# Full wwPDB EM Validation Report

May 19, 2025 – 07:30 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 9EGX / pdb_00009egx |
| EMDB ID | : | EMD-48039 |
| Title | : | RNA polymerase II-DSIF-SPT6-PAF1c-TFIIS-IWS1-hexasome, bp +27 |
| Authors | : | Markert, J.; Farnung, L. |
| Deposited on | : | 2024-11-21 |
| Resolution | : | 2.90 Å(reported) |

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

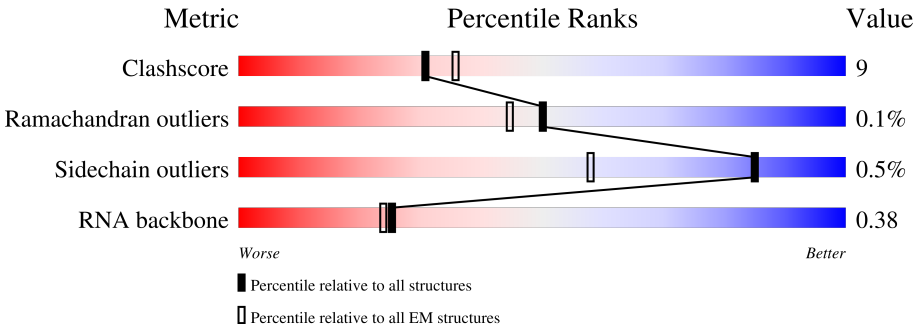
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev118 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0rc1 |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.43.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Clashscore | 210492 | 15764 |
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |
| RNA backbone | 6643 | 2191 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 1984 | 58% 14% 28% |
| 2 | B | 1251 | 74% 15% 10% |
| 3 | C | 275 | 80% 14% 6% |
| 4 | D | 142 | 82% 7% 11% |
| 5 | E | 210 | 83% 17% |
| 6 | F | 127 | 47% 14% 39% |
| 7 | G | 172 | 83% 16% |

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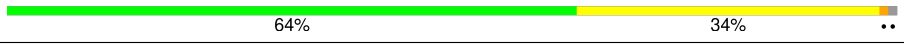
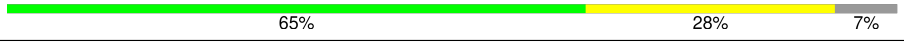
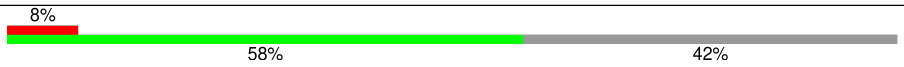
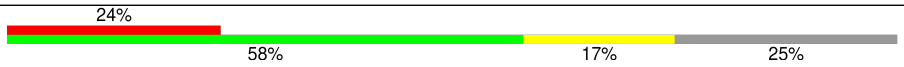
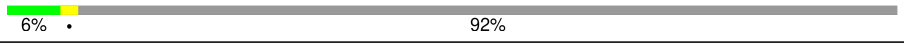
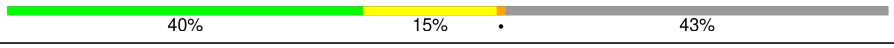
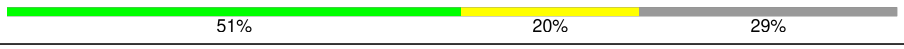
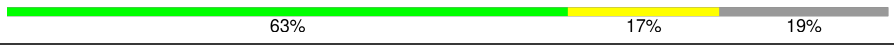
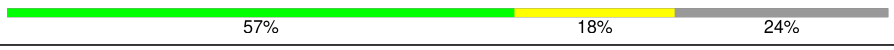
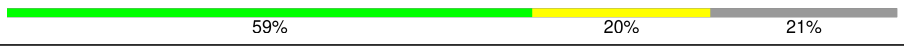
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 8 | H | 150 |   |
| 9 | I | 125 |   |
| 10 | J | 67 |   |
| 11 | K | 117 |   |
| 12 | L | 58 |   |
| 13 | M | 1729 |   |
| 14 | N | 206 |   |
| 15 | O | 821 |   |
| 16 | P | 21 |   |
| 17 | Q | 1179 |   |
| 18 | R | 713 |   |
| 19 | S | 304 |   |
| 20 | T | 215 |   |
| 21 | U | 666 |   |
| 22 | V | 531 |   |
| 23 | W | 305 |   |
| 24 | X | 531 |   |
| 25 | Y | 121 |   |
| 26 | Z | 1087 |   |
| 27 | a | 136 |   |
| 27 | e | 136 |   |
| 28 | b | 103 |   |
| 28 | f | 103 |   |
| 29 | c | 130 |   |
| 30 | d | 123 |   |

## 2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 65003 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase subunit.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | | |
| 1 | A | 1426 | 11210 | 7040 | 2013 | 2086 | 2 | 69 | 0 | 0 |

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | B | 1122 | 8980 | 5684 | 1576 | 1656 | 64 | 0 | 0 |

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | C | 258 | 2072 | 1300 | 356 | 410 | 6 | 0 | 0 |

- Molecule 4 is a protein called RNA polymerase Rpb4/RPC9 core domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | D | 126 | 1004 | 630 | 170 | 200 | 4 | 0 | 0 |

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit E.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | E | 209 | 1720 | 1089 | 300 | 323 | 8 | 0 | 0 |

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | F | 78 | 626 | 401 | 106 | 114 | 5 | 0 | 0 |

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 171 | Total | C | N | O | S | 0 | 0 |
| | | | 1333 | 866 | 214 | 245 | 8 | | |

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1197 | 759 | 195 | 238 | 5 | | |

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 582 | 168 | 181 | 11 | | |

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 66 | Total | C | N | O | S | 0 | 0 |
| | | | 524 | 339 | 88 | 91 | 6 | | |

- Molecule 11 is a protein called RNA polymerase II subunit J.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 115 | Total | C | N | O | S | 0 | 0 |
| | | | 920 | 593 | 152 | 173 | 2 | | |

- Molecule 12 is a protein called RNA polymerase II subunit K.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 397 | 246 | 77 | 68 | 6 | | |

- Molecule 13 is a protein called Transcription elongation factor SPT6.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 13 | M | 1002 | Total | C | N | O | 0 | 0 |
| | | | 4309 | 2295 | 1003 | 1011 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| M | -2 | SER | - | expression tag | UNP Q7KZ85 |
| M | -1 | ASN | - | expression tag | UNP Q7KZ85 |
| M | 0 | ALA | - | expression tag | UNP Q7KZ85 |

- Molecule 14 is a DNA chain called Non-template DNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | N | 148 | Total | C | N | O | P | 0 | 0 |
| | | | 3048 | 1446 | 555 | 899 | 148 | | |

- Molecule 15 is a protein called Protein IWS1 homolog.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 15 | O | 132 | Total | C | N | O | 0 | 0 |
| | | | 656 | 392 | 132 | 132 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| O | -1 | SER | - | expression tag | UNP Q96ST2 |
| O | 0 | ASN | - | expression tag | UNP Q96ST2 |
| O | 1 | ALA | - | expression tag | UNP Q96ST2 |

- Molecule 16 is a RNA chain called RNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | P | 21 | Total | C | N | O | P | 0 | 0 |
| | | | 432 | 193 | 59 | 159 | 21 | | |

- Molecule 17 is a protein called RNA polymerase-associated protein CTR9 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | Q | 890 | Total | C | N | O | S | 0 | 0 |
| | | | 6427 | 4026 | 1164 | 1218 | 19 | | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Q | 1174 | GLU | - | expression tag | UNP Q6PD62 |
| Q | 1175 | ASN | - | expression tag | UNP Q6PD62 |
| Q | 1176 | LEU | - | expression tag | UNP Q6PD62 |
| Q | 1177 | TYR | - | expression tag | UNP Q6PD62 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Q | 1178 | PHE | - | expression tag | UNP Q6PD62 |
| Q | 1179 | GLN | - | expression tag | UNP Q6PD62 |

- Molecule 18 is a protein called RNA polymerase-associated protein RTF1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | R | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1428 | 866 | 281 | 280 | 1 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| R | -2 | SER | - | expression tag | UNP Q92541 |
| R | -1 | ASN | - | expression tag | UNP Q92541 |
| R | 0 | ALA | - | expression tag | UNP Q92541 |

- Molecule 19 is a protein called Transcription elongation factor A protein 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 19 | S | 161 | Total | C | N | O | 0 | 0 |
| | | | 657 | 334 | 161 | 162 | | |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| S | -2 | SER | - | expression tag | UNP P23193 |
| S | -1 | ASN | - | expression tag | UNP P23193 |
| S | 0 | ALA | - | expression tag | UNP P23193 |

- Molecule 20 is a DNA chain called Template DNA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | T | 159 | Total | C | N | O | P | 0 | 0 |
| | | | 3245 | 1540 | 608 | 939 | 158 | | |

- Molecule 21 is a protein called RNA polymerase-associated protein LEO1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 21 | U | 125 | Total | C | N | O | 0 | 0 |
| | | | 617 | 367 | 125 | 125 | | |

- Molecule 22 is a protein called RNA polymerase II-associated factor 1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | V | 244 | Total | C | N | O | S | 0 | 0 |
| | | | 1378 | 842 | 267 | 267 | 2 | | |

- Molecule 23 is a protein called WDR61.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | W | 300 | Total | C | N | O | S | 0 | 0 |
| | | | 2333 | 1483 | 392 | 454 | 4 | | |

- Molecule 24 is a protein called Parafibromin.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 24 | X | 43 | Total | C | N | O | 0 | 0 |
| | | | 353 | 220 | 69 | 64 | | |

- Molecule 25 is a protein called Transcription elongation factor SPT4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | Y | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 911 | 570 | 159 | 173 | 9 | | |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| Y | -3 | GLY | - | expression tag | UNP P63272 |
| Y | -2 | PRO | - | expression tag | UNP P63272 |
| Y | -1 | GLY | - | expression tag | UNP P63272 |
| Y | 0 | SER | - | expression tag | UNP P63272 |

- Molecule 26 is a protein called Transcription elongation factor SPT5.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | Z | 510 | Total | C | N | O | P | S | 0 | 0 |
| | | | 4025 | 2552 | 709 | 745 | 1 | 18 | | |

- Molecule 27 is a protein called Histone H3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | a | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 627 | 397 | 116 | 111 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | e | 97 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 504 | 155 | 139 | 3 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| a | 36 | MET | LYS | engineered mutation | UNP A0A310TTQ1 |
| e | 36 | MET | LYS | engineered mutation | UNP A0A310TTQ1 |

- Molecule 28 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | b | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 662 | 418 | 129 | 114 | 1 | | |
| 28 | f | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 619 | 391 | 120 | 107 | 1 | | |

- Molecule 29 is a protein called Histone H2A type 1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 29 | c | 103 | Total | C | N | O | 0 | 0 |
| | | | 795 | 501 | 155 | 139 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| c | 99 | ARG | GLY | conflict | UNP P06897 |
| c | 123 | SER | ALA | conflict | UNP P06897 |

- Molecule 30 is a protein called Histone H2B 1.1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | d | 95 | Total | C | N | O | S | 0 | 0 |
| | | | 745 | 469 | 134 | 140 | 2 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| d | 0 | MET | - | initiating methionine | UNP P02281 |
| d | 29 | THR | SER | engineered mutation | UNP P02281 |

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 31 | A | 2 | Total Zn<br>2 2 | 0 |
| 31 | B | 1 | Total Zn<br>1 1 | 0 |
| 31 | C | 1 | Total Zn<br>1 1 | 0 |
| 31 | I | 2 | Total Zn<br>2 2 | 0 |
| 31 | J | 1 | Total Zn<br>1 1 | 0 |
| 31 | L | 1 | Total Zn<br>1 1 | 0 |
| 31 | Y | 1 | Total Zn<br>1 1 | 0 |

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

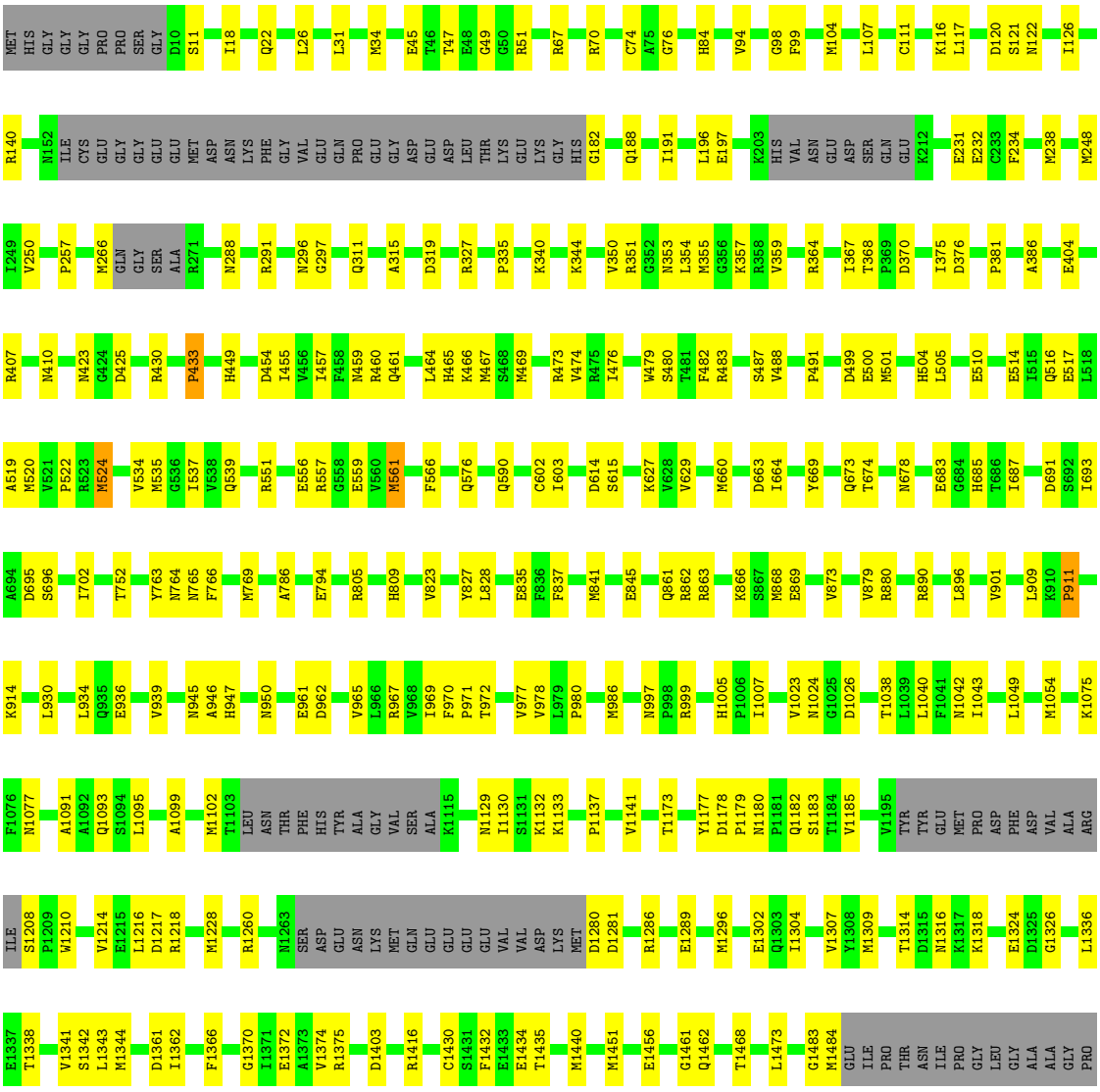
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 32 | A | 1 | Total Mg<br>1 1 | 0 |

