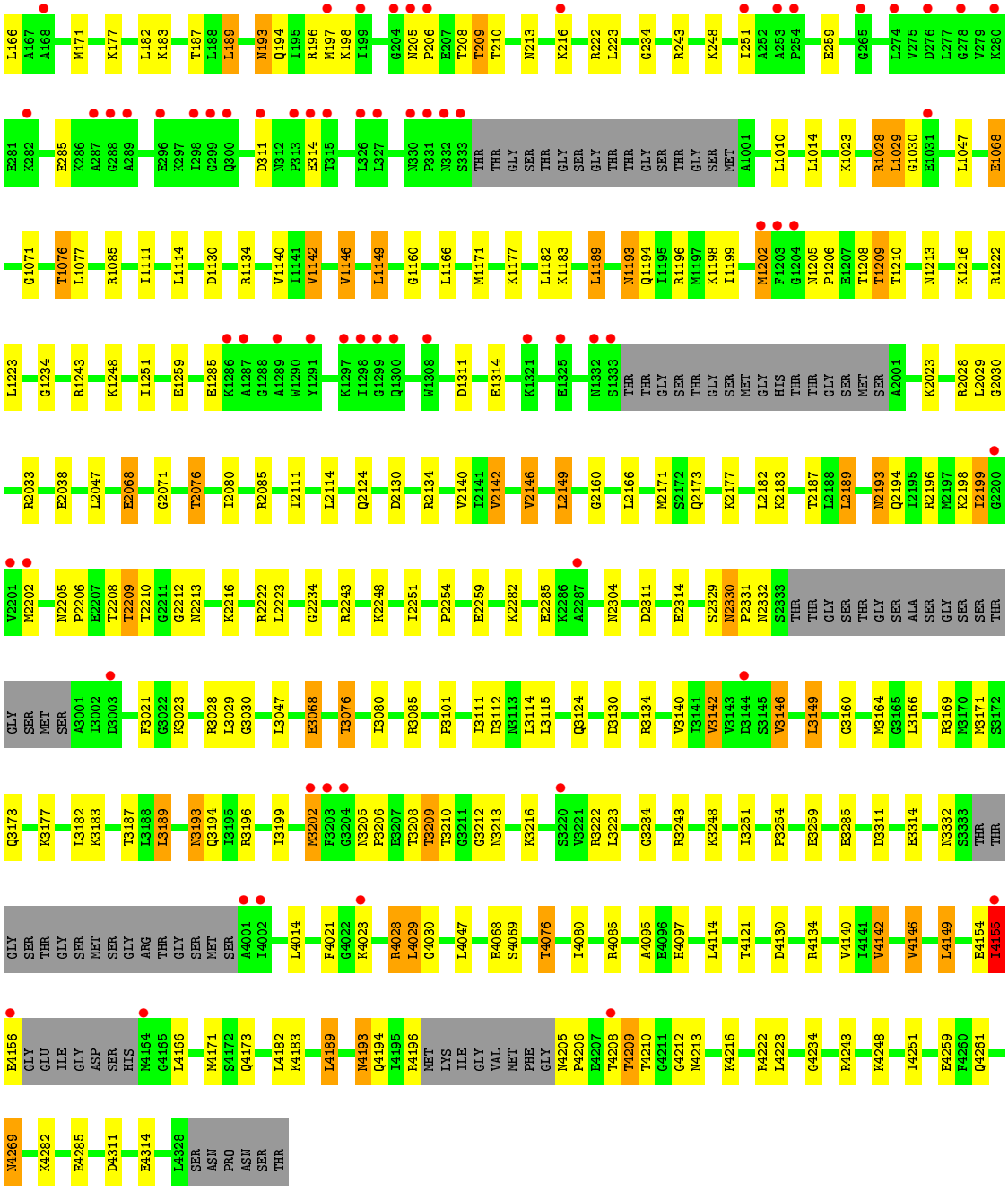
Chain F:



• Molecule 3: Protein recA

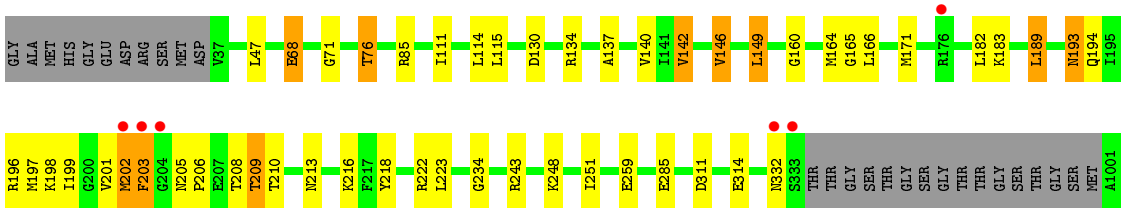
Chain A:

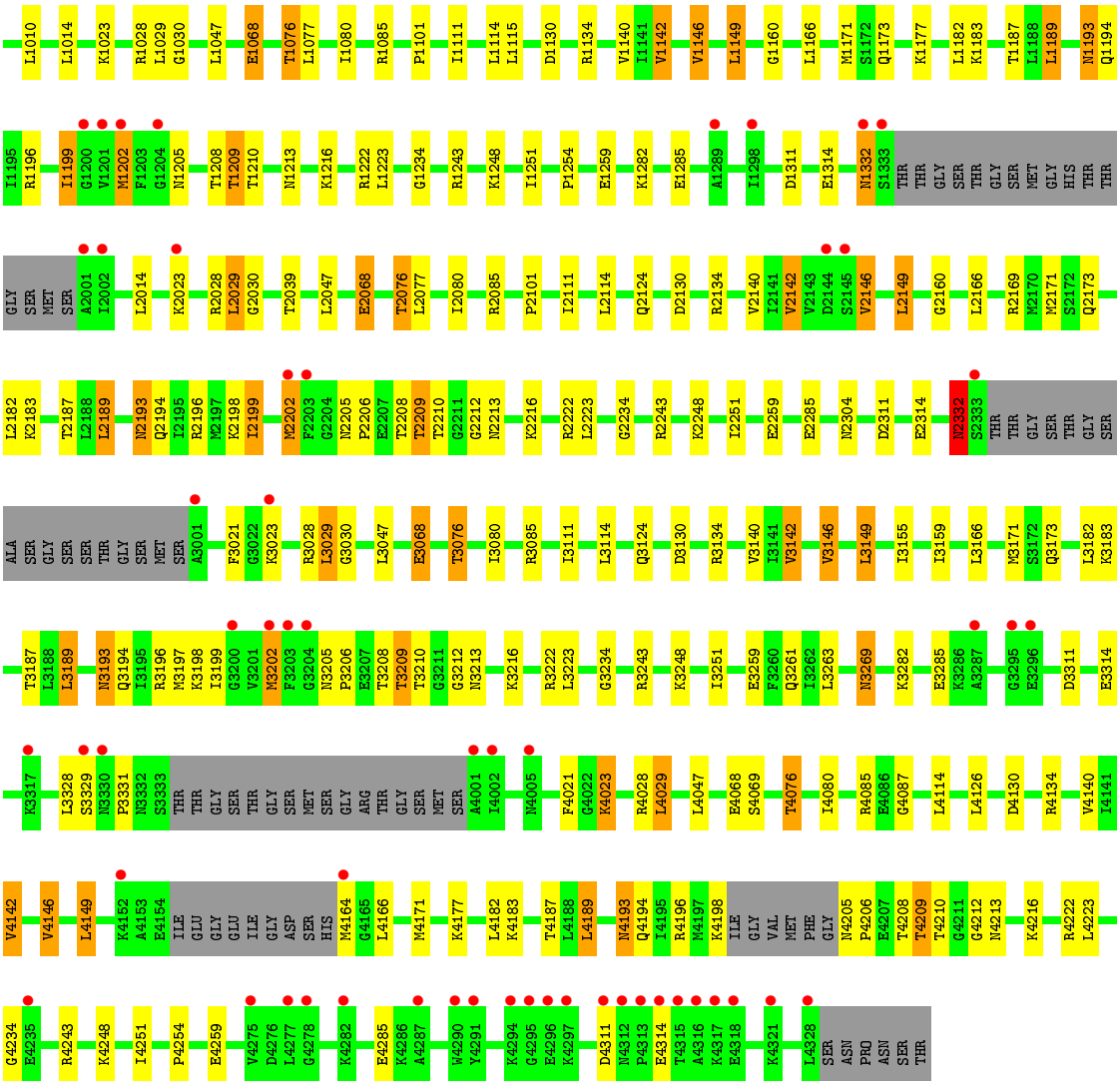





• Molecule 3: Protein recA

Chain D:


L1010 L1014 K1023 R1028 L1029 G1030 L1047 E1068 T1076 L1077 I1080 R1085 P1101 I1111 L1114 L1115 D1130 R1134 V1140 I1141 V1142 V1146 L1149 G1160 L1166 M1171 S1172 Q1173 K1177 L1182 K1183 T1187 L1188 L1189 N1193 Q1194
I1195 R1196 I1199 G1200 V1201 M1202 F1203 G1204 N1205 T1208 T1209 T1210 N1213 K1216 R1222 L1223 G1234 R1243 K1248 I1251 P1254 E1259 K1282 E1285 A1289 I1298 D1311 E1314 N1332 S1333 THR THR GLY SER THR GLY SER MET GLY HIS THR THR
GLY SER MET SER A2001 I2002 L2014 K2023 R2028 L2029 G2030 T2039 L2047 E2068 T2076 L2077 I2080 R2085 P2101 I2111 L2114 Q2124 D2130 R2134 V2140 I2141 V2142 V2143 D2144 S2145 V2146 L2149 G2160 L2166 R2169 M2170 M2171 S2172 Q2173
L2182 K2183 T2187 L2188 L2189 N2193 Q2194 I2195 R2196 M2197 K2198 I2199 M2202 F2203 G2204 N2205 P2206 E2207 T2208 T2209 T2210 G2211 G2212 N2213 K2216 R2222 L2223 G2234 R2243 K2248 I2251 E2259 E2285 N2304 D2311 E2314 N2332 S2333 THR THR GLY SER THR GLY SER
ALA SER GLY SER SER THR GLY SER MET SER A3001 F3021 G3022 K3023 R3028 L3029 G3030 L3047 E3068 T3076 I3080 R3085 I3111 L3114 Q3124 D3130 R3134 V3140 I3141 V3142 V3146 L3149 I3155 I3159 L3166 M3171 S3172 Q3173 L3182 K3183
T3187 L3188 L3189 N3193 Q3194 I3195 R3196 M3197 K3198 I3199 G3200 V3201 M3202 F3203 G3204 N3205 P3206 E3207 T3208 T3209 T3210 G3211 G3212 N3213 K3216 R3222 L3223 G3234 R3243 K3248 I3251 E3259 F3260 Q3261 I3262 L3263 N3269 K3282 E3285 K3286 A3287 G3295 E3296 D3311 E3314
K3317 L3328 S3329 N3330 P3331 N3332 S3333 THR THR GLY SER THR GLY SER MET SER GLY ARG THR GLY SER MET SER A4001 I4002 N4005 P4021 G4022 K4023 R4028 L4029 L4047 E4068 S4069 T4076 I4080 R4085 E4086 G4087 L4114 L4126 D4130 R4134 V4140 I4141
V4142 V4146 L4149 K4152 A4153 E4154 ILE GLU GLY GLU ILE GLY ASP SER HIS M4164 G4165 L4166 M4171 K4177 L4182 K4183 T4187 L4188 L4189 N4193 Q4194 I4195 R4196 M4197 K4198 ILE GLY VAL MET PHE GLY N4205 P4206 E4207 T4208 T4209 T4210 G4211 G4212 N4213 K4216 R4222 L4223
G4234 E4235 R4243 K4248 I4251 P4254 E4259 V4275 D4276 L4277 G4278 K4282 E4285 K4286 A4287 W4290 Y4291 K4294 G4295 E4296 K4297 D4311 N4312 P4313 E4314 T4315 A4316 K4317 E4318 K4321 L4328 SER ASN PRO ASN SER THR

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 21 21 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 159.00Å 300.50Å 80.10Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.00 – 3.15<br>39.75 – 2.98 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 89.9 (40.00-3.15)<br>86.7 (39.75-2.98) | Depositor<br>EDS |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.10 (at 3.01Å) | Xtriage |
| Refinement program | REFMAC 5.3.0036 | Depositor |
| R, $R_{free}$ | 0.217 , 0.243<br>0.271 , 0.307 | Depositor<br>DCC |
| $R_{free}$ test set | 1239 reflections (2.03%) | DCC |
| Wilson B-factor (Å$^2$) | 70.4 | Xtriage |
| Anisotropy | 0.133 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.28 , 19.0 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.32$ | Xtriage |
| Outliers | 1 of 72645 reflections (0.001%) | Xtriage |
| $F_o$,$F_c$ correlation | 0.89 | EDS |
| Total number of atoms | 25312 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: ALF, MG, ADP

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 | B | 1.15 | 0/260 | 1.79 | 7/397 (1.8%) |
| 1 | E | 1.13 | 0/260 | 1.97 | 12/397 (3.0%) |
| 2 | C | 3.88 | 1/146 (0.7%) | 2.40 | 4/225 (1.8%) |
| 2 | F | 6.25 | 1/146 (0.7%) | 2.40 | 5/225 (2.2%) |
| 3 | A | 0.39 | 0/12264 | 0.54 | 0/16503 |
| 3 | D | 0.39 | 0/12264 | 0.54 | 0/16501 |
| All | All | 0.70 | 2/25340 (0.0%) | 0.67 | 28/34248 (0.1%) |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 2 | F | 2007 | DG | P-O5' | -75.00 | 0.84 | 1.59 |
| 2 | C | 2007 | DG | P-O5' | -45.55 | 1.14 | 1.59 |

All (28) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | F | 2007 | DG | P-O5'-C5' | 25.73 | 162.07 | 120.90 |
| 2 | C | 2007 | DG | O5'-P-OP2 | -20.43 | 86.18 | 110.70 |
| 2 | C | 2007 | DG | O5'-P-OP1 | 18.46 | 132.85 | 110.70 |
| 1 | E | 1006 | DC | O4'-C4'-C3' | -8.95 | 100.63 | 106.00 |
| 2 | F | 2008 | DG | O4'-C1'-N9 | -8.52 | 102.04 | 108.00 |
| 1 | B | 1006 | DC | O4'-C4'-C3' | -8.51 | 100.89 | 106.00 |
| 1 | E | 1006 | DC | C1'-O4'-C4' | -8.17 | 101.93 | 110.10 |
| 2 | C | 2008 | DG | O4'-C1'-N9 | -8.07 | 102.35 | 108.00 |
| 1 | B | 1006 | DC | C1'-O4'-C4' | -7.84 | 102.26 | 110.10 |
| 2 | F | 2007 | DG | O5'-P-OP2 | 7.55 | 119.76 | 110.70 |
| 1 | E | 1010 | DT | O4'-C1'-N1 | 6.91 | 112.84 | 108.00 |
| 1 | B | 1010 | DT | N3-C2-O2 | -6.80 | 118.22 | 122.30 |
| 1 | E | 1002 | DT | P-O3'-C3' | 6.64 | 127.67 | 119.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | B | 1010 | DT | O4'-C1'-N1 | 6.28 | 112.39 | 108.00 |
| 1 | E | 1002 | DT | O4'-C1'-N1 | 6.28 | 112.39 | 108.00 |
| 1 | E | 1007 | DA | O4'-C4'-C3' | -5.70 | 102.22 | 104.50 |
| 2 | F | 2007 | DG | O4'-C1'-C2' | -5.69 | 101.35 | 105.90 |
| 2 | F | 2009 | DT | C1'-O4'-C4' | -5.49 | 104.61 | 110.10 |
| 1 | B | 1007 | DA | O4'-C1'-N9 | 5.43 | 111.80 | 108.00 |
| 1 | B | 1011 | DT | C1'-O4'-C4' | -5.35 | 104.75 | 110.10 |
| 1 | E | 1004 | DC | O4'-C1'-N1 | -5.31 | 104.28 | 108.00 |
| 2 | C | 2007 | DG | O4'-C1'-C2' | -5.22 | 101.72 | 105.90 |
| 1 | E | 1007 | DA | C1'-O4'-C4' | -5.15 | 104.95 | 110.10 |
| 1 | E | 1007 | DA | O4'-C1'-N9 | 5.15 | 111.61 | 108.00 |
| 1 | E | 1007 | DA | C4'-C3'-C2' | 5.14 | 107.72 | 103.10 |
| 1 | E | 1006 | DC | O4'-C1'-N1 | 5.13 | 111.59 | 108.00 |
| 1 | B | 1008 | DC | C1'-O4'-C4' | -5.11 | 105.00 | 110.10 |
| 1 | E | 1008 | DC | C1'-O4'-C4' | -5.05 | 105.05 | 110.10 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | B | 236 | 0 | 139 | 9 | 0 |
| 1 | E | 236 | 0 | 139 | 19 | 0 |
| 2 | C | 130 | 0 | 69 | 0 | 0 |
| 2 | F | 130 | 0 | 69 | 0 | 0 |
| 3 | A | 12125 | 0 | 12451 | 176 | 0 |
| 3 | D | 12125 | 0 | 12456 | 190 | 1 |
| 4 | A | 5 | 0 | 0 | 0 | 0 |
| 4 | D | 5 | 0 | 0 | 0 | 0 |
| 5 | A | 25 | 0 | 0 | 0 | 0 |
| 5 | D | 25 | 0 | 0 | 2 | 0 |
| 6 | A | 135 | 0 | 60 | 6 | 0 |
| 6 | D | 135 | 0 | 60 | 4 | 0 |
| All | All | 25312 | 0 | 25443 | 364 | 1 |

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 7.