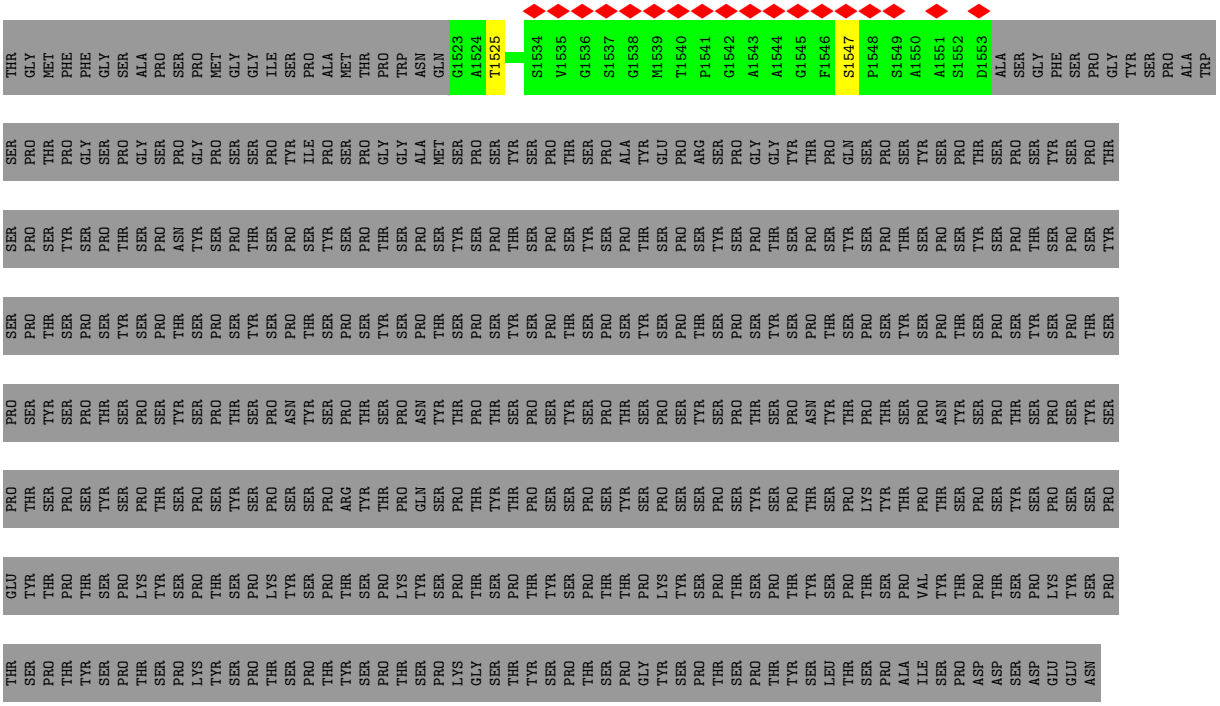
# 3 Residue-property plots (i)

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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-directed RNA polymerase subunit

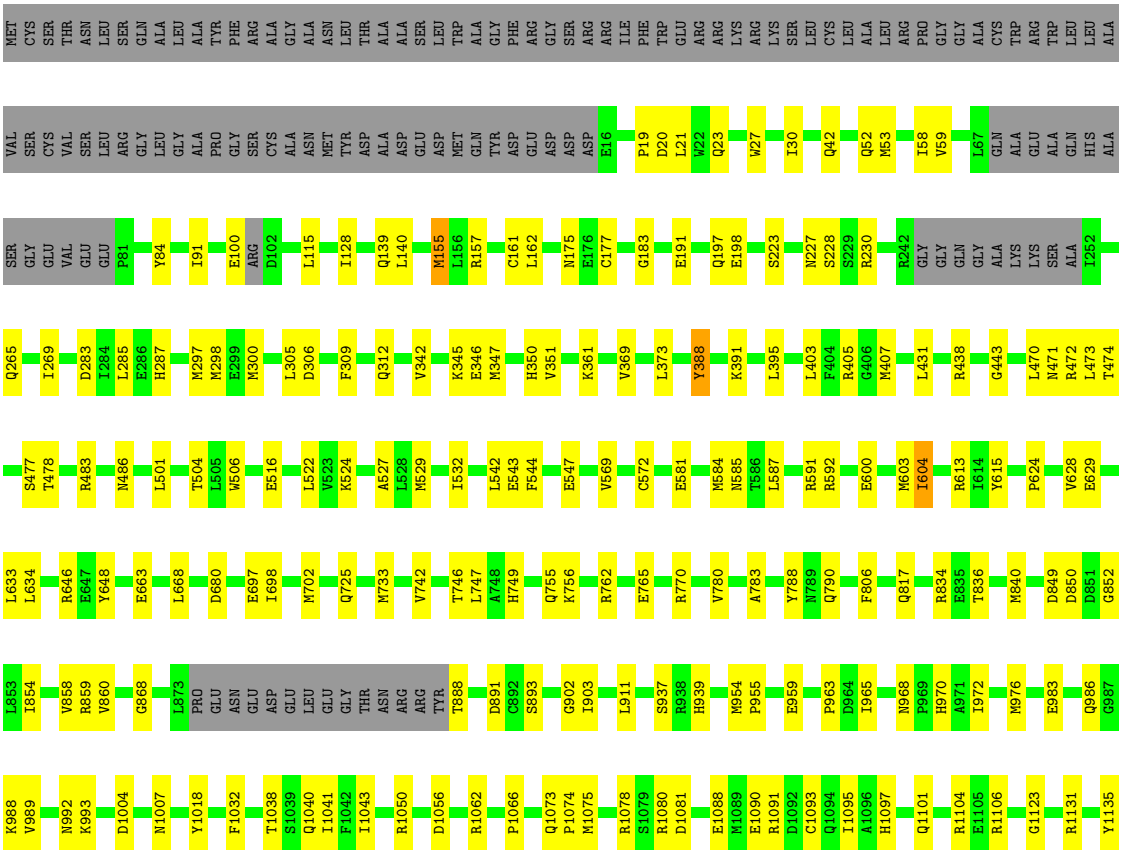
Chain A:

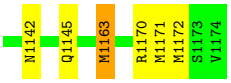





• Molecule 2: DNA-directed RNA polymerase subunit beta

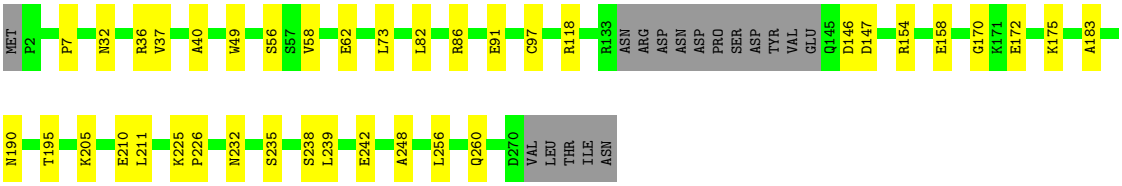
Chain B:




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

Chain C:

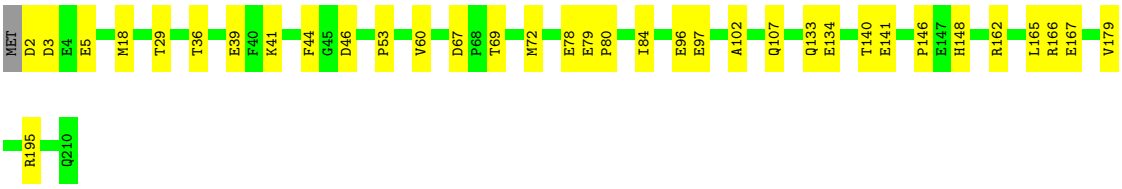

• Molecule 4: RNA polymerase Rpb4/RPC9 core domain-containing protein

Chain D:



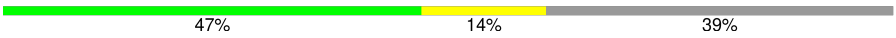
• Molecule 5: DNA-directed RNA polymerase II subunit E

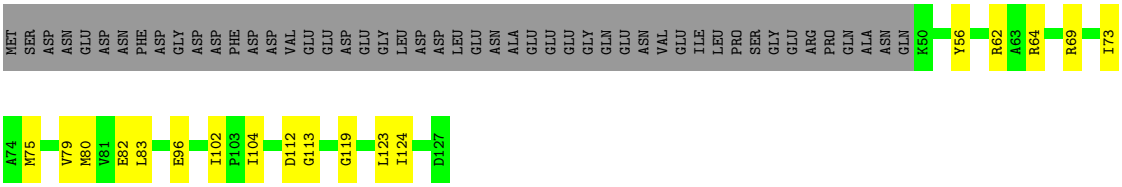
Chain E:


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



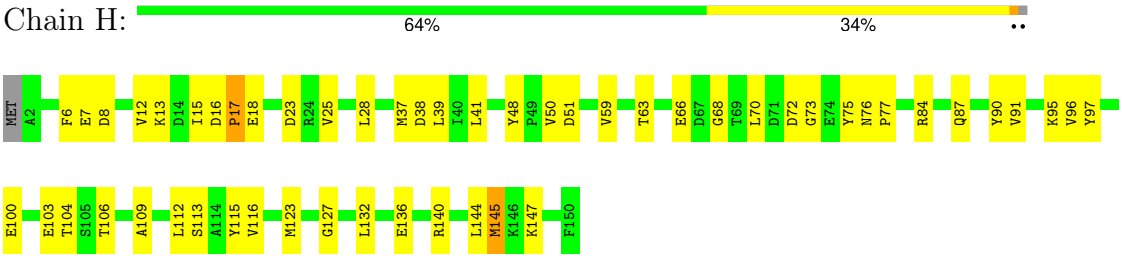

• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



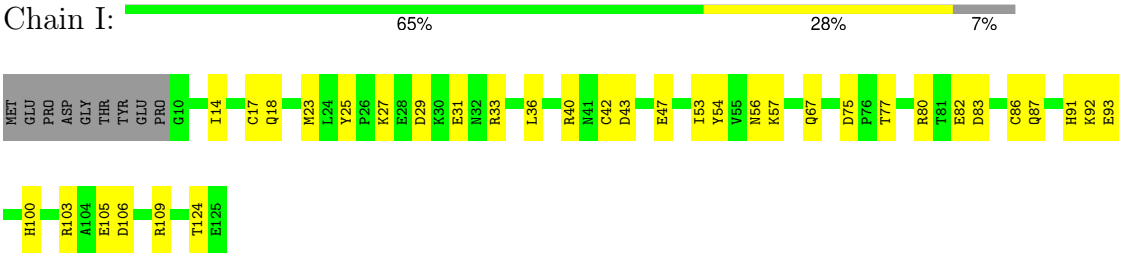
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



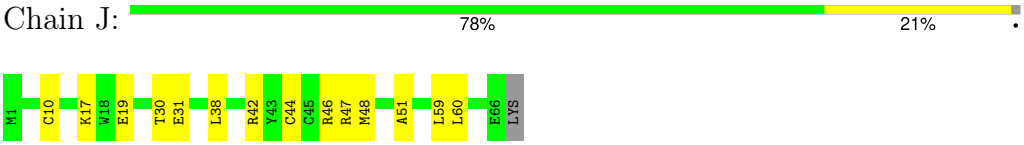

• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



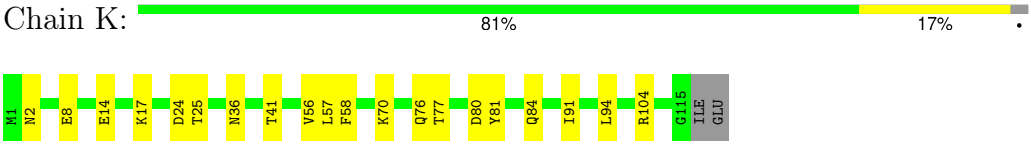

• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



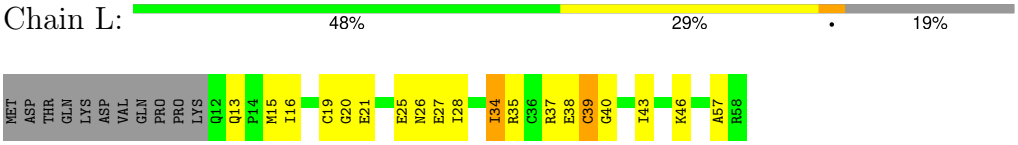

• Molecule 11: RNA polymerase II subunit J

Chain K:



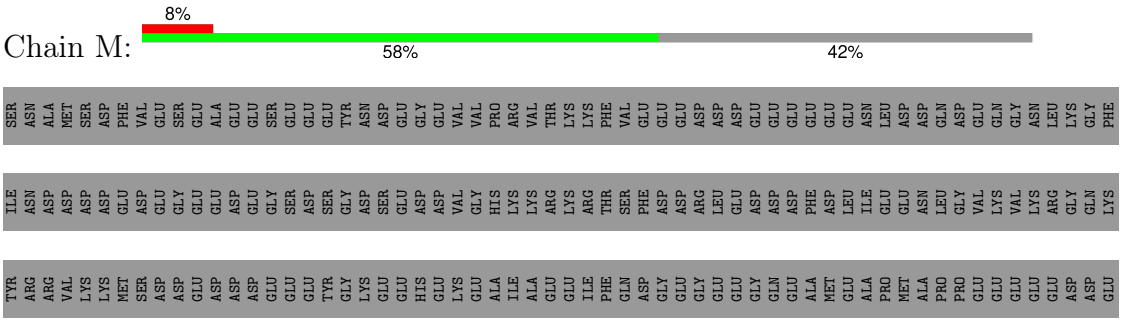

• Molecule 12: RNA polymerase II subunit K

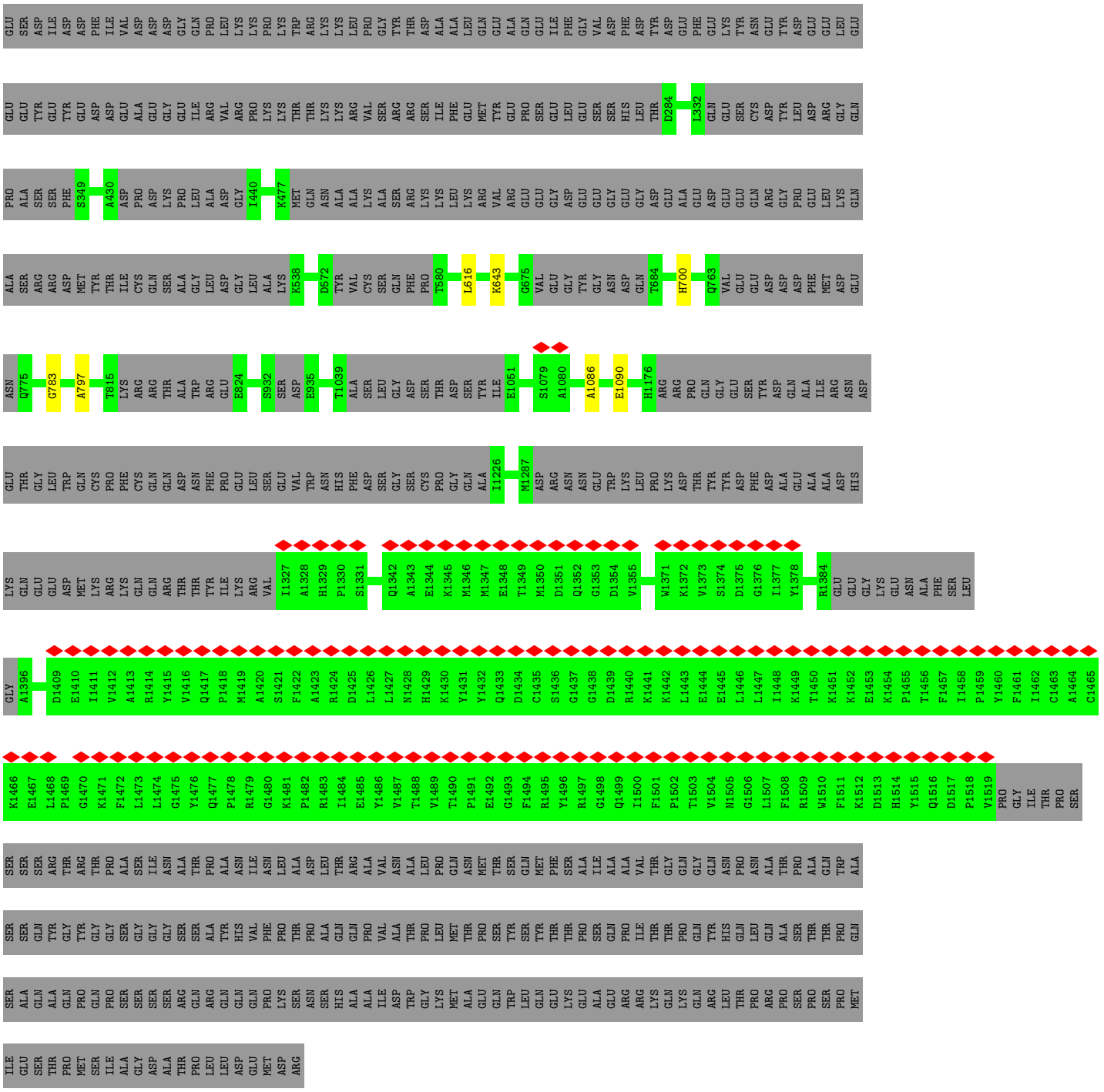
Chain L:




• Molecule 13: Transcription elongation factor SPT6

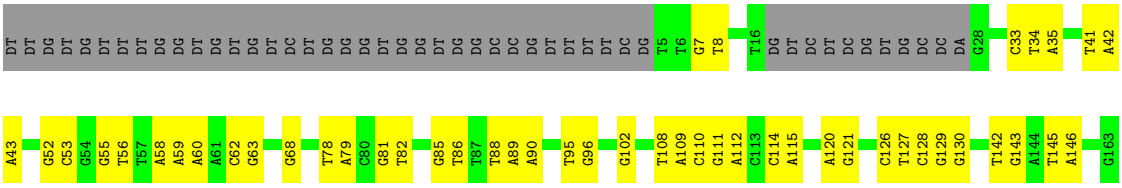
Chain M:





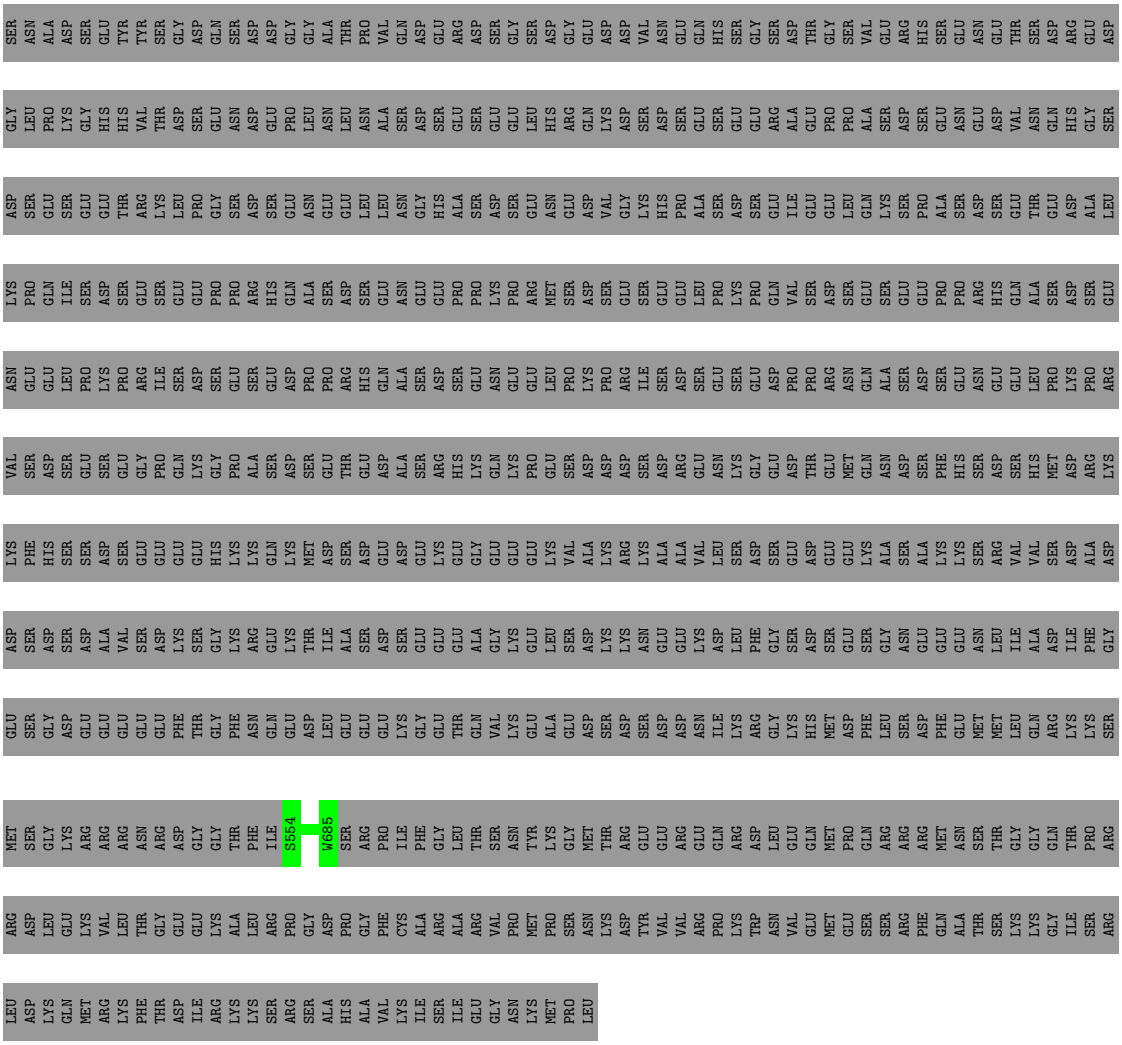
• Molecule 14: Non-template DNA

Chain N:

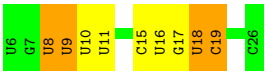

• Molecule 15: Protein IWS1 homolog

Chain O:

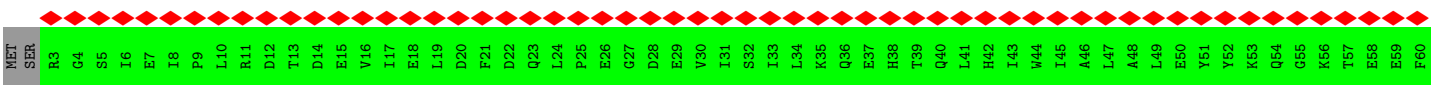

• Molecule 16: RNA

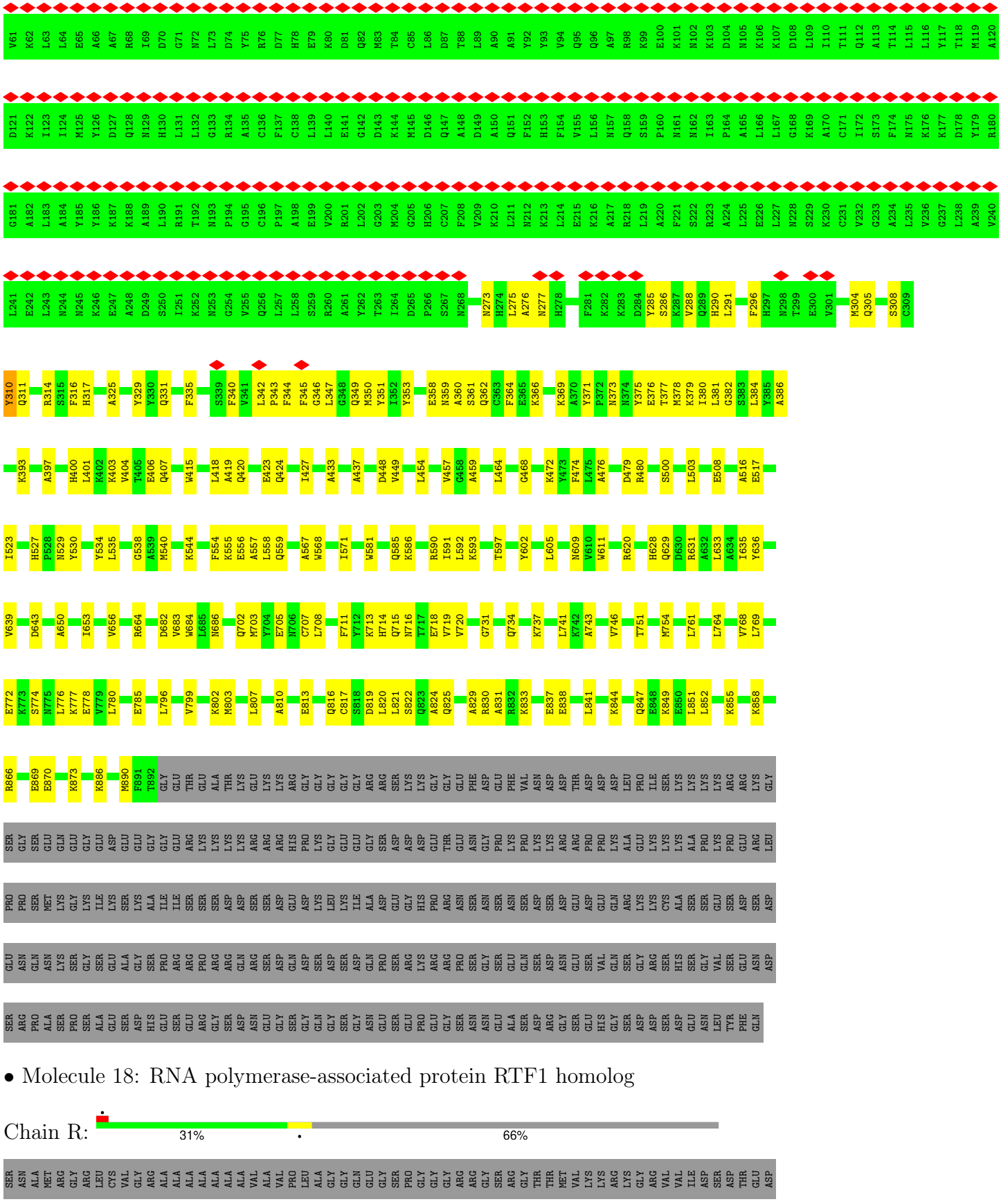
Chain P:


• Molecule 17: RNA polymerase-associated protein CTR9 homolog

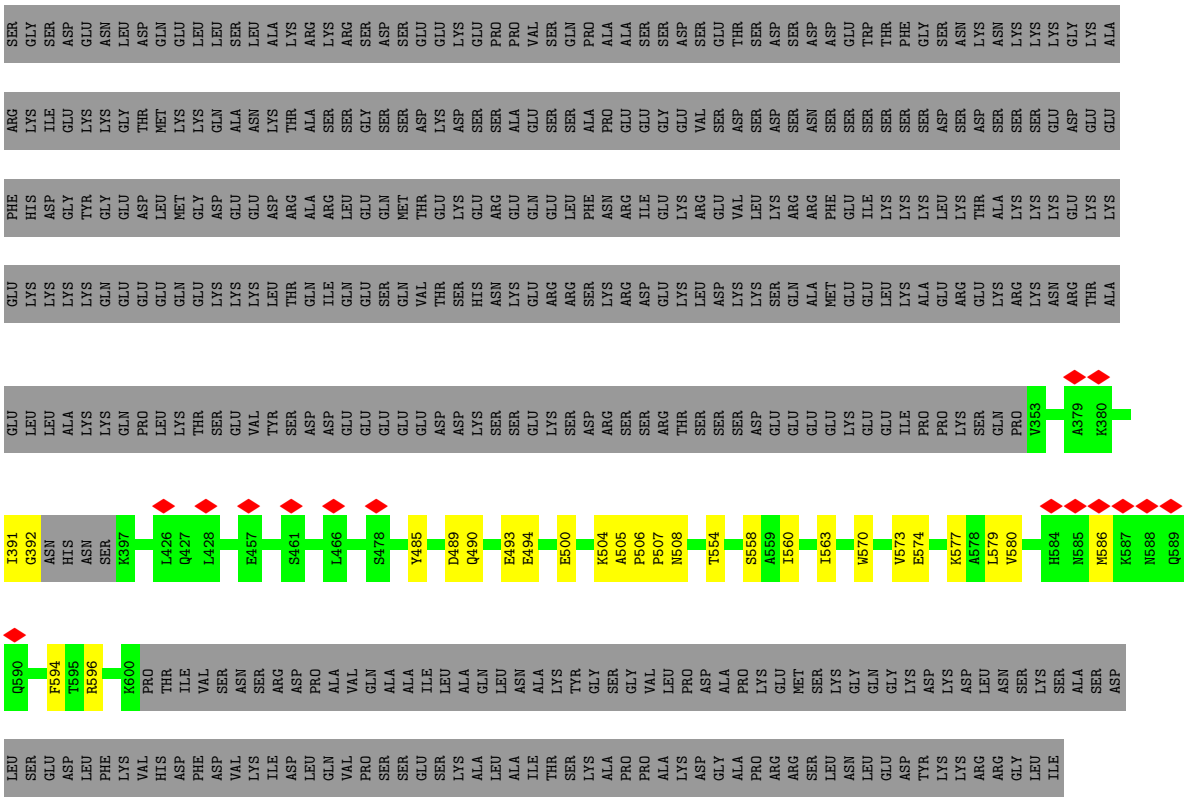
Chain Q:



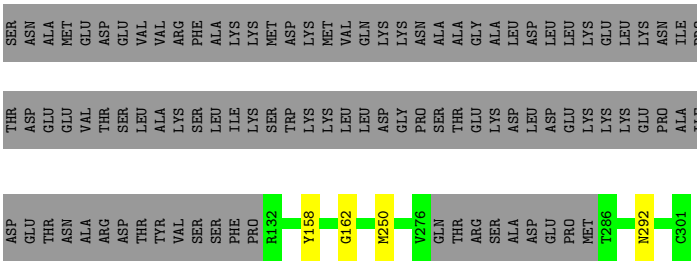

• Molecule 18: RNA polymerase-associated protein RTF1 homolog

Chain R:



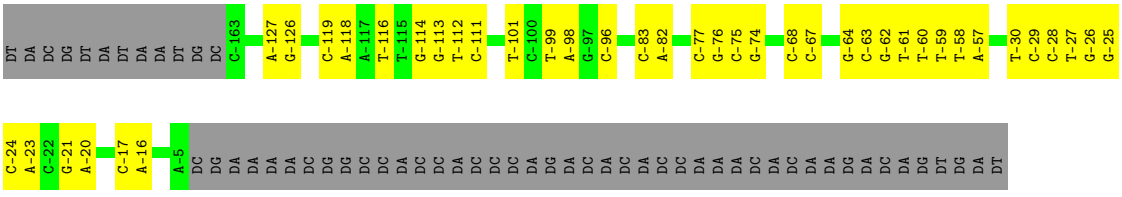
• Molecule 19: Transcription elongation factor A protein 1

Chain S:

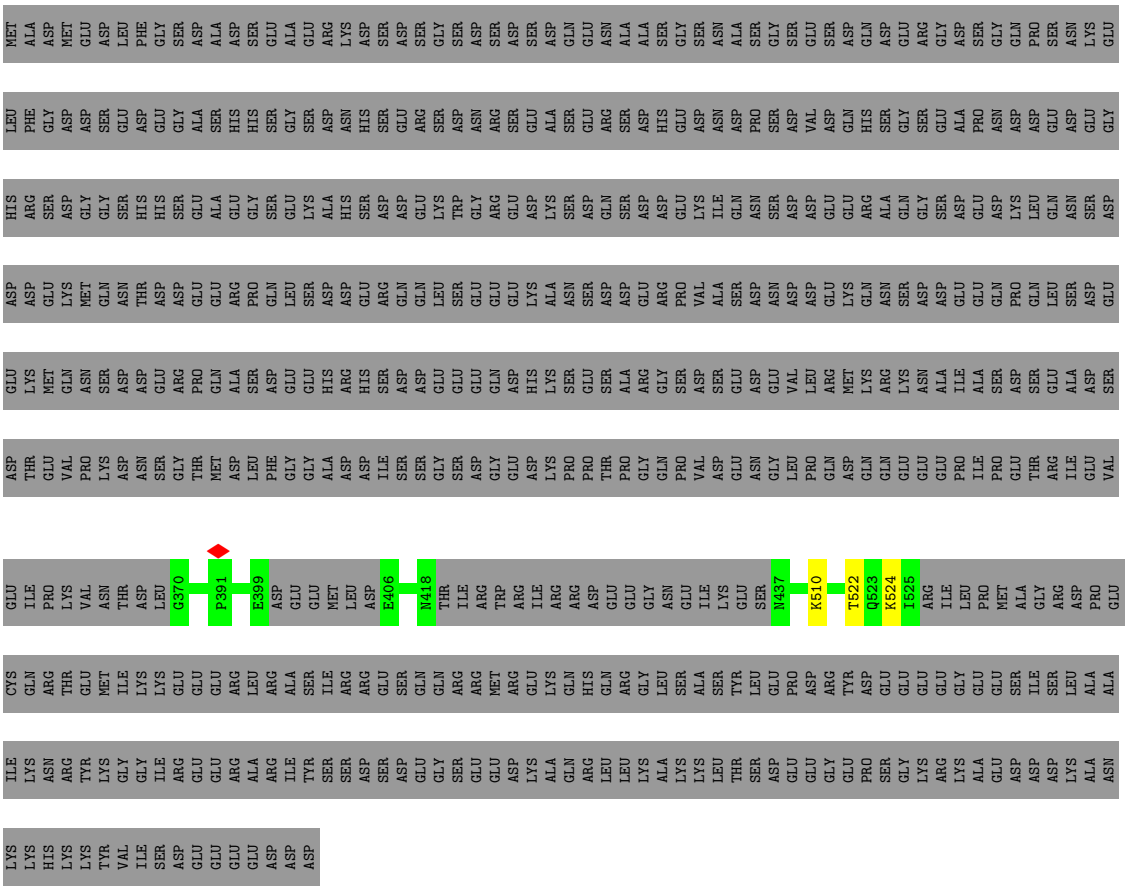
• Molecule 20: Template DNA

Chain T:

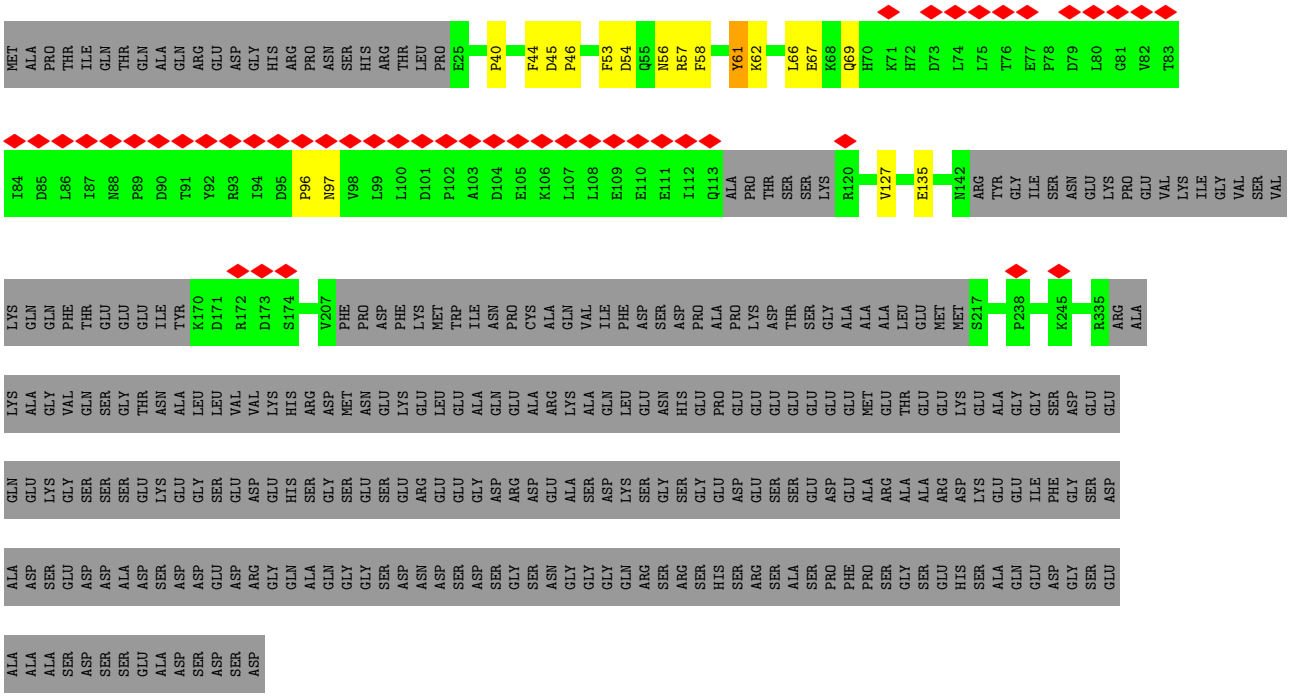
• Molecule 21: RNA polymerase-associated protein LEO1

Chain U:



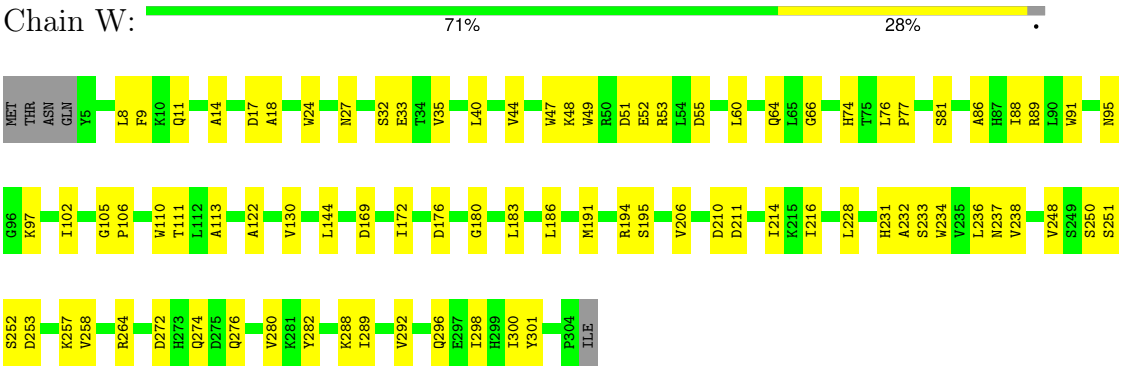

• Molecule 22: RNA polymerase II-associated factor 1 homolog

Chain V:

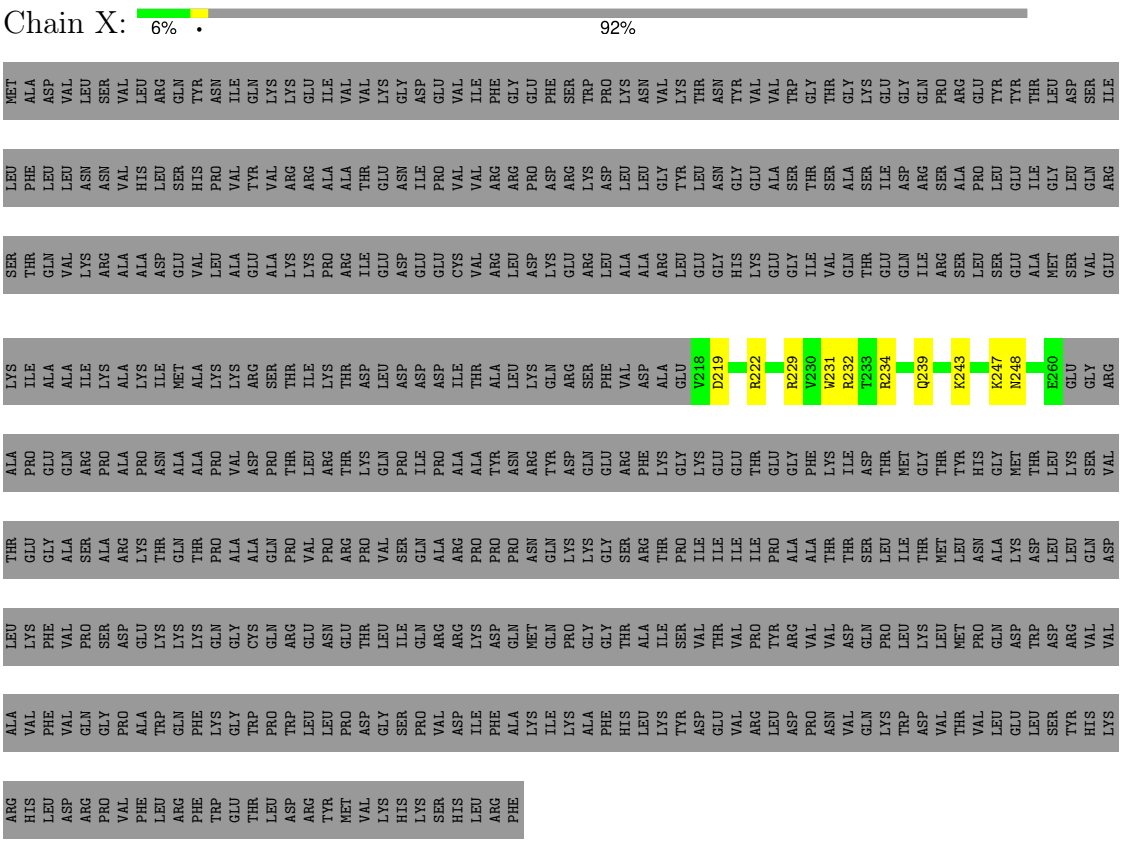
• Molecule 23: WDR61

Chain W:



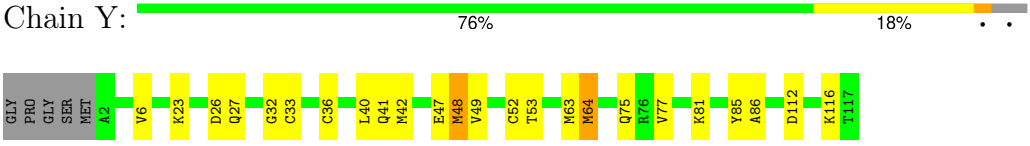

• Molecule 24: Parafibromin

Chain X:



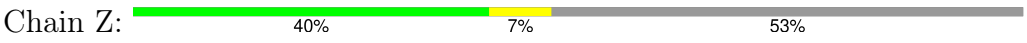

• Molecule 25: Transcription elongation factor SPT4

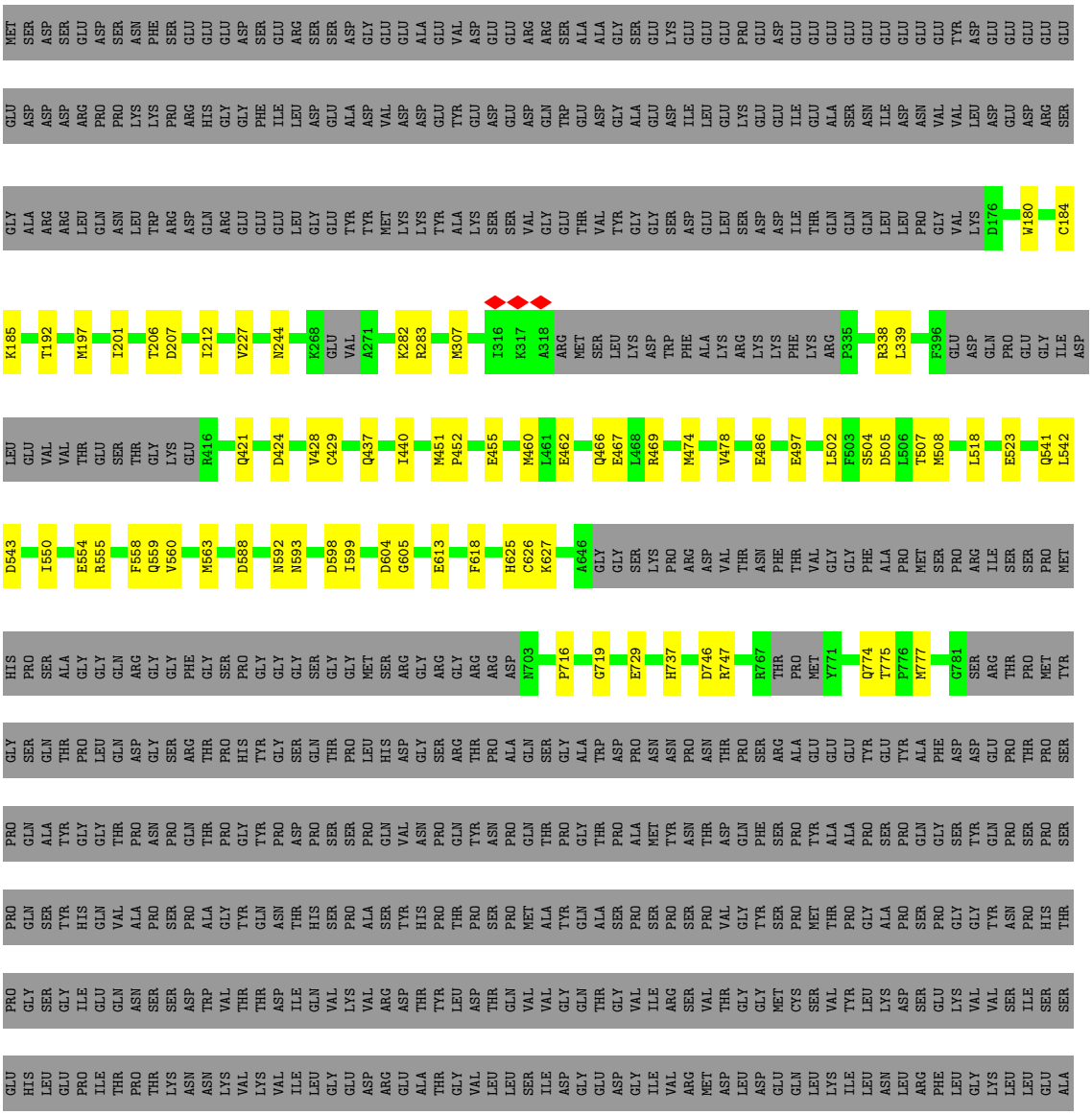
Chain Y:




• Molecule 26: Transcription elongation factor SPT5

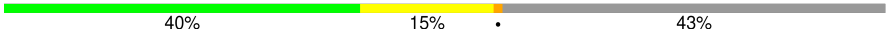
Chain Z:

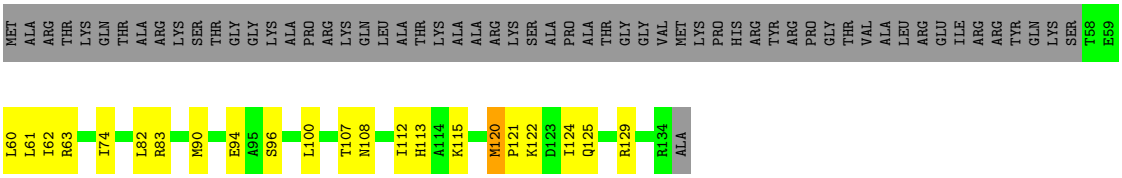




• Molecule 27: Histone H3

Chain a:



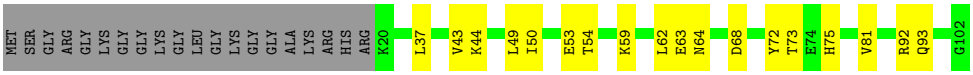
• Molecule 27: Histone H3

Chain e:



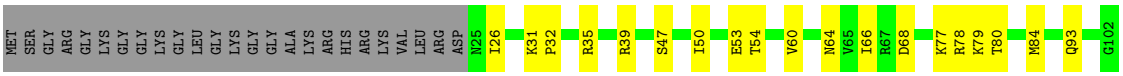
• Molecule 28: Histone H4

Chain b:


• Molecule 28: Histone H4

Chain f:

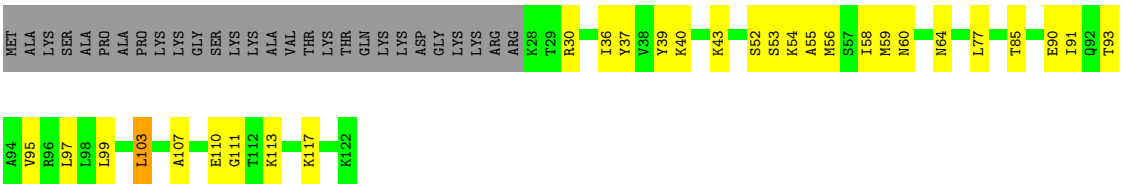

• Molecule 29: Histone H2A type 1

Chain c:



• Molecule 30: Histone H2B 1.1

Chain d:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 1139653 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 50 | Depositor |
| Minimum defocus (nm) | 900 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 BIOQUANTUM (6k x 4k) | Depositor |
| Maximum map value | 0.708 | Depositor |
| Minimum map value | -0.178 | Depositor |
| Average map value | 0.001 | Depositor |
| Map value standard deviation | 0.014 | Depositor |
| Recommended contour level | 0.02 | Depositor |
| Map size (Å) | 549.46, 549.46, 549.46 | wwPDB |
| Map dimensions | 500, 500, 500 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.09892, 1.09892, 1.09892 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, ZN, TPO

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 | 0.16 | 0/11384 | 0.39 | 2/15361 (0.0%) |
| 2 | B | 0.14 | 0/9158 | 0.34 | 0/12360 |
| 3 | C | 0.14 | 0/2115 | 0.33 | 0/2873 |
| 4 | D | 0.11 | 0/1017 | 0.31 | 0/1368 |
| 5 | E | 0.13 | 0/1751 | 0.33 | 0/2366 |
| 6 | F | 0.16 | 0/636 | 0.39 | 0/859 |
| 7 | G | 0.15 | 0/1364 | 0.36 | 0/1853 |
| 8 | H | 0.18 | 0/1219 | 0.44 | 1/1644 (0.1%) |
| 9 | I | 0.18 | 0/964 | 0.43 | 0/1305 |
| 10 | J | 0.17 | 0/533 | 0.41 | 0/719 |
| 11 | K | 0.15 | 0/939 | 0.36 | 0/1271 |
| 12 | L | 0.22 | 0/403 | 0.57 | 0/536 |
| 13 | M | 0.07 | 0/4330 | 0.22 | 0/5591 |
| 14 | N | 0.20 | 0/3417 | 0.41 | 0/5275 |
| 15 | O | 0.08 | 0/655 | 0.22 | 0/913 |
| 16 | P | 0.11 | 0/477 | 0.28 | 0/738 |
| 17 | Q | 0.15 | 0/6531 | 0.40 | 2/8861 (0.0%) |
| 18 | R | 0.13 | 0/1437 | 0.35 | 0/1972 |
| 19 | S | 0.08 | 0/659 | 0.18 | 0/827 |
| 20 | T | 0.18 | 0/3642 | 0.36 | 0/5614 |
| 21 | U | 0.08 | 0/613 | 0.28 | 0/847 |
| 22 | V | 0.12 | 0/1386 | 0.34 | 2/1909 (0.1%) |
| 23 | W | 0.25 | 1/2392 (0.0%) | 0.47 | 3/3257 (0.1%) |
| 24 | X | 0.31 | 0/356 | 0.46 | 0/478 |
| 25 | Y | 0.14 | 0/927 | 0.34 | 0/1250 |
| 26 | Z | 0.11 | 0/4084 | 0.31 | 0/5498 |
| 27 | a | 0.19 | 0/634 | 0.52 | 0/851 |
| 27 | e | 0.17 | 0/812 | 0.43 | 0/1088 |
| 28 | b | 0.18 | 0/669 | 0.43 | 0/894 |
| 28 | f | 0.19 | 0/626 | 0.46 | 0/837 |
| 29 | c | 0.17 | 0/805 | 0.40 | 0/1088 |
| 30 | d | 0.21 | 0/756 | 0.47 | 0/1015 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| All | All | 0.16 | 1/66691 (0.0%) | 0.37 | 10/91318 (0.0%) |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 23 | W | 106 | PRO | CG-CD | -8.41 | 1.28 | 1.51 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 23 | W | 106 | PRO | CA-N-CD | -13.85 | 92.11 | 111.50 |
| 1 | A | 911 | PRO | CA-N-CD | -10.54 | 97.24 | 112.00 |
| 23 | W | 106 | PRO | N-CD-CG | -10.21 | 91.55 | 103.80 |
| 1 | A | 433 | PRO | CA-N-CD | -8.53 | 100.06 | 112.00 |
| 17 | Q | 772 | GLU | CA-C-N | 7.58 | 135.34 | 121.70 |
| 17 | Q | 772 | GLU | C-N-CA | 7.58 | 135.34 | 121.70 |
| 8 | H | 17 | PRO | CA-N-CD | -6.84 | 102.43 | 112.00 |
| 23 | W | 52 | GLU | CA-CB-CG | 6.46 | 127.03 | 114.10 |
| 22 | V | 61 | TYR | CA-C-N | 6.03 | 132.55 | 121.70 |
| 22 | V | 61 | TYR | C-N-CA | 6.03 | 132.55 | 121.70 |

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 | A | 11210 | 0 | 11292 | 222 | 0 |
| 2 | B | 8980 | 0 | 9019 | 170 | 0 |
| 3 | C | 2072 | 0 | 2020 | 30 | 0 |
| 4 | D | 1004 | 0 | 980 | 10 | 0 |
| 5 | E | 1720 | 0 | 1737 | 27 | 0 |
| 6 | F | 626 | 0 | 657 | 17 | 0 |
| 7 | G | 1333 | 0 | 1321 | 21 | 0 |
| 8 | H | 1197 | 0 | 1156 | 35 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 9 | I | 942 | 0 | 872 | 35 | 0 |
| 10 | J | 524 | 0 | 541 | 14 | 0 |
| 11 | K | 920 | 0 | 942 | 17 | 0 |
| 12 | L | 397 | 0 | 405 | 16 | 0 |
| 13 | M | 4309 | 0 | 1506 | 3 | 0 |
| 14 | N | 3048 | 0 | 1669 | 37 | 0 |
| 15 | O | 656 | 0 | 290 | 0 | 0 |
| 16 | P | 432 | 0 | 219 | 3 | 0 |
| 17 | Q | 6427 | 0 | 5646 | 167 | 0 |
| 18 | R | 1428 | 0 | 922 | 22 | 0 |
| 19 | S | 657 | 0 | 199 | 3 | 0 |
| 20 | T | 3245 | 0 | 1780 | 39 | 0 |
| 21 | U | 617 | 0 | 263 | 1 | 0 |
| 22 | V | 1378 | 0 | 806 | 19 | 0 |
| 23 | W | 2333 | 0 | 2246 | 61 | 0 |
| 24 | X | 353 | 0 | 371 | 9 | 0 |
| 25 | Y | 911 | 0 | 907 | 20 | 0 |
| 26 | Z | 4025 | 0 | 4041 | 53 | 0 |
| 27 | a | 627 | 0 | 658 | 31 | 0 |
| 27 | e | 801 | 0 | 838 | 29 | 0 |
| 28 | b | 662 | 0 | 709 | 30 | 0 |
| 28 | f | 619 | 0 | 659 | 20 | 0 |
| 29 | c | 795 | 0 | 846 | 29 | 0 |
| 30 | d | 745 | 0 | 773 | 36 | 0 |
| 31 | A | 2 | 0 | 0 | 0 | 0 |
| 31 | B | 1 | 0 | 0 | 0 | 0 |
| 31 | C | 1 | 0 | 0 | 0 | 0 |
| 31 | I | 2 | 0 | 0 | 0 | 0 |
| 31 | J | 1 | 0 | 0 | 0 | 0 |
| 31 | L | 1 | 0 | 0 | 0 | 0 |
| 31 | Y | 1 | 0 | 0 | 0 | 0 |
| 32 | A | 1 | 0 | 0 | 0 | 0 |
| All | All | 65003 | 0 | 56290 | 1044 | 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 9.

All (1044) 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) |
|---|---|---|---|
| 29:c:92:GLU:HB3 | 30:d:103:LEU:HD11 | 1.48 | 0.95 |