All (364) 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) |
|---|---|---|---|
| 3:A:68:GLU:HG2 | 3:A:1216:LYS:HB3 | 1.39 | 1.02 |
| 3:D:68:GLU:HG2 | 3:D:1216:LYS:HB3 | 1.47 | 0.97 |
| 3:D:160:GLY:H | 3:D:1173:GLN:HE22 | 1.14 | 0.94 |
| 3:A:2068:GLU:HG2 | 3:A:3216:LYS:HB3 | 1.54 | 0.87 |
| 3:D:1194:GLN:HE21 | 3:D:1196:ARG:HH12 | 1.23 | 0.86 |
| 3:D:4194:GLN:HE21 | 3:D:4196:ARG:HH12 | 1.23 | 0.86 |
| 3:D:2194:GLN:HE21 | 3:D:2196:ARG:HH12 | 1.24 | 0.85 |
| 3:A:194:GLN:HE21 | 3:A:196:ARG:HH12 | 1.25 | 0.85 |
| 3:A:3194:GLN:HE21 | 3:A:3196:ARG:HH12 | 1.25 | 0.85 |
| 3:D:1193:ASN:HD22 | 3:D:1194:GLN:H | 1.25 | 0.84 |
| 3:A:3206:PRO:HG3 | 3:D:3202:MET:HB3 | 1.58 | 0.84 |
| 3:D:2193:ASN:HD22 | 3:D:2194:GLN:H | 1.26 | 0.84 |
| 3:D:3068:GLU:HG2 | 3:D:4216:LYS:HB3 | 1.56 | 0.84 |
| 3:A:4282:LYS:HG3 | 3:D:1282:LYS:HG3 | 1.59 | 0.83 |
| 3:A:1194:GLN:HE21 | 3:A:1196:ARG:HH12 | 1.24 | 0.83 |
| 3:A:3193:ASN:HD22 | 3:A:3194:GLN:H | 1.26 | 0.83 |
| 3:D:1068:GLU:HG2 | 3:D:2216:LYS:HB3 | 1.61 | 0.82 |
| 3:A:4194:GLN:HE21 | 3:A:4196:ARG:HH12 | 1.26 | 0.82 |
| 3:D:194:GLN:HE21 | 3:D:196:ARG:HH12 | 1.25 | 0.82 |
| 3:A:2193:ASN:HD22 | 3:A:2194:GLN:H | 1.27 | 0.81 |
| 3:A:2194:GLN:HE21 | 3:A:2196:ARG:HH12 | 1.24 | 0.81 |
| 3:D:3194:GLN:HE21 | 3:D:3196:ARG:HH12 | 1.26 | 0.81 |
| 3:A:193:ASN:HD22 | 3:A:194:GLN:H | 1.28 | 0.80 |
| 3:A:1193:ASN:HD22 | 3:A:1194:GLN:H | 1.28 | 0.80 |
| 3:D:160:GLY:H | 3:D:1173:GLN:NE2 | 1.81 | 0.79 |
| 3:D:4193:ASN:HD22 | 3:D:4194:GLN:H | 1.29 | 0.79 |
| 3:D:3193:ASN:HD22 | 3:D:3194:GLN:H | 1.29 | 0.79 |
| 1:E:1002:DT:H2' | 1:E:1003:DT:C6 | 2.19 | 0.78 |
| 3:D:2068:GLU:HG2 | 3:D:3216:LYS:HB3 | 1.66 | 0.77 |
| 3:D:193:ASN:HD22 | 3:D:194:GLN:H | 1.32 | 0.77 |
| 3:A:1068:GLU:HG2 | 3:A:2216:LYS:HB3 | 1.66 | 0.77 |
| 1:E:1002:DT:P | 3:D:165:GLY:HA2 | 2.25 | 0.77 |
| 3:A:71:GLY:HA2 | 6:A:502:ADP:H5'1 | 1.66 | 0.76 |
| 3:A:111:ILE:HG22 | 3:A:1030:GLY:CA | 2.14 | 0.76 |
| 3:A:4193:ASN:HD22 | 3:A:4194:GLN:H | 1.32 | 0.75 |
| 3:A:3068:GLU:HG2 | 3:A:4216:LYS:HB3 | 1.66 | 0.75 |
| 3:D:111:ILE:HG22 | 3:D:1030:GLY:CA | 2.19 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:68:GLU:HG2 | 3:A:1216:LYS:CB | 2.17 | 0.72 |
| 3:A:3146:VAL:HA | 3:A:3149:LEU:HD22 | 1.77 | 0.67 |
| 3:D:201:VAL:HA | 3:D:203:PHE:CZ | 2.29 | 0.67 |
| 3:D:1193:ASN:HD22 | 3:D:1194:GLN:N | 1.91 | 0.67 |
| 3:D:2193:ASN:HD22 | 3:D:2194:GLN:N | 1.92 | 0.66 |
| 3:D:4146:VAL:HA | 3:D:4149:LEU:HD22 | 1.77 | 0.66 |
| 3:D:201:VAL:HA | 3:D:203:PHE:CE1 | 2.30 | 0.66 |
| 3:D:3146:VAL:HA | 3:D:3149:LEU:HD22 | 1.78 | 0.66 |
| 3:A:2193:ASN:HD22 | 3:A:2194:GLN:N | 1.94 | 0.65 |
| 3:D:2160:GLY:H | 3:D:3173:GLN:HE22 | 1.41 | 0.65 |
| 3:D:3076:THR:HG21 | 3:D:3142:VAL:HG21 | 1.78 | 0.65 |
| 3:A:2068:GLU:HG2 | 3:A:3216:LYS:CB | 2.26 | 0.65 |
| 3:D:146:VAL:HA | 3:D:149:LEU:HD22 | 1.78 | 0.65 |
| 3:D:2160:GLY:H | 3:D:3173:GLN:NE2 | 1.95 | 0.65 |
| 3:A:193:ASN:HD22 | 3:A:194:GLN:N | 1.94 | 0.65 |
| 3:D:4193:ASN:HD22 | 3:D:4194:GLN:N | 1.95 | 0.65 |
| 3:D:3068:GLU:HG2 | 3:D:4216:LYS:CB | 2.27 | 0.65 |
| 3:A:4146:VAL:HA | 3:A:4149:LEU:HD22 | 1.78 | 0.65 |
| 3:A:2329:SER:O | 3:A:2330:ASN:HB2 | 1.94 | 0.65 |
| 3:A:112:ASP:O | 3:A:1028:ARG:HG2 | 1.97 | 0.64 |
| 3:A:1193:ASN:HD22 | 3:A:1194:GLN:N | 1.95 | 0.64 |
| 3:A:3193:ASN:HD22 | 3:A:3194:GLN:N | 1.94 | 0.64 |
| 3:A:146:VAL:HA | 3:A:149:LEU:HD22 | 1.79 | 0.64 |
| 3:D:3193:ASN:OD1 | 3:D:3209:THR:HG23 | 1.98 | 0.64 |
| 3:A:1146:VAL:HA | 3:A:1149:LEU:HD22 | 1.78 | 0.64 |
| 3:D:1111:ILE:HG22 | 3:D:2030:GLY:CA | 2.26 | 0.64 |
| 3:A:2146:VAL:HA | 3:A:2149:LEU:HD22 | 1.80 | 0.64 |
| 3:D:68:GLU:HG2 | 3:D:1216:LYS:CB | 2.26 | 0.64 |
| 3:A:3193:ASN:OD1 | 3:A:3209:THR:HG23 | 1.99 | 0.63 |
| 3:A:111:ILE:HG22 | 3:A:1030:GLY:N | 2.13 | 0.63 |
| 3:A:1071:GLY:HA2 | 6:A:1502:ADP:H5'1 | 1.79 | 0.63 |
| 3:D:193:ASN:OD1 | 3:D:209:THR:HG23 | 1.98 | 0.63 |
| 3:A:76:THR:HG21 | 3:A:142:VAL:HG21 | 1.80 | 0.63 |
| 1:E:1013:DT:C7 | 3:D:3197:MET:HG3 | 2.29 | 0.63 |
| 3:A:115:LEU:HD21 | 3:A:1014:LEU:HD21 | 1.81 | 0.63 |
| 3:D:2146:VAL:HA | 3:D:2149:LEU:HD22 | 1.80 | 0.63 |
| 1:B:1007:DA:H5' | 3:A:2212:GLY:HA2 | 1.80 | 0.63 |
| 1:E:1013:DT:H71 | 3:D:3197:MET:HG3 | 1.81 | 0.62 |
| 3:A:1076:THR:HG21 | 3:A:1142:VAL:HG21 | 1.81 | 0.62 |
| 3:D:3193:ASN:HD22 | 3:D:3194:GLN:N | 1.96 | 0.62 |
| 3:A:4193:ASN:HD22 | 3:A:4194:GLN:N | 1.97 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:2193:ASN:OD1 | 3:D:2209:THR:HG23 | 2.00 | 0.62 |
| 3:A:193:ASN:OD1 | 3:A:209:THR:HG23 | 2.00 | 0.62 |
| 3:D:4076:THR:HG21 | 3:D:4142:VAL:HG21 | 1.82 | 0.62 |
| 3:D:4193:ASN:OD1 | 3:D:4209:THR:HG23 | 1.99 | 0.62 |
| 3:D:1146:VAL:HA | 3:D:1149:LEU:HD22 | 1.80 | 0.62 |
| 3:A:4076:THR:HG21 | 3:A:4142:VAL:HG21 | 1.82 | 0.61 |
| 3:A:4193:ASN:OD1 | 3:A:4209:THR:HG23 | 2.00 | 0.61 |
| 3:D:2124:GLN:HG3 | 3:D:3021:PHE:CD1 | 2.36 | 0.61 |
| 3:A:2160:GLY:H | 3:A:3173:GLN:NE2 | 1.98 | 0.61 |
| 3:A:3076:THR:HG21 | 3:A:3142:VAL:HG21 | 1.82 | 0.61 |
| 3:D:1193:ASN:OD1 | 3:D:1209:THR:HG23 | 2.00 | 0.61 |
| 3:A:2330:ASN:H | 3:A:2331:PRO:HD3 | 1.65 | 0.60 |
| 3:A:1193:ASN:OD1 | 3:A:1209:THR:HG23 | 2.02 | 0.60 |
| 3:D:111:ILE:HG22 | 3:D:1030:GLY:HA2 | 1.83 | 0.60 |
| 1:E:1003:DT:O2 | 3:D:199:ILE:HG22 | 2.00 | 0.60 |
| 3:D:76:THR:HG21 | 3:D:142:VAL:HG21 | 1.84 | 0.60 |
| 3:A:2193:ASN:OD1 | 3:A:2209:THR:HG23 | 2.01 | 0.60 |
| 3:D:1076:THR:HG21 | 3:D:1142:VAL:HG21 | 1.82 | 0.60 |
| 3:A:3111:ILE:HG22 | 3:A:4030:GLY:CA | 2.32 | 0.60 |
| 3:D:193:ASN:HD22 | 3:D:194:GLN:N | 1.98 | 0.59 |
| 1:B:1002:DT:H2' | 1:B:1003:DT:C6 | 2.38 | 0.59 |
| 3:A:4121:THR:HG22 | 3:A:4155:ILE:HD12 | 1.85 | 0.59 |
| 3:A:150:THR:HB | 3:A:155:ILE:HD11 | 1.83 | 0.59 |
| 3:A:2160:GLY:H | 3:A:3173:GLN:HE22 | 1.50 | 0.59 |
| 1:E:1010:DT:H5' | 3:D:3212:GLY:HA2 | 1.84 | 0.59 |
| 3:D:2076:THR:HG21 | 3:D:2142:VAL:HG21 | 1.84 | 0.59 |
| 3:A:2076:THR:HG21 | 3:A:2142:VAL:HG21 | 1.85 | 0.59 |
| 3:D:2111:ILE:HG22 | 3:D:3030:GLY:CA | 2.33 | 0.58 |
| 3:D:3328:LEU:HB2 | 3:D:3331:PRO:HG3 | 1.84 | 0.58 |
| 3:D:4198:LYS:HG2 | 3:D:4206:PRO:O | 2.03 | 0.58 |
| 3:D:3111:ILE:HG23 | 3:D:4029:LEU:HD13 | 1.86 | 0.58 |
| 1:E:1007:DA:H5' | 3:D:2212:GLY:HA2 | 1.86 | 0.58 |
| 3:D:202:MET:HG2 | 3:D:202:MET:O | 2.03 | 0.57 |
| 3:A:4213:ASN:OD1 | 3:A:4216:LYS:HE2 | 2.04 | 0.57 |
| 3:D:3243:ARG:NH1 | 3:D:3259:GLU:OE2 | 2.37 | 0.57 |
| 3:D:1243:ARG:NH1 | 3:D:1259:GLU:OE2 | 2.38 | 0.57 |
| 3:D:213:ASN:OD1 | 3:D:216:LYS:HE2 | 2.05 | 0.57 |
| 3:D:2243:ARG:NH1 | 3:D:2259:GLU:OE2 | 2.38 | 0.57 |
| 3:D:1194:GLN:NE2 | 3:D:1196:ARG:HH12 | 1.99 | 0.57 |
| 3:A:1243:ARG:NH1 | 3:A:1259:GLU:OE2 | 2.38 | 0.56 |
| 1:E:1013:DT:H5' | 3:D:4212:GLY:HA2 | 1.86 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:2329:SER:O | 3:A:2330:ASN:CB | 2.53 | 0.56 |
| 3:D:3213:ASN:OD1 | 3:D:3216:LYS:HE2 | 2.05 | 0.56 |
| 3:A:2213:ASN:OD1 | 3:A:2216:LYS:HE2 | 2.05 | 0.56 |
| 3:D:1160:GLY:H | 3:D:2173:GLN:NE2 | 2.03 | 0.56 |
| 3:A:198:LYS:HG2 | 3:A:206:PRO:O | 2.05 | 0.56 |
| 3:D:2213:ASN:OD1 | 3:D:2216:LYS:HE2 | 2.05 | 0.56 |
| 3:D:3222:ARG:HG3 | 3:D:3248:LYS:HB3 | 1.87 | 0.56 |
| 3:D:1213:ASN:OD1 | 3:D:1216:LYS:HE2 | 2.05 | 0.56 |
| 3:A:2149:LEU:HD23 | 3:A:2171:MET:HE1 | 1.87 | 0.56 |
| 3:D:3076:THR:CG2 | 3:D:3142:VAL:HG21 | 2.35 | 0.56 |
| 3:A:4243:ARG:NH1 | 3:A:4259:GLU:OE2 | 2.39 | 0.56 |
| 3:D:4213:ASN:OD1 | 3:D:4216:LYS:HE2 | 2.05 | 0.56 |
| 3:A:2194:GLN:NE2 | 3:A:2196:ARG:HH12 | 2.01 | 0.55 |
| 3:A:3222:ARG:HG3 | 3:A:3248:LYS:HB3 | 1.88 | 0.55 |
| 3:A:2304:ASN:ND2 | 3:D:2304:ASN:OD1 | 2.27 | 0.55 |
| 3:A:76:THR:CG2 | 3:A:142:VAL:HG21 | 2.37 | 0.55 |
| 3:A:3243:ARG:NH1 | 3:A:3259:GLU:OE2 | 2.39 | 0.55 |
| 3:D:2222:ARG:HG3 | 3:D:2248:LYS:HB3 | 1.89 | 0.55 |
| 3:A:3213:ASN:OD1 | 3:A:3216:LYS:HE2 | 2.07 | 0.55 |
| 1:E:1013:DT:H5" | 3:D:4213:ASN:ND2 | 2.21 | 0.55 |
| 3:A:3076:THR:CG2 | 3:A:3142:VAL:HG21 | 2.36 | 0.55 |
| 3:D:1076:THR:CG2 | 3:D:1142:VAL:HG21 | 2.37 | 0.55 |
| 3:A:243:ARG:NH1 | 3:A:259:GLU:OE2 | 2.40 | 0.54 |
| 3:A:149:LEU:HD23 | 3:A:171:MET:HE1 | 1.90 | 0.54 |
| 3:A:1111:ILE:HG22 | 3:A:2030:GLY:CA | 2.37 | 0.54 |
| 3:D:4243:ARG:NH1 | 3:D:4259:GLU:OE2 | 2.41 | 0.54 |
| 3:A:4076:THR:CG2 | 3:A:4142:VAL:HG21 | 2.38 | 0.54 |
| 1:E:1010:DT:C2 | 3:D:2199:ILE:HD12 | 2.43 | 0.54 |
| 3:D:4194:GLN:NE2 | 3:D:4196:ARG:HH12 | 2.00 | 0.54 |
| 3:D:1160:GLY:H | 3:D:2173:GLN:HE22 | 1.56 | 0.54 |
| 3:A:4261:GLN:HB2 | 3:A:4269:ASN:HB3 | 1.89 | 0.54 |
| 3:D:149:LEU:HD23 | 3:D:171:MET:HE1 | 1.89 | 0.54 |
| 3:A:1076:THR:CG2 | 3:A:1142:VAL:HG21 | 2.37 | 0.54 |
| 3:D:4076:THR:CG2 | 3:D:4142:VAL:HG21 | 2.38 | 0.54 |
| 3:A:213:ASN:OD1 | 3:A:216:LYS:HE2 | 2.08 | 0.54 |
| 3:D:222:ARG:HG3 | 3:D:248:LYS:HB3 | 1.91 | 0.53 |
| 3:D:1068:GLU:HG2 | 3:D:2216:LYS:CB | 2.37 | 0.53 |
| 3:D:243:ARG:NH1 | 3:D:259:GLU:OE2 | 2.41 | 0.53 |
| 3:A:2243:ARG:NH1 | 3:A:2259:GLU:OE2 | 2.40 | 0.53 |
| 3:A:111:ILE:HG22 | 3:A:1030:GLY:HA2 | 1.89 | 0.53 |
| 3:D:4222:ARG:HG3 | 3:D:4248:LYS:HB3 | 1.89 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:4206:PRO:HG3 | 3:D:2202:MET:HB3 | 1.90 | 0.53 |
| 3:A:1160:GLY:H | 3:A:2173:GLN:NE2 | 2.06 | 0.53 |
| 3:A:1222:ARG:HG3 | 3:A:1248:LYS:HB3 | 1.90 | 0.53 |
| 3:A:1213:ASN:OD1 | 3:A:1216:LYS:HE2 | 2.07 | 0.53 |
| 3:A:222:ARG:HG3 | 3:A:248:LYS:HB3 | 1.90 | 0.53 |
| 3:D:2076:THR:CG2 | 3:D:2142:VAL:HG21 | 2.38 | 0.53 |
| 3:A:194:GLN:NE2 | 3:A:196:ARG:HH12 | 2.01 | 0.53 |
| 3:A:4222:ARG:HG3 | 3:A:4248:LYS:HB3 | 1.90 | 0.52 |
| 3:D:1222:ARG:HG3 | 3:D:1248:LYS:HB3 | 1.91 | 0.52 |
| 3:A:3206:PRO:HG3 | 3:D:3202:MET:CB | 2.34 | 0.52 |
| 3:D:194:GLN:NE2 | 3:D:196:ARG:HH12 | 2.03 | 0.52 |
| 3:D:2149:LEU:HD23 | 3:D:2171:MET:HE1 | 1.90 | 0.52 |
| 3:A:4069:SER:HB3 | 6:A:4502:ADP:H3' | 1.91 | 0.52 |
| 1:E:1013:DT:H73 | 3:D:3198:LYS:O | 2.09 | 0.52 |
| 3:D:76:THR:CG2 | 3:D:142:VAL:HG21 | 2.39 | 0.52 |
| 3:D:1254:PRO:HG3 | 6:D:502:ADP:O2' | 2.10 | 0.52 |
| 3:A:2222:ARG:HG3 | 3:A:2248:LYS:HB3 | 1.90 | 0.52 |
| 3:D:2194:GLN:NE2 | 3:D:2196:ARG:HH12 | 2.00 | 0.52 |
| 3:A:3124:GLN:HG3 | 3:A:4021:PHE:CD1 | 2.45 | 0.52 |
| 3:D:198:LYS:HG2 | 3:D:206:PRO:O | 2.09 | 0.51 |
| 3:D:1194:GLN:HE22 | 3:D:1196:ARG:HH22 | 1.56 | 0.51 |
| 1:E:1007:DA:C6 | 3:D:1199:ILE:HG13 | 2.45 | 0.51 |
| 3:A:2076:THR:CG2 | 3:A:2142:VAL:HG21 | 2.39 | 0.51 |