*Continued on next page...*

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:Q:866:ARG:HH12 | 17:Q:870:GLU:HB2 | 1.33 | 0.94 |
| 2:B:911:LEU:HG | 12:L:34:ILE:HD11 | 1.54 | 0.87 |
| 8:H:37:MET:HG2 | 8:H:127:GLY:HA3 | 1.57 | 0.86 |
| 17:Q:713:LYS:HD3 | 17:Q:715:GLN:H | 1.43 | 0.84 |
| 1:A:1344:MET:HE3 | 5:E:133:GLN:HG3 | 1.60 | 0.83 |
| 1:A:823:VAL:HG22 | 1:A:835:GLU:HB2 | 1.60 | 0.83 |
| 1:A:51:ARG:H | 1:A:51:ARG:HD3 | 1.45 | 0.82 |
| 17:Q:276:ALA:HB1 | 17:Q:288:VAL:HG23 | 1.60 | 0.81 |
| 27:a:60:LEU:HD11 | 27:a:90:MET:HE1 | 1.62 | 0.81 |
| 17:Q:684:TRP:HA | 17:Q:703:MET:HE2 | 1.61 | 0.81 |
| 1:A:467:MET:HE1 | 1:A:524:MET:HG2 | 1.61 | 0.80 |
| 1:A:557:ARG:O | 1:A:561:MET:HB2 | 1.80 | 0.80 |
| 17:Q:371:TYR:OH | 22:V:69:GLN:NE2 | 2.15 | 0.80 |
| 2:B:604:ILE:HG22 | 2:B:613:ARG:H | 1.47 | 0.80 |
| 2:B:859:ARG:HA | 2:B:859:ARG:NH1 | 1.97 | 0.80 |
| 14:N:115:DA:N1 | 20:T:-114:DG:O6 | 2.15 | 0.79 |
| 1:A:914:LYS:H | 1:A:914:LYS:HE2 | 1.47 | 0.79 |
| 2:B:298:MET:HE3 | 9:I:14:ILE:H | 1.49 | 0.78 |
| 10:J:19:GLU:OE1 | 10:J:19:GLU:N | 2.16 | 0.77 |
| 1:A:1179:PRO:O | 9:I:33:ARG:NH2 | 2.18 | 0.77 |
| 8:H:17:PRO:HD2 | 8:H:18:GLU:H | 1.49 | 0.76 |
| 2:B:859:ARG:HD3 | 26:Z:737:HIS:HA | 1.67 | 0.76 |
| 2:B:790:GLN:O | 2:B:968:ASN:ND2 | 2.19 | 0.76 |
| 27:a:125:GLN:NE2 | 28:b:53:GLU:OE1 | 2.18 | 0.76 |
| 17:Q:310:TYR:CE2 | 17:Q:343:PRO:HA | 2.21 | 0.75 |
| 29:c:104:GLN:HB2 | 30:d:54:LYS:HZ2 | 1.51 | 0.75 |
| 14:N:115:DA:C2 | 20:T:-114:DG:C6 | 2.75 | 0.75 |
| 17:Q:605:LEU:O | 17:Q:609:ASN:ND2 | 2.20 | 0.74 |
| 26:Z:451:MET:HB2 | 26:Z:460:MET:HG2 | 1.67 | 0.74 |
| 3:C:36:ARG:NH1 | 11:K:41:THR:OG1 | 2.21 | 0.74 |
| 1:A:914:LYS:HE2 | 1:A:914:LYS:N | 2.04 | 0.73 |
| 29:c:50:TYR:HB3 | 30:d:91:ILE:HD11 | 1.70 | 0.73 |
| 1:A:1208:SER:HG | 1:A:1210:TRP:NE1 | 1.86 | 0.72 |
| 17:Q:378:MET:HE1 | 22:V:56:ASN:HD21 | 1.53 | 0.72 |
| 9:I:92:LYS:HE2 | 9:I:92:LYS:H | 1.54 | 0.72 |
| 1:A:1208:SER:OG | 1:A:1210:TRP:NE1 | 2.23 | 0.72 |
| 11:K:14:GLU:N | 11:K:14:GLU:OE2 | 2.22 | 0.72 |
| 28:b:75:HIS:HD2 | 30:d:93:THR:HG21 | 1.54 | 0.72 |
| 1:A:140:ARG:NH2 | 1:A:234:PHE:O | 2.23 | 0.71 |
| 1:A:965:VAL:O | 1:A:969:ILE:HG22 | 1.90 | 0.71 |
| 17:Q:682:ASP:O | 17:Q:686:ASN:ND2 | 2.22 | 0.71 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:Q:768:VAL:HG21 | 17:Q:778:GLU:HG3 | 1.72 | 0.71 |
| 1:A:1099:ALA:HA | 1:A:1102:MET:HE3 | 1.73 | 0.71 |
| 1:A:1342:SER:O | 1:A:1344:MET:N | 2.23 | 0.71 |
| 27:a:82:LEU:HD11 | 28:b:81:VAL:HG23 | 1.71 | 0.71 |
| 9:I:47:GLU:OE1 | 9:I:47:GLU:N | 2.24 | 0.70 |
| 1:A:827:TYR:HE2 | 2:B:976:MET:HE3 | 1.56 | 0.70 |
| 17:Q:517:GLU:HG3 | 17:Q:540:MET:HE3 | 1.72 | 0.70 |
| 20:T:-126:DG:OP1 | 30:d:39:TYR:OH | 2.09 | 0.70 |
| 9:I:100:HIS:ND1 | 9:I:100:HIS:O | 2.23 | 0.70 |
| 17:Q:534:TYR:OH | 17:Q:556:GLU:OE1 | 2.10 | 0.70 |
| 1:A:111:CYS:SG | 1:A:188:GLN:NE2 | 2.65 | 0.70 |
| 1:A:514:GLU:OE1 | 2:B:1101:GLN:NE2 | 2.24 | 0.70 |
| 2:B:725:GLN:NE2 | 2:B:937:SER:O | 2.24 | 0.70 |
| 11:K:36:ASN:OD1 | 11:K:70:LYS:NZ | 2.25 | 0.70 |
| 14:N:115:DA:N1 | 20:T:-114:DG:C6 | 2.60 | 0.70 |
| 28:f:26:ILE:H | 28:f:26:ILE:HD12 | 1.56 | 0.70 |
| 17:Q:329:TYR:HB3 | 17:Q:347:LEU:HD22 | 1.72 | 0.70 |
| 14:N:68:DG:OP1 | 27:e:42:ARG:NH2 | 2.25 | 0.69 |
| 27:a:120:MET:HE2 | 27:a:122:LYS:HG2 | 1.73 | 0.69 |
| 26:Z:504:SER:OG | 26:Z:507:THR:O | 2.10 | 0.69 |
| 1:A:576:GLN:O | 1:A:590:GLN:NE2 | 2.25 | 0.69 |
| 2:B:756:LYS:NZ | 22:V:135:GLU:O | 2.26 | 0.69 |
| 30:d:107:ALA:HA | 30:d:110:GLU:CD | 2.18 | 0.69 |
| 17:Q:803:MET:HE1 | 17:Q:807:LEU:HD21 | 1.75 | 0.68 |
| 18:R:485:TYR:OH | 18:R:489:ASP:OD2 | 2.12 | 0.68 |
| 2:B:591:ARG:NH2 | 2:B:663:GLU:OE2 | 2.25 | 0.68 |
| 27:e:64:LYS:HZ2 | 27:e:89:VAL:HG12 | 1.58 | 0.68 |
| 1:A:1372:GLU:OE2 | 5:E:195:ARG:NH1 | 2.27 | 0.68 |
| 17:Q:866:ARG:O | 17:Q:866:ARG:NH1 | 2.27 | 0.68 |
| 23:W:8:LEU:HD13 | 23:W:288:LYS:HE3 | 1.75 | 0.68 |
| 1:A:1375:ARG:NE | 1:A:1403:ASP:OD1 | 2.26 | 0.67 |
| 17:Q:769:LEU:HD13 | 17:Q:824:ALA:HB2 | 1.75 | 0.67 |
| 2:B:230:ARG:HH22 | 2:B:346:GLU:HA | 1.59 | 0.67 |
| 8:H:38:ASP:OD1 | 8:H:39:LEU:N | 2.28 | 0.67 |
| 1:A:353:ASN:ND2 | 2:B:1073:GLN:OE1 | 2.27 | 0.67 |
| 2:B:1142:ASN:ND2 | 2:B:1145:GLN:O | 2.27 | 0.67 |
| 17:Q:817:CYS:HA | 17:Q:820:LEU:HD12 | 1.75 | 0.67 |
| 17:Q:711:PHE:HE2 | 23:W:233:SER:HB3 | 1.59 | 0.67 |
| 2:B:228:SER:O | 2:B:405:ARG:NH1 | 2.27 | 0.67 |
| 17:Q:310:TYR:OH | 17:Q:342:LEU:O | 2.13 | 0.67 |
| 2:B:850:ASP:OD2 | 12:L:13:GLN:NE2 | 2.28 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:118:ARG:NH1 | 3:C:147:ASP:OD2 | 2.29 | 0.66 |
| 23:W:191:MET:HE3 | 23:W:211:ASP:HB3 | 1.78 | 0.66 |
| 1:A:381:PRO:HB3 | 1:A:480:SER:HA | 1.76 | 0.66 |
| 17:Q:418:LEU:HD12 | 17:Q:433:ALA:HB2 | 1.77 | 0.66 |
| 1:A:946:ALA:O | 1:A:950:ASN:ND2 | 2.28 | 0.66 |
| 29:c:57:TYR:HB3 | 30:d:110:GLU:OE1 | 1.96 | 0.66 |
| 2:B:954:MET:HG3 | 2:B:955:PRO:HD2 | 1.78 | 0.66 |
| 2:B:1004:ASP:OD1 | 18:R:596:ARG:NH2 | 2.29 | 0.66 |
| 17:Q:713:LYS:HD3 | 17:Q:714:HIS:H | 1.58 | 0.66 |
| 24:X:219:ASP:HB2 | 24:X:222:ARG:HH21 | 1.60 | 0.66 |
| 17:Q:479:ASP:HB2 | 17:Q:480:ARG:HH12 | 1.59 | 0.66 |
| 17:Q:708:LEU:HD21 | 17:Q:719:VAL:HG21 | 1.77 | 0.66 |
| 2:B:733:MET:HE3 | 2:B:749:HIS:HB3 | 1.78 | 0.66 |
| 17:Q:353:TYR:OH | 22:V:57:ARG:O | 2.12 | 0.65 |
| 14:N:7:DG:H2" | 14:N:8:DT:H71 | 1.78 | 0.65 |
| 23:W:231:HIS:ND1 | 23:W:251:SER:OG | 2.28 | 0.65 |
| 1:A:516:GLN:HA | 1:A:520:MET:HE3 | 1.78 | 0.65 |
| 10:J:17:LYS:HD3 | 10:J:38:LEU:HB3 | 1.79 | 0.65 |
| 17:Q:401:LEU:HA | 17:Q:404:VAL:HG22 | 1.78 | 0.65 |
| 23:W:81:SER:HB3 | 23:W:91:TRP:HE1 | 1.61 | 0.65 |
| 1:A:423:ASN:ND2 | 1:A:425:ASP:OD1 | 2.29 | 0.65 |
| 27:e:83:ARG:HG3 | 28:f:80:THR:HG23 | 1.77 | 0.65 |
| 2:B:600:GLU:N | 2:B:600:GLU:OE1 | 2.30 | 0.65 |
| 4:D:39:MET:HE2 | 4:D:39:MET:HA | 1.78 | 0.65 |
| 1:A:1049:LEU:HG | 1:A:1054:MET:HE3 | 1.79 | 0.65 |
| 27:e:56:LYS:HE3 | 27:e:56:LYS:HA | 1.78 | 0.65 |
| 9:I:56:ASN:HD22 | 9:I:57:LYS:N | 1.95 | 0.64 |
| 12:L:27:GLU:OE2 | 12:L:27:GLU:N | 2.27 | 0.64 |
| 14:N:81:DG:H2' | 14:N:82:DT:C6 | 2.31 | 0.64 |
| 17:Q:799:VAL:O | 17:Q:802:LYS:NZ | 2.31 | 0.64 |
| 10:J:17:LYS:HG2 | 10:J:38:LEU:HD13 | 1.79 | 0.64 |
| 4:D:76:ASN:O | 4:D:79:THR:OG1 | 2.15 | 0.64 |
| 17:Q:397:ALA:O | 17:Q:401:LEU:HD12 | 1.98 | 0.64 |
| 1:A:866:LYS:HZ3 | 2:B:1091:ARG:HH22 | 1.45 | 0.64 |
| 28:b:92:ARG:HH22 | 30:d:97:LEU:HB3 | 1.62 | 0.64 |
| 2:B:309:PHE:O | 2:B:312:GLN:NE2 | 2.31 | 0.64 |
| 5:E:41:LYS:NZ | 5:E:46:ASP:OD1 | 2.29 | 0.64 |
| 8:H:103:GLU:HG3 | 8:H:109:ALA:HB2 | 1.78 | 0.64 |
| 27:e:59:GLU:OE1 | 27:e:59:GLU:N | 2.30 | 0.64 |
| 6:F:124:ILE:HD12 | 6:F:124:ILE:H | 1.63 | 0.63 |
| 1:A:504:HIS:HB3 | 2:B:1106:ARG:NH2 | 2.13 | 0.63 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:W:40:LEU:HD12 | 23:W:66:GLY:HA3 | 1.79 | 0.63 |
| 1:A:465:HIS:CD2 | 1:A:467:MET:HB2 | 2.34 | 0.63 |
| 23:W:248:VAL:HG12 | 23:W:258:VAL:HG22 | 1.80 | 0.63 |
| 3:C:175:LYS:NZ | 12:L:57:ALA:O | 2.30 | 0.63 |
| 2:B:19:PRO:O | 2:B:21:LEU:N | 2.31 | 0.63 |
| 5:E:78:GLU:OE1 | 5:E:78:GLU:N | 2.31 | 0.63 |
| 1:A:524:MET:HE1 | 2:B:1097:HIS:CD2 | 2.34 | 0.63 |
| 1:A:1208:SER:O | 1:A:1260:ARG:NH1 | 2.32 | 0.63 |
| 27:e:80:THR:O | 28:f:79:LYS:NZ | 2.31 | 0.63 |
| 1:A:674:THR:O | 1:A:678:ASN:ND2 | 2.31 | 0.63 |
| 1:A:1132:LYS:N | 1:A:1132:LYS:HE2 | 2.13 | 0.63 |
| 8:H:95:LYS:HG3 | 8:H:140:ARG:HH11 | 1.64 | 0.63 |
| 20:T:-99:DT:H2" | 20:T:-98:DA:C8 | 2.34 | 0.63 |
| 23:W:95:ASN:O | 23:W:97:LYS:NZ | 2.31 | 0.62 |
| 9:I:91:HIS:CE1 | 9:I:93:GLU:HB3 | 2.35 | 0.62 |
| 12:L:35:ARG:NH1 | 18:R:493:GLU:OE2 | 2.32 | 0.62 |
| 25:Y:63:MET:HE1 | 25:Y:77:VAL:HG23 | 1.80 | 0.62 |
| 1:A:866:LYS:CG | 1:A:1432:PHE:HB2 | 2.28 | 0.62 |
| 3:C:242:GLU:OE1 | 3:C:242:GLU:N | 2.31 | 0.62 |
| 18:R:504:LYS:HE2 | 18:R:507:PRO:HG2 | 1.82 | 0.62 |
| 23:W:292:VAL:HG12 | 23:W:298:ILE:HG12 | 1.81 | 0.62 |
| 1:A:296:ASN:OD1 | 1:A:297:GLY:N | 2.33 | 0.62 |
| 1:A:74:CYS:SG | 1:A:84:HIS:CE1 | 2.92 | 0.62 |
| 23:W:194:ARG:HD3 | 23:W:210:ASP:OD1 | 1.98 | 0.62 |
| 1:A:454:ASP:OD1 | 1:A:455:ILE:N | 2.32 | 0.62 |
| 1:A:67:ARG:NH2 | 16:P:15:C:OP2 | 2.32 | 0.62 |
| 12:L:39:CYS:SG | 12:L:40:GLY:N | 2.72 | 0.62 |
| 1:A:1208:SER:HG | 1:A:1210:TRP:CD1 | 2.18 | 0.62 |
| 1:A:862:ARG:NH1 | 2:B:1088:GLU:OE1 | 2.32 | 0.61 |
| 17:Q:664:ARG:O | 17:Q:664:ARG:NE | 2.33 | 0.61 |
| 2:B:155:MET:HE3 | 2:B:183:GLY:HA2 | 1.83 | 0.61 |
| 26:Z:541:GLN:NE2 | 26:Z:543:ASP:O | 2.33 | 0.61 |
| 9:I:31:GLU:N | 9:I:31:GLU:OE1 | 2.33 | 0.61 |
| 25:Y:41:GLN:HG3 | 25:Y:41:GLN:O | 1.99 | 0.61 |
| 23:W:236:LEU:N | 23:W:250:SER:O | 2.32 | 0.61 |
| 1:A:1130:ILE:O | 1:A:1130:ILE:HD12 | 2.00 | 0.61 |
| 2:B:309:PHE:CZ | 9:I:40:ARG:HB3 | 2.35 | 0.61 |
| 9:I:92:LYS:HE2 | 9:I:92:LYS:N | 2.14 | 0.61 |
| 8:H:66:GLU:N | 8:H:66:GLU:OE1 | 2.34 | 0.61 |
| 26:Z:338:ARG:HE | 26:Z:339:LEU:H | 1.49 | 0.61 |
| 30:d:55:ALA:O | 30:d:59:MET:HG2 | 2.01 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:300:MET:HG2 | 2:B:373:LEU:HD22 | 1.82 | 0.60 |
| 3:C:205:LYS:HD2 | 3:C:211:LEU:HD11 | 1.83 | 0.60 |
| 1:A:466:LYS:HG2 | 1:A:524:MET:HE2 | 1.83 | 0.60 |
| 1:A:1416:ARG:NH2 | 20:T:-30:DT:O2 | 2.34 | 0.60 |
| 29:c:104:GLN:HB2 | 30:d:54:LYS:NZ | 2.15 | 0.60 |
| 8:H:104:THR:HG23 | 8:H:106:THR:H | 1.66 | 0.60 |
| 2:B:522:LEU:O | 2:B:524:LYS:NZ | 2.30 | 0.60 |
| 10:J:10:CYS:SG | 10:J:42:ARG:NH2 | 2.74 | 0.60 |
| 20:T:-64:DG:N3 | 27:e:40:ARG:NH2 | 2.49 | 0.60 |
| 30:d:53:SER:HA | 30:d:56:MET:SD | 2.42 | 0.60 |
| 1:A:805:ARG:NH1 | 9:I:77:THR:OG1 | 2.34 | 0.60 |
| 2:B:191:GLU:OE1 | 2:B:191:GLU:N | 2.33 | 0.60 |
| 27:a:74:ILE:HG12 | 28:b:59:LYS:NZ | 2.16 | 0.60 |
| 2:B:347:MET:O | 2:B:361:LYS:NZ | 2.35 | 0.60 |