| 3:A:3194:GLN:NE2 | 3:A:3196:ARG:HH12 | 2.01 | 0.50 |
| 3:A:2194:GLN:HE22 | 3:A:2196:ARG:HH22 | 1.59 | 0.50 |
| 1:E:1003:DT:H2' | 3:D:197:MET:O | 2.11 | 0.50 |
| 3:D:111:ILE:HG22 | 3:D:1030:GLY:N | 2.27 | 0.50 |
| 3:D:4194:GLN:HE22 | 3:D:4196:ARG:HH22 | 1.58 | 0.50 |
| 3:A:101:PRO:HB3 | 3:A:1029:LEU:HD22 | 1.93 | 0.50 |
| 3:D:4069:SER:HA | 6:D:4502:ADP:O3A | 2.12 | 0.50 |
| 1:B:1009:DC:O2 | 3:A:3169:ARG:NH1 | 2.44 | 0.50 |
| 3:D:201:VAL:HG23 | 3:D:203:PHE:CD1 | 2.46 | 0.50 |
| 3:A:3194:GLN:HE22 | 3:A:3196:ARG:HH22 | 1.60 | 0.49 |
| 3:A:3160:GLY:H | 3:A:4173:GLN:NE2 | 2.10 | 0.49 |
| 3:D:194:GLN:HE22 | 3:D:196:ARG:HH22 | 1.58 | 0.49 |
| 3:D:2068:GLU:HG2 | 3:D:3216:LYS:CB | 2.40 | 0.49 |
| 3:D:2194:GLN:HE22 | 3:D:2196:ARG:HH22 | 1.58 | 0.49 |
| 3:A:194:GLN:HE22 | 3:A:196:ARG:HH22 | 1.59 | 0.49 |
| 3:A:1194:GLN:NE2 | 3:A:1196:ARG:HH12 | 2.00 | 0.49 |
| 1:B:1010:DT:H2' | 1:B:1011:DT:C6 | 2.47 | 0.49 |
| 3:D:1182:LEU:HD11 | 3:D:1189:LEU:HD12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:1194:GLN:HE21 | 3:D:1196:ARG:NH1 | 2.03 | 0.49 |
| 3:A:3111:ILE:HG22 | 3:A:4030:GLY:N | 2.27 | 0.49 |
| 3:D:2101:PRO:HB3 | 3:D:3029:LEU:HD22 | 1.95 | 0.49 |
| 3:A:2124:GLN:HG3 | 3:A:3021:PHE:CD1 | 2.48 | 0.49 |
| 3:D:3261:GLN:HB2 | 3:D:3269:ASN:HB3 | 1.95 | 0.48 |
| 3:D:3194:GLN:HE22 | 3:D:3196:ARG:HH22 | 1.61 | 0.48 |
| 3:A:1194:GLN:HE22 | 3:A:1196:ARG:HH22 | 1.59 | 0.48 |
| 3:A:1160:GLY:H | 3:A:2173:GLN:HE22 | 1.62 | 0.48 |
| 3:A:182:LEU:HD11 | 3:A:189:LEU:HD12 | 1.96 | 0.48 |
| 3:A:3254:PRO:HG3 | 6:A:2502:ADP:O2' | 2.13 | 0.48 |
| 3:D:1194:GLN:NE2 | 3:D:1196:ARG:HH22 | 2.12 | 0.48 |
| 3:D:1115:LEU:HD21 | 3:D:2014:LEU:HD21 | 1.95 | 0.48 |
| 3:A:1182:LEU:HD11 | 3:A:1189:LEU:HD12 | 1.95 | 0.48 |
| 3:D:137:ALA:HB1 | 3:D:1010:LEU:HB2 | 1.95 | 0.48 |
| 3:D:182:LEU:HD11 | 3:D:189:LEU:HD12 | 1.96 | 0.47 |
| 3:A:4194:GLN:NE2 | 3:A:4196:ARG:HH12 | 2.04 | 0.47 |
| 3:A:3160:GLY:H | 3:A:4173:GLN:HE22 | 1.61 | 0.47 |
| 3:A:4282:LYS:HG3 | 3:D:1282:LYS:CG | 2.40 | 0.47 |
| 3:A:1149:LEU:HD23 | 3:A:1171:MET:HE1 | 1.96 | 0.47 |
| 3:D:2194:GLN:NE2 | 3:D:2196:ARG:HH22 | 2.13 | 0.47 |
| 3:D:115:LEU:HD21 | 3:D:1014:LEU:HD21 | 1.97 | 0.47 |
| 3:D:4194:GLN:NE2 | 3:D:4196:ARG:HH22 | 2.13 | 0.47 |
| 3:A:4194:GLN:HE22 | 3:A:4196:ARG:HH22 | 1.61 | 0.47 |
| 3:D:194:GLN:NE2 | 3:D:196:ARG:HH22 | 2.11 | 0.47 |
| 3:A:111:ILE:CG2 | 3:A:1030:GLY:HA2 | 2.44 | 0.47 |
| 3:D:1149:LEU:HD23 | 3:D:1171:MET:HE1 | 1.95 | 0.47 |
| 3:A:2038:GLU:HA | 3:A:2332:ASN:HD21 | 1.80 | 0.47 |
| 3:D:2182:LEU:HD11 | 3:D:2189:LEU:HD12 | 1.96 | 0.47 |
| 3:D:3149:LEU:HD23 | 3:D:3171:MET:HE1 | 1.96 | 0.47 |
| 3:D:2111:ILE:HG22 | 3:D:3030:GLY:N | 2.30 | 0.47 |
| 3:A:4182:LEU:HD11 | 3:A:4189:LEU:HD12 | 1.95 | 0.47 |
| 3:D:2130:ASP:OD2 | 3:D:2134:ARG:NH1 | 2.47 | 0.47 |
| 3:D:1068:GLU:HA | 5:D:1501:ALF:F1 | 2.05 | 0.46 |
| 3:A:3068:GLU:HG2 | 3:A:4216:LYS:CB | 2.40 | 0.46 |
| 1:B:1011:DT:H2' | 1:B:1012:DT:C6 | 2.50 | 0.46 |
| 3:D:3182:LEU:HD11 | 3:D:3189:LEU:HD12 | 1.97 | 0.46 |
| 3:A:3149:LEU:HD23 | 3:A:3171:MET:HE1 | 1.96 | 0.46 |
| 1:E:1011:DT:H2' | 1:E:1012:DT:C6 | 2.50 | 0.46 |
| 3:A:2194:GLN:HE21 | 3:A:2196:ARG:NH1 | 2.04 | 0.46 |
| 3:D:3194:GLN:NE2 | 3:D:3196:ARG:HH12 | 2.02 | 0.46 |
| 3:D:4182:LEU:HD11 | 3:D:4189:LEU:HD12 | 1.97 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:3112:ASP:O | 3:A:4028:ARG:HG2 | 2.16 | 0.46 |
| 3:A:3111:ILE:HG23 | 3:A:4029:LEU:HD13 | 1.98 | 0.46 |
| 3:A:3111:ILE:HG22 | 3:A:4030:GLY:HA2 | 1.98 | 0.46 |
| 1:E:1006:DC:H5' | 3:D:2169:ARG:HA | 1.97 | 0.46 |
| 3:A:194:GLN:NE2 | 3:A:196:ARG:HH22 | 2.13 | 0.45 |
| 3:A:2194:GLN:NE2 | 3:A:2196:ARG:HH22 | 2.14 | 0.45 |
| 3:A:3080:ILE:HD11 | 3:A:3142:VAL:CG1 | 2.46 | 0.45 |
| 1:B:1010:DT:C2 | 3:A:2199:ILE:HD12 | 2.51 | 0.45 |
| 3:D:1111:ILE:HG22 | 3:D:2030:GLY:HA2 | 1.96 | 0.45 |
| 3:A:111:ILE:HG23 | 3:A:1029:LEU:HB3 | 1.98 | 0.45 |
| 3:D:1111:ILE:HG22 | 3:D:2030:GLY:N | 2.31 | 0.45 |
| 1:E:1013:DT:H72 | 3:D:3197:MET:HG3 | 1.99 | 0.45 |
| 3:A:159:ILE:HG12 | 3:A:1177:LYS:HD3 | 1.98 | 0.45 |
| 3:D:111:ILE:CG2 | 3:D:1030:GLY:HA2 | 2.47 | 0.45 |
| 3:D:3263:LEU:HG | 3:D:3269:ASN:HB2 | 1.99 | 0.45 |
| 1:B:1013:DT:H5' | 3:A:4212:GLY:HA2 | 1.97 | 0.45 |
| 3:A:2182:LEU:HD11 | 3:A:2189:LEU:HD12 | 1.99 | 0.45 |
| 3:A:2111:ILE:HG22 | 3:A:3030:GLY:CA | 2.46 | 0.45 |
| 3:D:4149:LEU:HD23 | 3:D:4171:MET:HE1 | 1.99 | 0.45 |
| 3:A:2130:ASP:OD2 | 3:A:2134:ARG:NH1 | 2.50 | 0.45 |
| 3:D:4177:LYS:HB3 | 3:D:4177:LYS:HE2 | 1.82 | 0.45 |
| 3:D:149:LEU:HD23 | 3:D:171:MET:CE | 2.47 | 0.45 |
| 1:E:1013:DT:H71 | 3:D:3197:MET:CG | 2.45 | 0.44 |
| 3:A:1194:GLN:NE2 | 3:A:1196:ARG:HH22 | 2.14 | 0.44 |
| 3:A:4194:GLN:NE2 | 3:A:4196:ARG:HH22 | 2.14 | 0.44 |
| 3:A:4154:GLU:C | 3:A:4156:GLU:H | 2.19 | 0.44 |
| 3:A:2149:LEU:HD23 | 3:A:2171:MET:CE | 2.47 | 0.44 |
| 3:D:130:ASP:OD2 | 3:D:134:ARG:NH1 | 2.50 | 0.44 |
| 3:A:1130:ASP:OD2 | 3:A:1134:ARG:NH1 | 2.51 | 0.44 |
| 3:A:3182:LEU:HD11 | 3:A:3189:LEU:HD12 | 1.99 | 0.44 |
| 1:E:1007:DA:C5' | 3:D:2212:GLY:HA2 | 2.47 | 0.44 |
| 3:D:2149:LEU:HD23 | 3:D:2171:MET:CE | 2.48 | 0.44 |
| 3:D:194:GLN:HE21 | 3:D:196:ARG:NH1 | 2.05 | 0.43 |
| 3:D:1080:ILE:HD11 | 3:D:1142:VAL:CG1 | 2.48 | 0.43 |
| 3:D:1130:ASP:OD2 | 3:D:1134:ARG:NH1 | 2.51 | 0.43 |
| 3:A:1111:ILE:HG22 | 3:A:2030:GLY:HA2 | 2.01 | 0.43 |
| 3:D:4254:PRO:HG3 | 6:D:3502:ADP:O2' | 2.18 | 0.43 |
| 3:D:3202:MET:HG2 | 3:D:3202:MET:H | 1.66 | 0.43 |
| 3:A:3101:PRO:HB3 | 3:A:4029:LEU:HD22 | 1.99 | 0.43 |
| 3:A:2177:LYS:HB3 | 3:A:2177:LYS:HE2 | 1.83 | 0.43 |
| 3:A:130:ASP:OD2 | 3:A:134:ARG:NH1 | 2.51 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:3130:ASP:OD2 | 3:D:3134:ARG:NH1 | 2.51 | 0.43 |
| 3:D:3080:ILE:HD11 | 3:D:3142:VAL:CG1 | 2.48 | 0.43 |
| 3:D:1149:LEU:HD23 | 3:D:1171:MET:CE | 2.48 | 0.43 |
| 3:A:2243:ARG:HG3 | 3:A:2259:GLU:HG2 | 2.00 | 0.43 |
| 3:A:3130:ASP:OD2 | 3:A:3134:ARG:NH1 | 2.51 | 0.43 |
| 3:D:2194:GLN:HE21 | 3:D:2196:ARG:NH1 | 2.04 | 0.43 |
| 3:D:3194:GLN:NE2 | 3:D:3196:ARG:HH22 | 2.16 | 0.43 |
| 3:D:4149:LEU:HD23 | 3:D:4171:MET:CE | 2.48 | 0.43 |
| 3:A:3194:GLN:NE2 | 3:A:3196:ARG:HH22 | 2.15 | 0.43 |
| 3:A:1149:LEU:HD23 | 3:A:1171:MET:CE | 2.48 | 0.43 |
| 3:A:4149:LEU:HD23 | 3:A:4171:MET:CE | 2.49 | 0.43 |
| 3:A:3182:LEU:HD23 | 3:A:3187:THR:HB | 2.00 | 0.43 |
| 3:D:4194:GLN:HE21 | 3:D:4196:ARG:NH1 | 2.03 | 0.43 |
| 3:D:2111:ILE:HG22 | 3:D:3030:GLY:HA2 | 2.01 | 0.43 |
| 3:D:2039:THR:HG23 | 3:D:2332:ASN:HD21 | 1.84 | 0.43 |
| 3:A:4080:ILE:HD11 | 3:A:4142:VAL:CG1 | 2.49 | 0.43 |
| 3:D:2243:ARG:HG3 | 3:D:2259:GLU:HG2 | 2.01 | 0.42 |
| 3:A:137:ALA:HB1 | 3:A:1010:LEU:HB2 | 2.00 | 0.42 |
| 3:A:1198:LYS:HG2 | 3:A:1206:PRO:O | 2.19 | 0.42 |
| 3:D:3124:GLN:HG3 | 3:D:4021:PHE:CD1 | 2.54 | 0.42 |
| 3:D:3198:LYS:HG2 | 3:D:3206:PRO:O | 2.20 | 0.42 |
| 3:D:1076:THR:HG22 | 3:D:1077:LEU:N | 2.34 | 0.42 |
| 3:D:3159:ILE:HD13 | 3:D:4126:LEU:HB3 | 2.02 | 0.42 |
| 3:A:3202:MET:H | 3:A:3202:MET:HG2 | 1.65 | 0.42 |
| 1:E:1013:DT:C7 | 3:D:3198:LYS:O | 2.67 | 0.42 |
| 3:D:2080:ILE:HD11 | 3:D:2142:VAL:CG1 | 2.48 | 0.42 |
| 3:A:2071:GLY:HA2 | 6:A:2502:ADP:H5'1 | 2.02 | 0.42 |
| 3:D:4130:ASP:OD2 | 3:D:4134:ARG:NH1 | 2.52 | 0.42 |
| 3:A:4095:ALA:O | 3:A:4097:HIS:HD2 | 2.03 | 0.42 |
| 3:A:4130:ASP:OD2 | 3:A:4134:ARG:NH1 | 2.53 | 0.42 |
| 3:D:1243:ARG:HG3 | 3:D:1259:GLU:HG2 | 2.01 | 0.42 |
| 3:A:1243:ARG:HG3 | 3:A:1259:GLU:HG2 | 2.02 | 0.42 |
| 3:A:2182:LEU:HD23 | 3:A:2187:THR:HB | 2.02 | 0.42 |
| 3:D:3194:GLN:HE21 | 3:D:3196:ARG:NH1 | 2.06 | 0.42 |
| 3:A:1068:GLU:HG2 | 3:A:2216:LYS:CB | 2.43 | 0.42 |
| 3:A:149:LEU:HD23 | 3:A:171:MET:CE | 2.48 | 0.42 |
| 3:D:2080:ILE:HD11 | 3:D:2142:VAL:HG13 | 2.02 | 0.42 |
| 3:A:2198:LYS:HG2 | 3:A:2206:PRO:O | 2.20 | 0.41 |
| 3:A:3177:LYS:HB3 | 3:A:3177:LYS:HE2 | 1.82 | 0.41 |
| 3:A:80:ILE:HD11 | 3:A:142:VAL:CG1 | 2.50 | 0.41 |
| 3:D:4023:LYS:H | 3:D:4023:LYS:HG2 | 1.74 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:A:3149:LEU:HD23 | 3:A:3171:MET:CE | 2.50 | 0.41 |
| 3:D:3149:LEU:HD23 | 3:D:3171:MET:CE | 2.50 | 0.41 |
| 3:D:71:GLY:HA2 | 6:D:502:ADP:H5'1 | 2.03 | 0.41 |
| 3:A:3080:ILE:HD11 | 3:A:3142:VAL:HG13 | 2.02 | 0.41 |
| 1:B:1003:DT:H2' | 3:A:197:MET:O | 2.20 | 0.41 |
| 3:A:243:ARG:HG3 | 3:A:259:GLU:HG2 | 2.02 | 0.41 |
| 3:D:4243:ARG:HG3 | 3:D:4259:GLU:HG2 | 2.03 | 0.41 |
| 3:D:2182:LEU:HD23 | 3:D:2187:THR:HB | 2.01 | 0.41 |
| 3:A:1202:MET:H | 3:A:1202:MET:HG2 | 1.64 | 0.41 |
| 3:D:3080:ILE:HD11 | 3:D:3142:VAL:HG13 | 2.02 | 0.41 |
| 3:A:177:LYS:HB3 | 3:A:177:LYS:HE2 | 1.85 | 0.41 |
| 3:D:4080:ILE:HD11 | 3:D:4142:VAL:CG1 | 2.50 | 0.41 |
| 3:D:1080:ILE:HD11 | 3:D:1142:VAL:HG13 | 2.02 | 0.41 |
| 3:A:2080:ILE:HD11 | 3:A:2142:VAL:CG1 | 2.50 | 0.41 |
| 3:D:3243:ARG:HG3 | 3:D:3259:GLU:HG2 | 2.02 | 0.41 |
| 3:A:182:LEU:HD23 | 3:A:187:THR:HB | 2.03 | 0.41 |
| 3:D:1202:MET:HG2 | 3:D:1202:MET:H | 1.65 | 0.41 |
| 3:D:1177:LYS:HB3 | 3:D:1177:LYS:HE2 | 1.84 | 0.41 |
| 3:D:3068:GLU:HA | 5:D:3501:ALF:F1 | 2.11 | 0.41 |
| 3:A:2330:ASN:N | 3:A:2331:PRO:HD3 | 2.35 | 0.41 |
| 3:A:2254:PRO:HG3 | 6:A:1502:ADP:O2' | 2.21 | 0.41 |
| 3:D:2076:THR:HG22 | 3:D:2077:LEU:N | 2.36 | 0.41 |
| 3:D:1182:LEU:HD23 | 3:D:1187:THR:HB | 2.03 | 0.41 |
| 3:D:3155:ILE:HA | 3:D:4177:LYS:HE3 | 2.03 | 0.41 |
| 3:A:4080:ILE:HD11 | 3:A:4142:VAL:HG13 | 2.03 | 0.40 |
| 3:A:3243:ARG:HG3 | 3:A:3259:GLU:HG2 | 2.04 | 0.40 |
| 3:A:1076:THR:HG22 | 3:A:1077:LEU:N | 2.36 | 0.40 |
| 3:D:4182:LEU:HD23 | 3:D:4187:THR:HB | 2.03 | 0.40 |
| 3:A:3115:LEU:HD21 | 3:A:4014:LEU:HD21 | 2.02 | 0.40 |
| 3:D:201:VAL:HG23 | 3:D:203:PHE:CE1 | 2.57 | 0.40 |
| 3:D:2146:VAL:O | 3:D:2149:LEU:HB2 | 2.22 | 0.40 |
| 3:D:3182:LEU:HD23 | 3:D:3187:THR:HB | 2.03 | 0.40 |
| 3:A:2033:ARG:NE | 3:A:2033:ARG:HA | 2.37 | 0.40 |
| 3:A:2282:LYS:HG3 | 3:D:3282:LYS:HG3 | 2.01 | 0.40 |
| 3:A:4149:LEU:HD23 | 3:A:4171:MET:HE1 | 2.01 | 0.40 |
| 3:A:4243:ARG:HG3 | 3:A:4259:GLU:HG2 | 2.02 | 0.40 |
| 3:A:2199:ILE:HD11 | 3:A:3164:MET:HE3 | 2.03 | 0.40 |
| 3:D:1101:PRO:HB3 | 3:D:2029:LEU:HD22 | 2.04 | 0.40 |
| 1:B:1010:DT:H5' | 3:A:3212:GLY:HA2 | 2.04 | 0.40 |
| 3:D:2198:LYS:HG2 | 3:D:2206:PRO:O | 2.22 | 0.40 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:D:218:TYR:OH | 3:D:4087:GLY:O[4_456] | 2.19 | 0.01 |

## 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 | |
|---|---|---|---|---|---|---|---|
| 3 | A | 1595/1706 (94%) | 1549 (97%) | 33 (2%) | 13 (1%) | 24 | 67 |
| 3 | D | 1595/1706 (94%) | 1539 (96%) | 43 (3%) | 13 (1%) | 24 | 67 |
| All | All | 3190/3412 (94%) | 3088 (97%) | 76 (2%) | 26 (1%) | 24 | 67 |

All (26) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 1023 | LYS |
| 3 | A | 2023 | LYS |
| 3 | A | 2330 | ASN |
| 3 | A | 3023 | LYS |
| 3 | A | 4023 | LYS |
| 3 | D | 1023 | LYS |
| 3 | D | 2023 | LYS |
| 3 | D | 3023 | LYS |
| 3 | D | 4023 | LYS |
| 3 | D | 1332 | ASN |
| 3 | D | 3269 | ASN |
| 3 | D | 332 | ASN |
| 3 | D | 2332 | ASN |
| 3 | A | 234 | GLY |
| 3 | A | 1234 | GLY |
| 3 | A | 2234 | GLY |
| 3 | A | 3234 | GLY |
| 3 | A | 3332 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 4234 | GLY |
| 3 | A | 4269 | ASN |
| 3 | D | 234 | GLY |
| 3 | D | 1234 | GLY |
| 3 | D | 2234 | GLY |
| 3 | D | 3234 | GLY |
| 3 | D | 4234 | GLY |
| 3 | A | 4155 | ILE |