| 17:Q:558:LEU:HD22 | 17:Q:571:ILE:HG13 | 1.82 | 0.60 |
| 12:L:38:GLU:O | 12:L:40:GLY:N | 2.35 | 0.60 |
| 1:A:1309:MET:O | 19:S:250:MET:N | 2.35 | 0.60 |
| 3:C:58:VAL:HG11 | 10:J:59:LEU:HB3 | 1.82 | 0.60 |
| 17:Q:358:GLU:O | 17:Q:361:SER:OG | 2.18 | 0.60 |
| 1:A:1324:GLU:N | 1:A:1324:GLU:OE1 | 2.35 | 0.60 |
| 2:B:470:LEU:HD21 | 2:B:478:THR:HG23 | 1.83 | 0.59 |
| 4:D:96:GLU:N | 4:D:96:GLU:OE1 | 2.35 | 0.59 |
| 1:A:691:ASP:OD2 | 1:A:765:ASN:ND2 | 2.35 | 0.59 |
| 1:A:1484:MET:SD | 1:A:1484:MET:N | 2.75 | 0.59 |
| 2:B:230:ARG:NH2 | 2:B:346:GLU:OE1 | 2.34 | 0.59 |
| 2:B:628:VAL:HG22 | 2:B:633:LEU:HG | 1.84 | 0.59 |
| 2:B:1032:PHE:O | 3:C:32:ASN:ND2 | 2.35 | 0.59 |
| 9:I:91:HIS:HE1 | 9:I:93:GLU:HB3 | 1.66 | 0.59 |
| 1:A:1302:GLU:OE1 | 1:A:1302:GLU:N | 2.35 | 0.59 |
| 17:Q:275:LEU:HD11 | 17:Q:291:LEU:HD12 | 1.84 | 0.59 |
| 2:B:765:GLU:OE1 | 2:B:770:ARG:NE | 2.35 | 0.59 |
| 2:B:817:GLN:N | 2:B:817:GLN:OE1 | 2.35 | 0.59 |
| 29:c:103:ALA:O | 30:d:54:LYS:NZ | 2.35 | 0.59 |
| 28:b:64:ASN:OD1 | 28:b:93:GLN:NE2 | 2.36 | 0.59 |
| 2:B:483:ARG:NH2 | 2:B:527:ALA:O | 2.35 | 0.59 |
| 1:A:1483:GLY:HA3 | 6:F:80:MET:HE3 | 1.85 | 0.59 |
| 17:Q:419:ALA:HB2 | 17:Q:433:ALA:HB3 | 1.84 | 0.59 |
| 25:Y:49:VAL:O | 25:Y:53:THR:OG1 | 2.18 | 0.59 |
| 5:E:2:ASP:OD1 | 5:E:3:ASP:N | 2.36 | 0.59 |
| 14:N:129:DG:H2" | 14:N:130:DG:N7 | 2.18 | 0.59 |
| 17:Q:423:GLU:OE1 | 24:X:231:TRP:NE1 | 2.33 | 0.59 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:f:32:PRO:HA | 28:f:35:ARG:HD3 | 1.85 | 0.59 |
| 1:A:556:GLU:OE1 | 1:A:556:GLU:N | 2.36 | 0.58 |
| 3:C:183:ALA:HB3 | 3:C:232:ASN:HB3 | 1.85 | 0.58 |
| 17:Q:702:GLN:O | 17:Q:705:GLU:HG3 | 2.03 | 0.58 |
| 27:a:61:LEU:HD12 | 28:b:37:LEU:HD23 | 1.85 | 0.58 |
| 23:W:113:ALA:HB3 | 23:W:122:ALA:HB3 | 1.84 | 0.58 |
| 1:A:1217:ASP:OD1 | 1:A:1218:ARG:N | 2.36 | 0.58 |
| 5:E:79:GLU:N | 5:E:79:GLU:OE1 | 2.37 | 0.58 |
| 27:a:90:MET:HE3 | 27:a:90:MET:O | 2.03 | 0.58 |
| 29:c:103:ALA:C | 30:d:54:LYS:HZ1 | 2.12 | 0.58 |
| 1:A:1456:GLU:N | 1:A:1456:GLU:OE1 | 2.35 | 0.58 |
| 8:H:17:PRO:HD2 | 8:H:18:GLU:N | 2.18 | 0.58 |
| 12:L:37:ARG:CZ | 12:L:37:ARG:HA | 2.34 | 0.58 |
| 1:A:866:LYS:NZ | 2:B:1091:ARG:HH22 | 2.01 | 0.58 |
| 2:B:100:GLU:N | 2:B:100:GLU:OE1 | 2.37 | 0.58 |
| 26:Z:282:LYS:HG3 | 26:Z:283:ARG:HG2 | 1.85 | 0.58 |
| 30:d:60:ASN:O | 30:d:64:ASN:ND2 | 2.36 | 0.58 |
| 2:B:986:GLN:HA | 2:B:989:VAL:HG12 | 1.86 | 0.58 |
| 12:L:21:GLU:OE1 | 12:L:21:GLU:N | 2.37 | 0.58 |
| 20:T:-58:DT:H2" | 20:T:-57:DA:N7 | 2.19 | 0.58 |
| 25:Y:81:LYS:O | 25:Y:85:TYR:OH | 2.17 | 0.58 |
| 26:Z:613:GLU:O | 26:Z:625:HIS:N | 2.36 | 0.58 |
| 11:K:80:ASP:OD1 | 11:K:80:ASP:N | 2.34 | 0.57 |
| 18:R:577:LYS:HA | 18:R:580:VAL:HG22 | 1.85 | 0.57 |
| 17:Q:347:LEU:HD12 | 17:Q:351:TYR:CZ | 2.39 | 0.57 |
| 1:A:866:LYS:HG3 | 1:A:1432:PHE:HB2 | 1.86 | 0.57 |
| 14:N:62:DC:N4 | 14:N:63:DG:O6 | 2.37 | 0.57 |
| 17:Q:380:ILE:HD12 | 17:Q:400:HIS:HE1 | 1.69 | 0.57 |
| 26:Z:598:ASP:OD1 | 26:Z:599:ILE:N | 2.38 | 0.57 |
| 2:B:53:MET:HA | 2:B:53:MET:HE3 | 1.84 | 0.57 |
| 17:Q:643:ASP:OD2 | 24:X:239:GLN:NE2 | 2.36 | 0.57 |
| 26:Z:563:MET:HE1 | 26:Z:618:PHE:CD2 | 2.39 | 0.57 |
| 28:b:68:ASP:OD2 | 28:b:93:GLN:NE2 | 2.37 | 0.57 |
| 1:A:368:THR:HG23 | 1:A:483:ARG:HG2 | 1.86 | 0.57 |
| 5:E:36:THR:N | 5:E:39:GLU:OE2 | 2.37 | 0.57 |
| 17:Q:737:LYS:HZ1 | 17:Q:764:LEU:HD13 | 1.69 | 0.57 |
| 1:A:977:VAL:HG21 | 1:A:1040:LEU:HD21 | 1.86 | 0.57 |
| 2:B:1142:ASN:HD21 | 2:B:1145:GLN:HG2 | 1.67 | 0.57 |
| 1:A:454:ASP:O | 1:A:474:VAL:HG23 | 2.04 | 0.57 |
| 1:A:896:LEU:HD13 | 1:A:980:PRO:HG3 | 1.87 | 0.57 |
| 1:A:70:ARG:HD2 | 2:B:1131:ARG:HH12 | 1.70 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:86:ARG:NH1 | 26:Z:716:PRO:O | 2.38 | 0.57 |
| 7:G:10:GLU:N | 7:G:10:GLU:OE1 | 2.38 | 0.57 |
| 5:E:96:GLU:OE1 | 5:E:96:GLU:N | 2.38 | 0.57 |
| 7:G:117:MET:HG3 | 7:G:128:TYR:HB3 | 1.85 | 0.57 |
| 23:W:64:GLN:OE1 | 23:W:89:ARG:NH2 | 2.38 | 0.57 |
| 1:A:464:LEU:O | 1:A:861:GLN:NE2 | 2.38 | 0.56 |
| 1:A:1296:MET:HE3 | 1:A:1296:MET:HA | 1.87 | 0.56 |
| 23:W:24:TRP:NE1 | 23:W:32:SER:O | 2.37 | 0.56 |
| 28:b:92:ARG:HH12 | 30:d:97:LEU:HD13 | 1.69 | 0.56 |
| 1:A:45:GLU:N | 1:A:45:GLU:OE1 | 2.37 | 0.56 |
| 1:A:505:LEU:H | 2:B:1106:ARG:NH2 | 2.03 | 0.56 |
| 2:B:309:PHE:O | 2:B:309:PHE:HD2 | 1.89 | 0.56 |
| 2:B:1080:ARG:HB2 | 2:B:1080:ARG:NH1 | 2.20 | 0.56 |
| 3:C:56:SER:HG | 3:C:158:GLU:H | 1.51 | 0.56 |
| 5:E:18:MET:HE1 | 5:E:60:VAL:HG11 | 1.88 | 0.56 |
| 5:E:97:GLU:N | 5:E:97:GLU:OE1 | 2.38 | 0.56 |
| 5:E:141:GLU:N | 5:E:141:GLU:OE1 | 2.38 | 0.56 |
| 8:H:90:TYR:CD2 | 8:H:145:MET:HE3 | 2.40 | 0.56 |
| 10:J:17:LYS:HZ3 | 10:J:17:LYS:HB2 | 1.71 | 0.56 |
| 23:W:169:ASP:N | 23:W:169:ASP:OD1 | 2.37 | 0.56 |
| 26:Z:604:ASP:OD1 | 26:Z:605:GLY:N | 2.38 | 0.56 |
| 2:B:834:ARG:HH11 | 2:B:840:MET:HE3 | 1.70 | 0.56 |
| 5:E:5:GLU:N | 5:E:5:GLU:OE1 | 2.38 | 0.56 |
| 23:W:86:ALA:HB1 | 23:W:105:GLY:HA2 | 1.87 | 0.56 |
| 26:Z:523:GLU:N | 26:Z:523:GLU:OE1 | 2.38 | 0.56 |
| 1:A:1038:THR:O | 1:A:1042:ASN:ND2 | 2.38 | 0.56 |
| 26:Z:626:CYS:SG | 26:Z:627:LYS:N | 2.78 | 0.56 |
| 2:B:407:MET:HE2 | 2:B:443:GLY:HA3 | 1.88 | 0.56 |
| 17:Q:866:ARG:NH1 | 17:Q:870:GLU:HB2 | 2.14 | 0.56 |
| 29:c:55:LEU:O | 29:c:59:THR:HG22 | 2.05 | 0.56 |
| 17:Q:317:HIS:HE2 | 22:V:58:PHE:HA | 1.71 | 0.56 |
| 28:b:75:HIS:CD2 | 30:d:93:THR:HG21 | 2.37 | 0.56 |
| 1:A:1344:MET:HE1 | 5:E:134:GLU:HA | 1.87 | 0.56 |
| 2:B:852:GLY:O | 2:B:868:GLY:N | 2.34 | 0.56 |
| 2:B:859:ARG:NH1 | 2:B:902:GLY:O | 2.32 | 0.55 |
| 2:B:1170:ARG:HB3 | 2:B:1172:MET:SD | 2.46 | 0.55 |
| 1:A:98:GLY:HA3 | 1:A:1440:MET:HE3 | 1.88 | 0.55 |
| 9:I:82:GLU:OE1 | 9:I:82:GLU:N | 2.39 | 0.55 |
| 11:K:58:PHE:HB3 | 11:K:76:GLN:HB3 | 1.88 | 0.55 |
| 17:Q:620:ARG:NH2 | 17:Q:629:GLN:OE1 | 2.39 | 0.55 |
| 17:Q:869:GLU:OE2 | 17:Q:873:LYS:NZ | 2.39 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:367:ILE:HG21 | 1:A:501:MET:HG3 | 1.89 | 0.55 |
| 2:B:198:GLU:N | 2:B:198:GLU:OE1 | 2.39 | 0.55 |
| 2:B:859:ARG:NH2 | 2:B:860:VAL:O | 2.39 | 0.55 |
| 5:E:166:ARG:HB2 | 5:E:166:ARG:HH11 | 1.72 | 0.55 |
| 14:N:102:DG:N2 | 20:T:-101:DT:O2 | 2.39 | 0.55 |
| 23:W:130:VAL:HB | 23:W:144:LEU:HD12 | 1.87 | 0.55 |
| 25:Y:112:ASP:OD2 | 25:Y:116:LYS:NZ | 2.40 | 0.55 |
| 2:B:859:ARG:NH1 | 2:B:903:ILE:HG12 | 2.22 | 0.55 |
| 26:Z:474:MET:HE2 | 26:Z:474:MET:HA | 1.87 | 0.55 |
| 1:A:116:LYS:NZ | 1:A:182:GLY:O | 2.38 | 0.55 |
| 1:A:359:VAL:HG11 | 2:B:1106:ARG:HE | 1.70 | 0.55 |
| 2:B:227:ASN:ND2 | 2:B:227:ASN:O | 2.40 | 0.55 |
| 25:Y:75:GLN:NE2 | 25:Y:86:ALA:O | 2.40 | 0.55 |
| 27:e:83:ARG:HA | 27:e:83:ARG:NH1 | 2.22 | 0.55 |
| 1:A:505:LEU:H | 2:B:1106:ARG:HH22 | 1.52 | 0.55 |
| 8:H:75:TYR:CD2 | 8:H:77:PRO:HD3 | 2.41 | 0.55 |
| 17:Q:316:PHE:HB2 | 17:Q:325:ALA:HB2 | 1.88 | 0.55 |
| 17:Q:508:GLU:HG3 | 17:Q:540:MET:SD | 2.47 | 0.55 |
| 27:a:113:HIS:NE2 | 27:e:110:CYS:SG | 2.80 | 0.55 |
| 1:A:367:ILE:HD11 | 1:A:499:ASP:HB2 | 1.89 | 0.55 |
| 1:A:559:GLU:N | 1:A:559:GLU:OE1 | 2.40 | 0.55 |
| 1:A:1137:PRO:HB2 | 1:A:1341:VAL:HG23 | 1.89 | 0.55 |
| 29:c:25:PHE:CZ | 29:c:59:THR:HG21 | 2.42 | 0.55 |
| 1:A:99:PHE:HB3 | 1:A:248:MET:SD | 2.46 | 0.54 |
| 1:A:376:ASP:OD2 | 1:A:473:ARG:NH1 | 2.40 | 0.54 |
| 1:A:827:TYR:CE2 | 2:B:976:MET:HE3 | 2.39 | 0.54 |
| 1:A:936:GLU:OE1 | 1:A:936:GLU:N | 2.39 | 0.54 |
| 2:B:285:LEU:HD11 | 2:B:305:LEU:HD21 | 1.89 | 0.54 |
| 26:Z:184:CYS:SG | 26:Z:185:LYS:N | 2.80 | 0.54 |
| 26:Z:613:GLU:N | 26:Z:625:HIS:O | 2.40 | 0.54 |
| 27:e:50:GLU:OE2 | 28:f:39:ARG:NE | 2.35 | 0.54 |
| 1:A:121:SER:HA | 1:A:126:ILE:HG21 | 1.90 | 0.54 |
| 1:A:1216:LEU:HD12 | 1:A:1228:MET:HE1 | 1.89 | 0.54 |
| 17:Q:286:SER:O | 17:Q:290:HIS:ND1 | 2.40 | 0.54 |
| 30:d:39:TYR:CE1 | 30:d:43:LYS:HE2 | 2.42 | 0.54 |
| 28:f:47:SER:HB3 | 28:f:50:ILE:HG12 | 1.88 | 0.54 |
| 14:N:110:DC:H2" | 14:N:111:DG:N7 | 2.22 | 0.54 |
| 23:W:48:LYS:N | 23:W:55:ASP:O | 2.32 | 0.54 |
| 29:c:50:TYR:CE1 | 30:d:111:GLY:HA3 | 2.43 | 0.54 |
| 1:A:909:LEU:C | 1:A:911:PRO:HD2 | 2.32 | 0.54 |
| 1:A:120:ASP:O | 1:A:122:ASN:N | 2.39 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:23:GLN:N | 2:B:23:GLN:OE1 | 2.38 | 0.54 |
| 2:B:849:ASP:OD2 | 12:L:46:LYS:NZ | 2.39 | 0.54 |
| 6:F:112:ASP:OD1 | 6:F:113:GLY:N | 2.39 | 0.54 |
| 25:Y:6:VAL:O | 25:Y:27:GLN:NE2 | 2.35 | 0.54 |
| 1:A:1361:ASP:OD1 | 1:A:1362:ILE:N | 2.41 | 0.54 |
| 2:B:197:GLN:NE2 | 2:B:486:ASN:O | 2.40 | 0.54 |
| 2:B:309:PHE:HE1 | 9:I:25:TYR:CE1 | 2.26 | 0.54 |
| 9:I:29:ASP:HB2 | 9:I:36:LEU:HD23 | 1.89 | 0.54 |
| 17:Q:331:GLN:HB3 | 17:Q:335:PHE:CZ | 2.42 | 0.54 |
| 20:T:-127:DA:OP1 | 30:d:53:SER:N | 2.41 | 0.54 |
| 2:B:30:ILE:HD11 | 2:B:698:ILE:HG21 | 1.90 | 0.54 |
| 10:J:44:CYS:O | 10:J:47:ARG:NH1 | 2.41 | 0.54 |
| 8:H:136:GLU:N | 8:H:136:GLU:OE1 | 2.41 | 0.54 |
| 9:I:103:ARG:HD2 | 9:I:103:ARG:O | 2.07 | 0.54 |
| 2:B:646:ARG:O | 2:B:648:TYR:N | 2.35 | 0.54 |
| 2:B:1040:GLN:NE2 | 3:C:195:THR:OG1 | 2.41 | 0.54 |
| 23:W:206:VAL:HG11 | 23:W:238:VAL:HG21 | 1.88 | 0.54 |
| 27:e:81:ASP:O | 28:f:79:LYS:HE2 | 2.08 | 0.54 |
| 2:B:52:GLN:HG3 | 2:B:53:MET:SD | 2.48 | 0.54 |
| 2:B:988:LYS:O | 2:B:992:ASN:ND2 | 2.41 | 0.54 |
| 6:F:69:ARG:O | 6:F:73:ILE:HG12 | 2.08 | 0.54 |
| 8:H:15:ILE:HG22 | 8:H:16:ASP:OD1 | 2.08 | 0.54 |
| 25:Y:33:CYS:HB3 | 25:Y:42:MET:HE2 | 1.90 | 0.54 |
| 27:e:115:LYS:HD3 | 27:e:115:LYS:N | 2.23 | 0.54 |
| 18:R:493:GLU:OE1 | 18:R:493:GLU:N | 2.41 | 0.53 |
| 23:W:35:VAL:N | 23:W:47:TRP:O | 2.29 | 0.53 |
| 17:Q:731:GLY:HA2 | 17:Q:734:GLN:HE22 | 1.73 | 0.53 |
| 26:Z:455:GLU:OE1 | 26:Z:455:GLU:N | 2.41 | 0.53 |
| 27:a:62:ILE:HG13 | 28:b:37:LEU:HD11 | 1.90 | 0.53 |
| 1:A:1468:THR:O | 6:F:64:ARG:NH1 | 2.41 | 0.53 |