### 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 |
|---|---|---|---|---|---|
| 3 | A | 1267/1339 (95%) | 1142 (90%) | 125 (10%) | 10 36 |
| 3 | D | 1267/1339 (95%) | 1136 (90%) | 131 (10%) | 9 34 |
| All | All | 2534/2678 (95%) | 2278 (90%) | 256 (10%) | 9 35 |

All (256) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 47 | LEU |
| 3 | A | 68 | GLU |
| 3 | A | 76 | THR |
| 3 | A | 85 | ARG |
| 3 | A | 114 | LEU |
| 3 | A | 140 | VAL |
| 3 | A | 142 | VAL |
| 3 | A | 146 | VAL |
| 3 | A | 149 | LEU |
| 3 | A | 166 | LEU |
| 3 | A | 183 | LYS |
| 3 | A | 189 | LEU |
| 3 | A | 193 | ASN |
| 3 | A | 205 | ASN |
| 3 | A | 208 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 209 | THR |
| 3 | A | 210 | THR |
| 3 | A | 223 | LEU |
| 3 | A | 251 | ILE |
| 3 | A | 285 | GLU |
| 3 | A | 311 | ASP |
| 3 | A | 314 | GLU |
| 3 | A | 1028 | ARG |
| 3 | A | 1029 | LEU |
| 3 | A | 1047 | LEU |
| 3 | A | 1068 | GLU |
| 3 | A | 1076 | THR |
| 3 | A | 1085 | ARG |
| 3 | A | 1114 | LEU |
| 3 | A | 1140 | VAL |
| 3 | A | 1142 | VAL |
| 3 | A | 1146 | VAL |
| 3 | A | 1149 | LEU |
| 3 | A | 1166 | LEU |
| 3 | A | 1183 | LYS |
| 3 | A | 1189 | LEU |
| 3 | A | 1193 | ASN |
| 3 | A | 1199 | ILE |
| 3 | A | 1202 | MET |
| 3 | A | 1205 | ASN |
| 3 | A | 1208 | THR |
| 3 | A | 1209 | THR |
| 3 | A | 1210 | THR |
| 3 | A | 1223 | LEU |
| 3 | A | 1251 | ILE |
| 3 | A | 1285 | GLU |
| 3 | A | 1311 | ASP |
| 3 | A | 1314 | GLU |
| 3 | A | 2028 | ARG |
| 3 | A | 2029 | LEU |
| 3 | A | 2047 | LEU |
| 3 | A | 2068 | GLU |
| 3 | A | 2076 | THR |
| 3 | A | 2085 | ARG |
| 3 | A | 2114 | LEU |
| 3 | A | 2140 | VAL |
| 3 | A | 2142 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 2146 | VAL |
| 3 | A | 2149 | LEU |
| 3 | A | 2166 | LEU |
| 3 | A | 2183 | LYS |
| 3 | A | 2189 | LEU |
| 3 | A | 2193 | ASN |
| 3 | A | 2199 | ILE |
| 3 | A | 2202 | MET |
| 3 | A | 2205 | ASN |
| 3 | A | 2208 | THR |
| 3 | A | 2209 | THR |
| 3 | A | 2210 | THR |
| 3 | A | 2223 | LEU |
| 3 | A | 2251 | ILE |
| 3 | A | 2285 | GLU |
| 3 | A | 2311 | ASP |
| 3 | A | 2314 | GLU |
| 3 | A | 3028 | ARG |
| 3 | A | 3029 | LEU |
| 3 | A | 3047 | LEU |
| 3 | A | 3068 | GLU |
| 3 | A | 3076 | THR |
| 3 | A | 3085 | ARG |
| 3 | A | 3114 | LEU |
| 3 | A | 3140 | VAL |
| 3 | A | 3142 | VAL |
| 3 | A | 3146 | VAL |
| 3 | A | 3149 | LEU |
| 3 | A | 3166 | LEU |
| 3 | A | 3183 | LYS |
| 3 | A | 3189 | LEU |
| 3 | A | 3193 | ASN |
| 3 | A | 3199 | ILE |
| 3 | A | 3202 | MET |
| 3 | A | 3205 | ASN |
| 3 | A | 3208 | THR |
| 3 | A | 3209 | THR |
| 3 | A | 3210 | THR |
| 3 | A | 3223 | LEU |
| 3 | A | 3251 | ILE |
| 3 | A | 3285 | GLU |
| 3 | A | 3311 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 3314 | GLU |
| 3 | A | 4028 | ARG |
| 3 | A | 4029 | LEU |
| 3 | A | 4047 | LEU |
| 3 | A | 4068 | GLU |
| 3 | A | 4076 | THR |
| 3 | A | 4085 | ARG |
| 3 | A | 4114 | LEU |
| 3 | A | 4140 | VAL |
| 3 | A | 4142 | VAL |
| 3 | A | 4146 | VAL |
| 3 | A | 4149 | LEU |
| 3 | A | 4155 | ILE |
| 3 | A | 4166 | LEU |
| 3 | A | 4183 | LYS |
| 3 | A | 4189 | LEU |
| 3 | A | 4193 | ASN |
| 3 | A | 4205 | ASN |
| 3 | A | 4208 | THR |
| 3 | A | 4209 | THR |
| 3 | A | 4210 | THR |
| 3 | A | 4223 | LEU |
| 3 | A | 4251 | ILE |
| 3 | A | 4285 | GLU |
| 3 | A | 4311 | ASP |
| 3 | A | 4314 | GLU |
| 3 | D | 47 | LEU |
| 3 | D | 68 | GLU |
| 3 | D | 76 | THR |
| 3 | D | 85 | ARG |
| 3 | D | 114 | LEU |
| 3 | D | 140 | VAL |
| 3 | D | 142 | VAL |
| 3 | D | 146 | VAL |
| 3 | D | 149 | LEU |
| 3 | D | 164 | MET |
| 3 | D | 166 | LEU |
| 3 | D | 183 | LYS |
| 3 | D | 189 | LEU |
| 3 | D | 193 | ASN |
| 3 | D | 202 | MET |
| 3 | D | 203 | PHE |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 205 | ASN |
| 3 | D | 208 | THR |
| 3 | D | 209 | THR |
| 3 | D | 210 | THR |
| 3 | D | 223 | LEU |
| 3 | D | 251 | ILE |
| 3 | D | 285 | GLU |
| 3 | D | 311 | ASP |
| 3 | D | 314 | GLU |
| 3 | D | 1028 | ARG |
| 3 | D | 1029 | LEU |
| 3 | D | 1047 | LEU |
| 3 | D | 1068 | GLU |
| 3 | D | 1076 | THR |
| 3 | D | 1085 | ARG |
| 3 | D | 1114 | LEU |
| 3 | D | 1140 | VAL |
| 3 | D | 1142 | VAL |
| 3 | D | 1146 | VAL |
| 3 | D | 1149 | LEU |
| 3 | D | 1166 | LEU |
| 3 | D | 1183 | LYS |
| 3 | D | 1189 | LEU |
| 3 | D | 1193 | ASN |
| 3 | D | 1199 | ILE |
| 3 | D | 1202 | MET |
| 3 | D | 1205 | ASN |
| 3 | D | 1208 | THR |
| 3 | D | 1209 | THR |
| 3 | D | 1210 | THR |
| 3 | D | 1223 | LEU |
| 3 | D | 1251 | ILE |
| 3 | D | 1285 | GLU |
| 3 | D | 1311 | ASP |
| 3 | D | 1314 | GLU |
| 3 | D | 1332 | ASN |
| 3 | D | 2028 | ARG |
| 3 | D | 2029 | LEU |
| 3 | D | 2047 | LEU |
| 3 | D | 2068 | GLU |
| 3 | D | 2076 | THR |
| 3 | D | 2085 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 2114 | LEU |
| 3 | D | 2140 | VAL |
| 3 | D | 2142 | VAL |
| 3 | D | 2146 | VAL |
| 3 | D | 2149 | LEU |
| 3 | D | 2166 | LEU |
| 3 | D | 2183 | LYS |
| 3 | D | 2189 | LEU |
| 3 | D | 2193 | ASN |
| 3 | D | 2199 | ILE |
| 3 | D | 2202 | MET |
| 3 | D | 2205 | ASN |
| 3 | D | 2208 | THR |
| 3 | D | 2209 | THR |
| 3 | D | 2210 | THR |
| 3 | D | 2223 | LEU |
| 3 | D | 2251 | ILE |
| 3 | D | 2285 | GLU |
| 3 | D | 2311 | ASP |
| 3 | D | 2314 | GLU |
| 3 | D | 2332 | ASN |
| 3 | D | 3028 | ARG |
| 3 | D | 3029 | LEU |
| 3 | D | 3047 | LEU |
| 3 | D | 3068 | GLU |
| 3 | D | 3076 | THR |
| 3 | D | 3085 | ARG |
| 3 | D | 3114 | LEU |
| 3 | D | 3140 | VAL |
| 3 | D | 3142 | VAL |
| 3 | D | 3146 | VAL |
| 3 | D | 3149 | LEU |
| 3 | D | 3166 | LEU |
| 3 | D | 3183 | LYS |
| 3 | D | 3189 | LEU |
| 3 | D | 3193 | ASN |
| 3 | D | 3199 | ILE |
| 3 | D | 3202 | MET |
| 3 | D | 3205 | ASN |
| 3 | D | 3208 | THR |
| 3 | D | 3209 | THR |
| 3 | D | 3210 | THR |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 3223 | LEU |
| 3 | D | 3251 | ILE |
| 3 | D | 3285 | GLU |
| 3 | D | 3311 | ASP |
| 3 | D | 3314 | GLU |
| 3 | D | 3329 | SER |
| 3 | D | 4028 | ARG |
| 3 | D | 4029 | LEU |
| 3 | D | 4047 | LEU |
| 3 | D | 4068 | GLU |
| 3 | D | 4076 | THR |
| 3 | D | 4085 | ARG |
| 3 | D | 4114 | LEU |
| 3 | D | 4140 | VAL |
| 3 | D | 4142 | VAL |
| 3 | D | 4146 | VAL |
| 3 | D | 4149 | LEU |
| 3 | D | 4164 | MET |
| 3 | D | 4166 | LEU |
| 3 | D | 4183 | LYS |
| 3 | D | 4189 | LEU |
| 3 | D | 4193 | ASN |
| 3 | D | 4205 | ASN |
| 3 | D | 4208 | THR |
| 3 | D | 4209 | THR |
| 3 | D | 4210 | THR |
| 3 | D | 4223 | LEU |
| 3 | D | 4251 | ILE |
| 3 | D | 4285 | GLU |
| 3 | D | 4311 | ASP |
| 3 | D | 4314 | GLU |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 97 | HIS |
| 3 | A | 181 | ASN |
| 3 | A | 193 | ASN |
| 3 | A | 194 | GLN |
| 3 | A | 205 | ASN |
| 3 | A | 300 | GLN |
| 3 | A | 304 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | A | 1097 | HIS |
| 3 | A | 1173 | GLN |
| 3 | A | 1181 | ASN |
| 3 | A | 1193 | ASN |
| 3 | A | 1194 | GLN |
| 3 | A | 1205 | ASN |
| 3 | A | 1300 | GLN |
| 3 | A | 1304 | ASN |
| 3 | A | 2097 | HIS |
| 3 | A | 2173 | GLN |
| 3 | A | 2181 | ASN |
| 3 | A | 2193 | ASN |
| 3 | A | 2194 | GLN |
| 3 | A | 2300 | GLN |
| 3 | A | 2304 | ASN |
| 3 | A | 2332 | ASN |
| 3 | A | 3097 | HIS |
| 3 | A | 3173 | GLN |
| 3 | A | 3181 | ASN |
| 3 | A | 3193 | ASN |
| 3 | A | 3194 | GLN |
| 3 | A | 3205 | ASN |
| 3 | A | 3300 | GLN |
| 3 | A | 3304 | ASN |
| 3 | A | 4097 | HIS |
| 3 | A | 4173 | GLN |
| 3 | A | 4181 | ASN |
| 3 | A | 4193 | ASN |
| 3 | A | 4194 | GLN |
| 3 | A | 4205 | ASN |
| 3 | A | 4300 | GLN |
| 3 | A | 4304 | ASN |
| 3 | D | 97 | HIS |
| 3 | D | 181 | ASN |
| 3 | D | 193 | ASN |
| 3 | D | 194 | GLN |
| 3 | D | 205 | ASN |
| 3 | D | 300 | GLN |
| 3 | D | 304 | ASN |
| 3 | D | 332 | ASN |
| 3 | D | 1097 | HIS |
| 3 | D | 1173 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | D | 1181 | ASN |
| 3 | D | 1193 | ASN |
| 3 | D | 1194 | GLN |
| 3 | D | 1205 | ASN |
| 3 | D | 1300 | GLN |
| 3 | D | 1304 | ASN |
| 3 | D | 1332 | ASN |
| 3 | D | 2097 | HIS |
| 3 | D | 2173 | GLN |
| 3 | D | 2181 | ASN |
| 3 | D | 2193 | ASN |
| 3 | D | 2194 | GLN |
| 3 | D | 2205 | ASN |
| 3 | D | 2300 | GLN |
| 3 | D | 2304 | ASN |
| 3 | D | 3097 | HIS |
| 3 | D | 3173 | GLN |
| 3 | D | 3181 | ASN |
| 3 | D | 3193 | ASN |
| 3 | D | 3194 | GLN |
| 3 | D | 3205 | ASN |
| 3 | D | 3300 | GLN |
| 3 | D | 3304 | ASN |
| 3 | D | 4097 | HIS |
| 3 | D | 4173 | GLN |
| 3 | D | 4181 | ASN |
| 3 | D | 4184 | GLN |
| 3 | D | 4193 | ASN |
| 3 | D | 4194 | GLN |
| 3 | D | 4205 | ASN |
| 3 | D | 4300 | GLN |
| 3 | D | 4304 | ASN |

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 for Mogul analysis.

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 | $\#\|Z\| > 2$ |
| 5 | ALF | A | 1501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | A | 1502 | 4 | 22,29,29 | 0.98 | 1 (4%) | 27,45,45 | 2.28 | 6 (22%) |
| 5 | ALF | A | 2501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | A | 2502 | 4 | 22,29,29 | 0.98 | 1 (4%) | 27,45,45 | 1.97 | 5 (18%) |
| 5 | ALF | A | 3501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | A | 3502 | 4 | 22,29,29 | 1.00 | 1 (4%) | 27,45,45 | 2.03 | 4 (14%) |
| 5 | ALF | A | 4501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | A | 4502 | 4 | 22,29,29 | 1.16 | 2 (9%) | 27,45,45 | 1.90 | 5 (18%) |
| 5 | ALF | A | 501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | A | 502 | 4 | 22,29,29 | 1.09 | 1 (4%) | 27,45,45 | 1.99 | 5 (18%) |
| 5 | ALF | D | 1501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | D | 1502 | 4 | 22,29,29 | 0.86 | 1 (4%) | 27,45,45 | 2.06 | 5 (18%) |
| 5 | ALF | D | 2501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | D | 2502 | 4 | 22,29,29 | 1.03 | 1 (4%) | 27,45,45 | 2.12 | 4 (14%) |
| 5 | ALF | D | 3501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | D | 3502 | 4 | 22,29,29 | 1.01 | 1 (4%) | 27,45,45 | 2.02 | 4 (14%) |
| 5 | ALF | D | 4501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | D | 4502 | 4 | 22,29,29 | 1.07 | 1 (4%) | 27,45,45 | 2.02 | 5 (18%) |
| 5 | ALF | D | 501 | - | 0,4,4 | 0.00 | - | 0,6,6 | 0.00 | - |
| 6 | ADP | D | 502 | 4 | 22,29,29 | 0.95 | 1 (4%) | 27,45,45 | 1.84 | 6 (22%) |

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 |
|---|---|---|---|---|---|---|---|
| 5 | ALF | A | 1501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | A | 1502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | A | 2501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | A | 2502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | A | 3501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | A | 3502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | A | 4501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | A | 4502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | A | 501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | A | 502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | D | 1501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | D | 1502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | D | 2501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | D | 2502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | D | 3501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | D | 3502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | D | 4501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | D | 4502 | 4 | - | 0/12/32/32 | 0/3/3/3 |
| 5 | ALF | D | 501 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | ADP | D | 502 | 4 | - | 0/12/32/32 | 0/3/3/3 |

All (11) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 6 | A | 4502 | ADP | O4'-C1' | 2.42 | 1.44 | 1.41 |
| 6 | D | 1502 | ADP | C5-C4 | 2.66 | 1.46 | 1.40 |
| 6 | A | 1502 | ADP | C5-C4 | 2.95 | 1.47 | 1.40 |
| 6 | A | 3502 | ADP | C5-C4 | 2.98 | 1.47 | 1.40 |
| 6 | D | 502 | ADP | C5-C4 | 3.07 | 1.47 | 1.40 |
| 6 | A | 2502 | ADP | C5-C4 | 3.11 | 1.47 | 1.40 |
| 6 | D | 3502 | ADP | C5-C4 | 3.18 | 1.47 | 1.40 |
| 6 | A | 4502 | ADP | C5-C4 | 3.32 | 1.48 | 1.40 |
| 6 | A | 502 | ADP | C5-C4 | 3.41 | 1.48 | 1.40 |
| 6 | D | 4502 | ADP | C5-C4 | 3.63 | 1.48 | 1.40 |
| 6 | D | 2502 | ADP | C5-C4 | 3.63 | 1.48 | 1.40 |

All (49) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | A | 1502 | ADP | N3-C2-N1 | -8.57 | 122.33 | 128.89 |
| 6 | D | 2502 | ADP | N3-C2-N1 | -7.99 | 122.78 | 128.89 |
| 6 | A | 3502 | ADP | N3-C2-N1 | -7.84 | 122.89 | 128.89 |
| 6 | D | 4502 | ADP | N3-C2-N1 | -7.39 | 123.24 | 128.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | A | 4502 | ADP | N3-C2-N1 | -7.36 | 123.26 | 128.89 |
| 6 | D | 1502 | ADP | N3-C2-N1 | -6.96 | 123.57 | 128.89 |
| 6 | A | 502 | ADP | N3-C2-N1 | -6.85 | 123.65 | 128.89 |
| 6 | D | 3502 | ADP | N3-C2-N1 | -6.32 | 124.05 | 128.89 |
| 6 | A | 2502 | ADP | N3-C2-N1 | -6.20 | 124.15 | 128.89 |
| 6 | D | 3502 | ADP | C2'-C1'-N9 | -5.90 | 105.27 | 114.29 |
| 6 | D | 1502 | ADP | C2'-C1'-N9 | -5.36 | 106.10 | 114.29 |
| 6 | D | 502 | ADP | N3-C2-N1 | -5.31 | 124.83 | 128.89 |
| 6 | A | 2502 | ADP | C2'-C1'-N9 | -4.96 | 106.72 | 114.29 |
| 6 | A | 1502 | ADP | C2'-C1'-N9 | -4.86 | 106.87 | 114.29 |
| 6 | D | 2502 | ADP | C2'-C1'-N9 | -4.64 | 107.21 | 114.29 |
| 6 | D | 502 | ADP | C2'-C1'-N9 | -4.51 | 107.40 | 114.29 |
| 6 | A | 3502 | ADP | C2'-C1'-N9 | -4.15 | 107.94 | 114.29 |
| 6 | D | 4502 | ADP | C2'-C1'-N9 | -4.14 | 107.96 | 114.29 |
| 6 | A | 502 | ADP | PA-O3A-PB | -3.83 | 119.84 | 132.67 |
| 6 | A | 502 | ADP | C2'-C1'-N9 | -3.80 | 108.48 | 114.29 |
| 6 | A | 2502 | ADP | PA-O3A-PB | -3.10 | 122.26 | 132.67 |
| 6 | D | 502 | ADP | C4-C5-N7 | -2.78 | 106.92 | 109.48 |
| 6 | A | 1502 | ADP | PA-O3A-PB | -2.68 | 123.67 | 132.67 |
| 6 | A | 4502 | ADP | C2'-C1'-N9 | -2.50 | 110.47 | 114.29 |
| 6 | A | 4502 | ADP | C4-C5-N7 | -2.46 | 107.21 | 109.48 |
| 6 | D | 1502 | ADP | C4-C5-N7 | -2.35 | 107.32 | 109.48 |
| 6 | D | 502 | ADP | PA-O3A-PB | -2.22 | 125.22 | 132.67 |
| 6 | D | 4502 | ADP | PA-O3A-PB | -2.16 | 125.44 | 132.67 |
| 6 | D | 2502 | ADP | PA-O3A-PB | -2.13 | 125.52 | 132.67 |
| 6 | D | 3502 | ADP | PA-O3A-PB | -2.11 | 125.59 | 132.67 |
| 6 | A | 502 | ADP | C4-C5-N7 | -2.07 | 107.58 | 109.48 |
| 6 | A | 2502 | ADP | C4-C5-N7 | -2.06 | 107.59 | 109.48 |
| 6 | D | 1502 | ADP | N6-C6-N1 | 2.02 | 123.54 | 119.20 |
| 6 | A | 1502 | ADP | C2-N1-C6 | 2.04 | 122.42 | 118.77 |
| 6 | A | 502 | ADP | O3B-PB-O2B | 2.07 | 115.24 | 107.38 |
| 6 | A | 4502 | ADP | C2-N1-C6 | 2.10 | 122.52 | 118.77 |
| 6 | D | 502 | ADP | O4'-C1'-N9 | 2.13 | 112.56 | 108.10 |
| 6 | A | 3502 | ADP | O2B-PB-O1B | 2.16 | 117.53 | 110.58 |
| 6 | A | 1502 | ADP | O3B-PB-O2B | 2.18 | 115.68 | 107.38 |
| 6 | D | 502 | ADP | O2B-PB-O1B | 2.21 | 117.68 | 110.58 |
| 6 | A | 1502 | ADP | N6-C6-N1 | 2.34 | 124.22 | 119.20 |
| 6 | A | 3502 | ADP | C2-N1-C6 | 2.37 | 123.00 | 118.77 |
| 6 | A | 2502 | ADP | O2B-PB-O1B | 2.45 | 118.47 | 110.58 |
| 6 | D | 4502 | ADP | O3B-PB-O2B | 2.46 | 116.73 | 107.38 |
| 6 | D | 3502 | ADP | O4'-C1'-N9 | 2.57 | 113.49 | 108.10 |
| 6 | D | 4502 | ADP | C2-N1-C6 | 2.59 | 123.39 | 118.77 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 6 | D | 1502 | ADP | O2B-PB-O1B | 2.64 | 119.09 | 110.58 |
| 6 | A | 4502 | ADP | O2B-PB-O1B | 2.65 | 119.11 | 110.58 |
| 6 | D | 2502 | ADP | C2-N1-C6 | 2.94 | 124.01 | 118.77 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 12 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 6 | A | 1502 | ADP | 2 | 0 |
| 6 | A | 2502 | ADP | 2 | 0 |
| 6 | A | 4502 | ADP | 1 | 0 |
| 6 | A | 502 | ADP | 1 | 0 |
| 5 | D | 1501 | ALF | 1 | 0 |
| 5 | D | 3501 | ALF | 1 | 0 |
| 6 | D | 3502 | ADP | 1 | 0 |
| 6 | D | 4502 | ADP | 1 | 0 |
| 6 | D | 502 | ADP | 2 | 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

## 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 | B | 12/15 (80%) | 0.10 | 1 (8%) 14 6 | 37, 42, 48, 48 | 0 |
| 1 | E | 12/15 (80%) | 0.08 | 0 100 100 | 38, 47, 53, 62 | 0 |
| 2 | C | 6/6 (100%) | 0.37 | 0 100 100 | 46, 48, 63, 66 | 1 (16%) |
| 2 | F | 6/6 (100%) | 0.27 | 0 100 100 | 48, 50, 55, 56 | 1 (16%) |
| 3 | A | 1609/1706 (94%) | 0.27 | 72 (4%) 37 21 | 39, 49, 64, 96 | 0 |
| 3 | D | 1609/1706 (94%) | 0.14 | 61 (3%) 44 27 | 39, 49, 65, 96 | 0 |
| All | All | 3254/3454 (94%) | 0.21 | 134 (4%) 41 25 | 37, 49, 64, 96 | 2 (0%) |

All (134) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | D | 4295 | GLY | 5.3 |
| 3 | A | 37 | VAL | 5.3 |
| 3 | A | 4164 | MET | 5.1 |
| 3 | A | 1333 | SER | 4.4 |
| 3 | D | 2001 | ALA | 4.4 |
| 3 | A | 1287 | ALA | 4.4 |
| 3 | D | 4297 | LYS | 4.3 |
| 3 | A | 3203 | PHE | 4.3 |
| 3 | D | 333 | SER | 4.2 |
| 3 | A | 288 | GLY | 4.2 |
| 3 | A | 3204 | GLY | 3.9 |
| 3 | A | 1202 | MET | 3.8 |
| 3 | A | 2202 | MET | 3.8 |
| 3 | A | 205 | ASN | 3.8 |
| 3 | D | 4291 | TYR | 3.8 |
| 3 | D | 3202 | MET | 3.8 |
| 3 | D | 3204 | GLY | 3.8 |
| 3 | A | 4155 | ILE | 3.7 |
| 3 | A | 276 | ASP | 3.7 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | A | 1289 | ALA | 3.7 |
| 3 | D | 3203 | PHE | 3.7 |
| 3 | A | 3202 | MET | 3.7 |
| 3 | A | 299 | GLY | 3.6 |
| 3 | A | 60 | ARG | 3.6 |
| 3 | A | 251 | ILE | 3.6 |
| 3 | D | 2002 | ILE | 3.5 |
| 3 | D | 4290 | TRP | 3.5 |
| 3 | A | 314 | GLU | 3.4 |
| 3 | D | 4001 | ALA | 3.3 |
| 3 | A | 1204 | GLY | 3.3 |
| 3 | D | 3001 | ALA | 3.3 |
| 3 | D | 4318 | GLU | 3.3 |
| 3 | D | 3330 | ASN | 3.2 |
| 3 | D | 4317 | LYS | 3.2 |
| 3 | A | 315 | THR | 3.1 |
| 3 | A | 331 | PRO | 3.1 |
| 3 | A | 282 | LYS | 3.1 |
| 3 | D | 4282 | LYS | 3.1 |
| 3 | D | 3023 | LYS | 3.1 |
| 3 | D | 4275 | VAL | 3.0 |
| 3 | A | 204 | GLY | 3.0 |
| 3 | A | 4001 | ALA | 3.0 |
| 3 | A | 55 | GLY | 3.0 |
| 3 | D | 3296 | GLU | 2.9 |
| 3 | A | 326 | LEU | 2.9 |
| 3 | D | 4313 | PRO | 2.9 |
| 3 | A | 253 | ALA | 2.9 |
| 3 | D | 3295 | GLY | 2.9 |
| 3 | D | 3287 | ALA | 2.8 |
| 3 | A | 1298 | ILE | 2.8 |
| 3 | A | 332 | ASN | 2.8 |
| 3 | A | 2287 | ALA | 2.7 |
| 3 | D | 4164 | MET | 2.7 |
| 3 | D | 4314 | GLU | 2.7 |
| 3 | D | 176 | ARG | 2.7 |
| 3 | A | 168 | ALA | 2.7 |
| 3 | A | 2200 | GLY | 2.7 |
| 3 | D | 4311 | ASP | 2.7 |
| 3 | A | 1286 | LYS | 2.6 |
| 3 | A | 333 | SER | 2.6 |
| 3 | A | 274 | LEU | 2.6 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | A | 1299 | GLY | 2.6 |
| 3 | D | 4315 | THR | 2.6 |
| 3 | D | 2023 | LYS | 2.6 |
| 3 | A | 4208 | THR | 2.6 |
| 3 | A | 1300 | GLN | 2.6 |
| 3 | A | 3003 | ASP | 2.6 |
| 3 | D | 4278 | GLY | 2.6 |
| 3 | D | 4321 | LYS | 2.6 |
| 3 | A | 197 | MET | 2.6 |
| 3 | A | 1297 | LYS | 2.5 |
| 3 | A | 4023 | LYS | 2.5 |
| 3 | A | 4002 | ILE | 2.5 |
| 3 | D | 4277 | LEU | 2.5 |
| 3 | D | 4294 | LYS | 2.5 |
| 3 | D | 332 | ASN | 2.5 |
| 3 | D | 4316 | ALA | 2.5 |
| 3 | A | 1321 | LYS | 2.5 |
| 3 | D | 4152 | LYS | 2.5 |
| 3 | D | 1202 | MET | 2.4 |
| 3 | D | 4312 | ASN | 2.4 |
| 3 | A | 53 | ALA | 2.4 |
| 3 | D | 4235 | GLU | 2.4 |
| 3 | D | 3329 | SER | 2.4 |
| 3 | D | 1333 | SER | 2.4 |
| 3 | D | 2333 | SER | 2.4 |
| 3 | D | 2145 | SER | 2.3 |
| 3 | A | 2201 | VAL | 2.3 |
| 3 | A | 1332 | ASN | 2.3 |
| 3 | A | 3220 | SER | 2.3 |
| 3 | A | 287 | ALA | 2.3 |
| 3 | A | 289 | ALA | 2.3 |
| 3 | D | 1200 | GLY | 2.3 |
| 3 | D | 4296 | GLU | 2.3 |
| 3 | A | 327 | LEU | 2.3 |
| 3 | A | 311 | ASP | 2.3 |
| 3 | A | 1308 | TRP | 2.3 |
| 3 | D | 2203 | PHE | 2.3 |
| 3 | D | 4328 | LEU | 2.3 |
| 3 | A | 298 | ILE | 2.3 |
| 3 | D | 1298 | ILE | 2.3 |
| 3 | D | 1289 | ALA | 2.3 |
| 3 | A | 1325 | GLU | 2.3 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 3 | A | 49 | ILE | 2.3 |
| 3 | D | 3317 | LYS | 2.2 |
| 3 | A | 280 | LYS | 2.2 |
| 3 | D | 1201 | VAL | 2.2 |
| 3 | A | 296 | GLU | 2.2 |
| 3 | A | 254 | PRO | 2.2 |
| 1 | B | 1002 | DT | 2.2 |
| 3 | A | 3144 | ASP | 2.2 |
| 3 | D | 2144 | ASP | 2.2 |
| 3 | D | 1204 | GLY | 2.2 |
| 3 | D | 202 | MET | 2.2 |
| 3 | A | 330 | ASN | 2.2 |
| 3 | D | 4005 | ASN | 2.2 |
| 3 | D | 204 | GLY | 2.1 |
| 3 | A | 1291 | TYR | 2.1 |
| 3 | A | 206 | PRO | 2.1 |
| 3 | A | 4156 | GLU | 2.1 |
| 3 | A | 300 | GLN | 2.1 |
| 3 | D | 4002 | ILE | 2.1 |
| 3 | D | 1332 | ASN | 2.1 |
| 3 | A | 1203 | PHE | 2.1 |
| 3 | D | 203 | PHE | 2.1 |
| 3 | D | 3200 | GLY | 2.1 |
| 3 | A | 199 | ILE | 2.1 |
| 3 | A | 216 | LYS | 2.1 |
| 3 | A | 1031 | GLU | 2.1 |
| 3 | D | 4287 | ALA | 2.1 |
| 3 | D | 2202 | MET | 2.1 |
| 3 | A | 265 | GLY | 2.0 |
| 3 | A | 278 | GLY | 2.0 |
| 3 | A | 313 | PRO | 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

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 | MG | A | 500 | 1/1 | 0.90 | 0.43 | 2.82 | 44,44,44,44 | 0 |
| 5 | ALF | A | 1501 | 5/5 | 0.93 | 0.30 | 1.47 | 35,35,38,41 | 0 |
| 5 | ALF | D | 3501 | 5/5 | 0.93 | 0.29 | 0.57 | 27,29,33,33 | 0 |
| 5 | ALF | D | 2501 | 5/5 | 0.96 | 0.36 | 0.37 | 24,26,29,30 | 0 |
| 5 | ALF | A | 501 | 5/5 | 0.92 | 0.30 | 0.32 | 38,39,44,46 | 0 |
| 6 | ADP | A | 502 | 27/27 | 0.91 | 0.26 | 0.06 | 42,44,48,49 | 0 |
| 5 | ALF | D | 501 | 5/5 | 0.97 | 0.31 | 0.05 | 30,30,32,35 | 0 |
| 5 | ALF | D | 1501 | 5/5 | 0.97 | 0.28 | -0.10 | 23,24,26,26 | 0 |
| 5 | ALF | A | 3501 | 5/5 | 0.94 | 0.28 | -0.33 | 28,28,31,32 | 0 |
| 6 | ADP | A | 3502 | 27/27 | 0.94 | 0.21 | -0.57 | 16,20,24,26 | 0 |
| 5 | ALF | D | 4501 | 5/5 | 0.90 | 0.17 | -0.58 | 41,41,43,43 | 0 |
| 6 | ADP | D | 3502 | 27/27 | 0.93 | 0.20 | -0.58 | 28,34,36,37 | 0 |
| 6 | ADP | A | 1502 | 27/27 | 0.96 | 0.20 | -0.65 | 27,30,35,35 | 0 |
| 5 | ALF | A | 4501 | 5/5 | 0.90 | 0.17 | -0.74 | 49,49,51,51 | 0 |
| 6 | ADP | D | 502 | 27/27 | 0.96 | 0.21 | -0.77 | 16,23,29,30 | 0 |
| 5 | ALF | A | 2501 | 5/5 | 0.96 | 0.26 | -0.94 | 24,25,27,28 | 0 |
| 6 | ADP | D | 4502 | 27/27 | 0.93 | 0.14 | -1.07 | 41,43,45,46 | 0 |
| 6 | ADP | A | 4502 | 27/27 | 0.93 | 0.14 | -1.24 | 31,42,44,45 | 0 |
| 6 | ADP | A | 2502 | 27/27 | 0.96 | 0.17 | -1.25 | 15,20,27,27 | 0 |
| 6 | ADP | D | 2502 | 27/27 | 0.95 | 0.19 | -1.31 | 25,27,29,30 | 0 |
| 6 | ADP | D | 1502 | 27/27 | 0.96 | 0.19 | -1.38 | 15,19,23,24 | 0 |
| 4 | MG | A | 3500 | 1/1 | 0.95 | 0.42 | - | 27,27,27,27 | 0 |
| 4 | MG | A | 4500 | 1/1 | 0.95 | 0.24 | - | 32,32,32,32 | 0 |
| 4 | MG | A | 1500 | 1/1 | 0.92 | 0.43 | - | 38,38,38,38 | 0 |
| 4 | MG | D | 500 | 1/1 | 0.92 | 0.39 | - | 34,34,34,34 | 0 |
| 4 | MG | D | 1500 | 1/1 | 0.96 | 0.41 | - | 28,28,28,28 | 0 |
| 4 | MG | D | 3500 | 1/1 | 0.87 | 0.36 | - | 31,31,31,31 | 0 |
| 4 | MG | A | 2500 | 1/1 | 0.94 | 0.42 | - | 25,25,25,25 | 0 |
| 4 | MG | D | 2500 | 1/1 | 0.94 | 0.55 | - | 32,32,32,32 | 0 |
| 4 | MG | D | 4500 | 1/1 | 0.80 | 0.19 | - | 39,39,39,39 | 0 |

## 6.5 Other polymers

There are no such residues in this entry.