| 28:b:75:HIS:CD2 | 30:d:77:LEU:HD12 | 2.42 | 0.53 |
| 2:B:1172:MET:HA | 2:B:1172:MET:HE3 | 1.90 | 0.53 |
| 3:C:7:PRO:O | 11:K:104:ARG:NH1 | 2.41 | 0.53 |
| 11:K:77:THR:OG1 | 11:K:81:TYR:O | 2.18 | 0.53 |
| 12:L:25:GLU:OE2 | 12:L:25:GLU:N | 2.42 | 0.53 |
| 2:B:756:LYS:N | 10:J:51:ALA:O | 2.34 | 0.53 |
| 2:B:859:ARG:HA | 2:B:859:ARG:HH11 | 1.73 | 0.53 |
| 1:A:537:ILE:HA | 1:A:539:GLN:HE22 | 1.74 | 0.53 |
| 1:A:930:LEU:HB3 | 1:A:939:VAL:HG12 | 1.90 | 0.53 |
| 2:B:516:GLU:N | 2:B:516:GLU:OE1 | 2.41 | 0.53 |
| 26:Z:542:LEU:HD21 | 26:Z:560:VAL:HG21 | 1.91 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:a:124:ILE:HB | 28:b:53:GLU:OE2 | 2.09 | 0.53 |
| 2:B:230:ARG:NH2 | 2:B:346:GLU:HA | 2.21 | 0.53 |
| 2:B:1040:GLN:OE1 | 2:B:1040:GLN:N | 2.42 | 0.53 |
| 27:a:82:LEU:HD12 | 27:a:83:ARG:N | 2.24 | 0.53 |
| 1:A:866:LYS:HG2 | 1:A:1432:PHE:HB2 | 1.89 | 0.53 |
| 5:E:84:ILE:HD12 | 14:N:43:DA:H5" | 1.90 | 0.53 |
| 14:N:114:DC:N4 | 14:N:115:DA:N6 | 2.56 | 0.53 |
| 17:Q:364:PHE:HB3 | 17:Q:380:ILE:HD11 | 1.91 | 0.53 |
| 23:W:172:ILE:HB | 23:W:186:LEU:HB2 | 1.91 | 0.53 |
| 25:Y:42:MET:HA | 25:Y:48:MET:HE2 | 1.91 | 0.53 |
| 2:B:968:ASN:HD21 | 2:B:970:HIS:HB2 | 1.73 | 0.53 |
| 5:E:67:ASP:OD1 | 5:E:69:THR:OG1 | 2.24 | 0.53 |
| 17:Q:378:MET:HE1 | 22:V:56:ASN:ND2 | 2.23 | 0.53 |
| 25:Y:26:ASP:OD1 | 25:Y:27:GLN:N | 2.41 | 0.53 |
| 26:Z:554:GLU:OE2 | 26:Z:559:GLN:NE2 | 2.42 | 0.53 |
| 30:d:95:VAL:HG13 | 30:d:99:LEU:HD12 | 1.91 | 0.53 |
| 1:A:315:ALA:O | 1:A:319:ASP:N | 2.39 | 0.53 |
| 17:Q:273:ASN:HD22 | 17:Q:304:MET:HE3 | 1.74 | 0.53 |
| 17:Q:366:LYS:HG3 | 17:Q:369:LYS:HZ3 | 1.73 | 0.53 |
| 17:Q:538:GLY:HA3 | 17:Q:554:PHE:CE1 | 2.44 | 0.53 |
| 17:Q:544:LYS:O | 23:W:191:MET:HE1 | 2.08 | 0.53 |
| 1:A:11:SER:O | 2:B:1135:TYR:OH | 2.22 | 0.52 |
| 1:A:375:ILE:HD12 | 1:A:535:MET:HE1 | 1.91 | 0.52 |
| 9:I:54:TYR:HE1 | 9:I:56:ASN:HB2 | 1.74 | 0.52 |
| 17:Q:359:ASN:O | 17:Q:362:GLN:HG3 | 2.09 | 0.52 |
| 1:A:76:GLY:HA2 | 2:B:1131:ARG:NH2 | 2.24 | 0.52 |
| 1:A:1302:GLU:O | 1:A:1304:ILE:N | 2.40 | 0.52 |
| 7:G:151:ARG:NE | 7:G:153:ASP:OD1 | 2.42 | 0.52 |
| 26:Z:466:GLN:OE1 | 26:Z:466:GLN:N | 2.43 | 0.52 |
| 30:d:107:ALA:O | 30:d:110:GLU:HG2 | 2.09 | 0.52 |
| 28:f:31:LYS:O | 28:f:35:ARG:HG3 | 2.09 | 0.52 |
| 1:A:986:MET:HE1 | 1:A:1075:LYS:HG3 | 1.90 | 0.52 |
| 3:C:260:GLN:HB2 | 11:K:91:ILE:HG21 | 1.90 | 0.52 |
| 18:R:574:GLU:HA | 18:R:577:LYS:HE3 | 1.90 | 0.52 |
| 23:W:33:GLU:O | 23:W:49:TRP:N | 2.43 | 0.52 |
| 2:B:859:ARG:HH11 | 2:B:903:ILE:HG12 | 1.75 | 0.52 |
| 2:B:1062:ARG:NH1 | 2:B:1081:ASP:O | 2.42 | 0.52 |
| 20:T:-118:DA:H4' | 29:c:29:ARG:HH12 | 1.75 | 0.52 |
| 26:Z:592:ASN:OD1 | 26:Z:593:ASN:N | 2.43 | 0.52 |
| 1:A:517:GLU:OE1 | 6:F:62:ARG:NH1 | 2.40 | 0.52 |
| 1:A:1430:CYS:HB2 | 1:A:1435:THR:HG23 | 1.91 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:968:ASN:ND2 | 2:B:970:HIS:HB2 | 2.25 | 0.52 |
| 17:Q:406:GLU:HG2 | 17:Q:407:GLN:H | 1.74 | 0.52 |
| 17:Q:479:ASP:CB | 17:Q:480:ARG:HH12 | 2.23 | 0.52 |
| 18:R:391:ILE:O | 26:Z:777:MET:HE3 | 2.09 | 0.52 |
| 23:W:289:ILE:HB | 23:W:301:TYR:HB2 | 1.92 | 0.52 |
| 14:N:60:DA:P | 28:f:32:PRO:HG3 | 2.49 | 0.52 |
| 1:A:1077:ASN:HB3 | 6:F:56:TYR:HE1 | 1.75 | 0.52 |
| 2:B:306:ASP:OD1 | 9:I:23:MET:HE3 | 2.10 | 0.52 |
| 2:B:1056:ASP:O | 2:B:1078:ARG:NH2 | 2.43 | 0.52 |
| 17:Q:713:LYS:HD3 | 17:Q:714:HIS:N | 2.25 | 0.52 |
| 23:W:210:ASP:HB3 | 23:W:234:TRP:CE2 | 2.45 | 0.52 |
| 9:I:87:GLN:OE1 | 9:I:87:GLN:N | 2.43 | 0.51 |
| 17:Q:310:TYR:HE2 | 17:Q:343:PRO:HA | 1.74 | 0.51 |
| 17:Q:713:LYS:HD3 | 17:Q:715:GLN:N | 2.21 | 0.51 |
| 2:B:542:LEU:HD21 | 2:B:569:VAL:HG11 | 1.92 | 0.51 |
| 17:Q:340:PHE:HE2 | 22:V:66:LEU:HD21 | 1.76 | 0.51 |
| 23:W:194:ARG:HD2 | 23:W:194:ARG:N | 2.25 | 0.51 |
| 1:A:480:SER:HB3 | 11:K:2:ASN:HD21 | 1.75 | 0.51 |
| 2:B:58:ILE:HD11 | 2:B:227:ASN:ND2 | 2.26 | 0.51 |
| 7:G:94:LYS:HD3 | 7:G:119:PHE:CD1 | 2.46 | 0.51 |
| 17:Q:567:ALA:O | 17:Q:571:ILE:HG12 | 2.11 | 0.51 |
| 17:Q:774:SER:O | 17:Q:830:ARG:NH1 | 2.38 | 0.51 |
| 1:A:967:ARG:NH2 | 1:A:1326:GLY:O | 2.43 | 0.51 |
| 2:B:298:MET:CE | 9:I:14:ILE:H | 2.19 | 0.51 |
| 2:B:587:LEU:HB3 | 2:B:603:MET:HE3 | 1.91 | 0.51 |
| 4:D:62:MET:O | 4:D:66:ASN:ND2 | 2.44 | 0.51 |
| 1:A:457:ILE:HG23 | 1:A:504:HIS:HB2 | 1.92 | 0.51 |
| 1:A:1461:GLY:O | 2:B:1104:ARG:NH1 | 2.44 | 0.51 |
| 2:B:470:LEU:HD22 | 2:B:472:ARG:HD2 | 1.93 | 0.51 |
| 2:B:474:THR:HG23 | 2:B:477:SER:H | 1.75 | 0.51 |
| 2:B:1142:ASN:ND2 | 2:B:1145:GLN:HG2 | 2.26 | 0.51 |
| 17:Q:415:TRP:HB2 | 17:Q:437:ALA:HB2 | 1.92 | 0.51 |
| 17:Q:479:ASP:HB2 | 17:Q:480:ARG:NH1 | 2.24 | 0.51 |
| 17:Q:653:ILE:HA | 17:Q:656:VAL:HG22 | 1.93 | 0.51 |
| 17:Q:841:LEU:HA | 17:Q:844:LYS:HG2 | 1.93 | 0.51 |
| 23:W:49:TRP:CZ3 | 23:W:300:ILE:HG13 | 2.45 | 0.51 |
| 23:W:206:VAL:HG22 | 23:W:216:ILE:HG12 | 1.93 | 0.51 |
| 23:W:272:ASP:O | 23:W:274:GLN:NE2 | 2.44 | 0.51 |
| 27:a:120:MET:HE3 | 27:a:121:PRO:HD2 | 1.93 | 0.51 |
| 11:K:56:VAL:HA | 11:K:77:THR:HG22 | 1.92 | 0.51 |
| 14:N:78:DT:H2" | 14:N:79:DA:N7 | 2.26 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:e:72:ARG:HH12 | 27:e:83:ARG:NH1 | 2.09 | 0.51 |
| 5:E:166:ARG:HB2 | 5:E:166:ARG:NH1 | 2.26 | 0.51 |
| 23:W:195:SER:OG | 23:W:236:LEU:O | 2.24 | 0.51 |
| 30:d:113:LYS:HE3 | 30:d:113:LYS:HA | 1.92 | 0.51 |
| 17:Q:776:LEU:HD22 | 17:Q:831:ALA:HA | 1.93 | 0.51 |
| 20:T:-112:DT:H2" | 20:T:-111:DC:C5 | 2.46 | 0.51 |
| 20:T:-61:DT:H2" | 20:T:-60:DT:H71 | 1.93 | 0.51 |
| 26:Z:307:MET:SD | 26:Z:307:MET:N | 2.84 | 0.51 |
| 3:C:73:LEU:O | 3:C:238:SER:OG | 2.27 | 0.51 |
| 11:K:8:GLU:OE1 | 11:K:8:GLU:N | 2.41 | 0.51 |
| 17:Q:713:LYS:CD | 17:Q:714:HIS:H | 2.23 | 0.51 |
| 20:T:-58:DT:H2" | 20:T:-57:DA:C8 | 2.46 | 0.51 |
| 2:B:963:PRO:HG3 | 2:B:1043:ILE:HD12 | 1.92 | 0.50 |
| 25:Y:47:GLU:N | 25:Y:47:GLU:OE1 | 2.42 | 0.50 |
| 27:a:74:ILE:HG12 | 28:b:59:LYS:HZ2 | 1.76 | 0.50 |
| 1:A:22:GLN:O | 2:B:1170:ARG:N | 2.45 | 0.50 |
| 2:B:854:ILE:HD11 | 2:B:858:VAL:HG11 | 1.93 | 0.50 |
| 17:Q:592:LEU:O | 17:Q:597:THR:OG1 | 2.21 | 0.50 |
| 1:A:107:LEU:HD22 | 1:A:191:ILE:HD13 | 1.94 | 0.50 |
| 17:Q:427:ILE:HG21 | 17:Q:464:LEU:HD21 | 1.91 | 0.50 |
| 1:A:869:GLU:OE2 | 2:B:1095:ILE:HD13 | 2.11 | 0.50 |
| 2:B:959:GLU:N | 2:B:959:GLU:OE1 | 2.44 | 0.50 |
| 17:Q:886:LYS:O | 17:Q:890:MET:HG2 | 2.11 | 0.50 |
| 20:T:-29:DC:H2' | 20:T:-28:DC:C6 | 2.47 | 0.50 |
| 26:Z:338:ARG:HE | 26:Z:338:ARG:HA | 1.76 | 0.50 |
| 1:A:1077:ASN:HB3 | 6:F:56:TYR:CE1 | 2.46 | 0.50 |
| 1:A:1314:THR:OG1 | 1:A:1316:ASN:OD1 | 2.23 | 0.50 |
| 2:B:115:LEU:HD23 | 12:L:43:ILE:HD13 | 1.94 | 0.50 |
| 3:C:235:SER:OG | 3:C:239:LEU:O | 2.26 | 0.50 |
| 8:H:72:ASP:OD1 | 8:H:73:GLY:N | 2.44 | 0.50 |
| 28:b:92:ARG:HH12 | 30:d:97:LEU:HB3 | 1.77 | 0.50 |
| 28:b:92:ARG:NH1 | 30:d:97:LEU:HD13 | 2.26 | 0.50 |
| 17:Q:329:TYR:HB3 | 17:Q:347:LEU:CD2 | 2.42 | 0.50 |
| 17:Q:384:LEU:HD13 | 17:Q:397:ALA:HB2 | 1.93 | 0.50 |
| 26:Z:421:GLN:N | 26:Z:421:GLN:OE1 | 2.45 | 0.50 |
| 2:B:755:GLN:NE2 | 10:J:48:MET:SD | 2.85 | 0.50 |
| 2:B:806:PHE:O | 2:B:1050:ARG:NH1 | 2.44 | 0.50 |
| 9:I:67:GLN:N | 9:I:67:GLN:OE1 | 2.44 | 0.50 |
| 12:L:16:ILE:HD12 | 12:L:26:ASN:O | 2.11 | 0.50 |
| 27:a:63:ARG:HG2 | 27:a:63:ARG:HH11 | 1.77 | 0.50 |
| 1:A:473:ARG:HG3 | 1:A:473:ARG:HH11 | 1.77 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:Q:586:LYS:HG2 | 17:Q:590:ARG:HD2 | 1.93 | 0.50 |
| 20:T:-28:DC:H5" | 20:T:-27:DT:H5" | 1.94 | 0.50 |
| 1:A:505:LEU:N | 2:B:1106:ARG:HH22 | 2.10 | 0.49 |
| 1:A:909:LEU:O | 1:A:911:PRO:HD2 | 2.12 | 0.49 |
| 2:B:733:MET:HG2 | 2:B:1050:ARG:O | 2.12 | 0.49 |
| 12:L:38:GLU:OE1 | 12:L:38:GLU:N | 2.42 | 0.49 |
| 29:c:85:LEU:O | 29:c:89:ASN:ND2 | 2.38 | 0.49 |
| 1:A:410:ASN:HD22 | 1:A:430:ARG:HG2 | 1.77 | 0.49 |
| 2:B:20:ASP:N | 2:B:680:ASP:OD2 | 2.41 | 0.49 |
| 14:N:114:DC:H2" | 14:N:115:DA:H5" | 1.93 | 0.49 |
| 4:D:62:MET:HE3 | 4:D:62:MET:HA | 1.94 | 0.49 |
| 17:Q:734:GLN:N | 17:Q:734:GLN:OE1 | 2.45 | 0.49 |
| 17:Q:830:ARG:HA | 17:Q:833:LYS:HE2 | 1.93 | 0.49 |
| 20:T:-96:DC:H5' | 27:a:83:ARG:HH21 | 1.77 | 0.49 |
| 26:Z:437:GLN:OE1 | 26:Z:437:GLN:N | 2.45 | 0.49 |
| 9:I:54:TYR:CE1 | 9:I:56:ASN:HB2 | 2.47 | 0.49 |
| 18:R:494:GLU:N | 18:R:494:GLU:OE1 | 2.44 | 0.49 |
| 22:V:45:ASP:HB3 | 24:X:232:ARG:HE | 1.76 | 0.49 |
| 1:A:683:GLU:O | 2:B:1038:THR:OG1 | 2.27 | 0.49 |
| 11:K:24:ASP:OD1 | 11:K:25:THR:N | 2.45 | 0.49 |
| 13:M:616:LEU:N | 13:M:643:LYS:O | 2.45 | 0.49 |
| 1:A:1451:MET:HE2 | 1:A:1451:MET:HA | 1.95 | 0.49 |
| 2:B:613:ARG:NH1 | 2:B:615:TYR:OH | 2.45 | 0.49 |
| 9:I:42:CYS:SG | 9:I:43:ASP:N | 2.86 | 0.49 |
| 17:Q:377:THR:HG21 | 17:Q:403:LYS:HD3 | 1.93 | 0.49 |
| 17:Q:633:LEU:HD12 | 17:Q:653:ILE:HG22 | 1.94 | 0.49 |
| 27:e:90:MET:HE2 | 27:e:90:MET:HA | 1.95 | 0.49 |
| 1:A:1095:LEU:HD12 | 1:A:1095:LEU:O | 2.12 | 0.49 |
| 14:N:55:DG:H2' | 14:N:56:DT:H71 | 1.95 | 0.49 |
| 14:N:120:DA:H2" | 14:N:121:DG:N7 | 2.28 | 0.49 |
| 29:c:81:ARG:HD2 | 29:c:85:LEU:HG | 1.93 | 0.49 |
| 27:e:121:PRO:HB3 | 28:f:53:GLU:HG3 | 1.93 | 0.49 |
| 1:A:1141:VAL:HB | 1:A:1336:LEU:HB2 | 1.95 | 0.49 |
| 1:A:1462:GLN:HA | 2:B:1104:ARG:HH12 | 1.78 | 0.49 |
| 3:C:225:LYS:HG3 | 3:C:226:PRO:HD2 | 1.95 | 0.49 |
| 17:Q:351:TYR:HB2 | 17:Q:360:ALA:HB2 | 1.95 | 0.49 |
| 1:A:535:MET:O | 1:A:669:TYR:OH | 2.20 | 0.49 |
| 17:Q:373:ASN:HB2 | 17:Q:376:GLU:HG2 | 1.94 | 0.49 |
| 25:Y:52:CYS:SG | 25:Y:53:THR:N | 2.85 | 0.49 |
| 26:Z:729:GLU:O | 26:Z:747:ARG:NH2 | 2.45 | 0.49 |
| 2:B:157:ARG:NH2 | 2:B:177:CYS:O | 2.46 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:836:THR:O | 2:B:888:THR:N | 2.46 | 0.49 |
| 8:H:100:GLU:O | 8:H:113:SER:N | 2.46 | 0.49 |
| 11:K:17:LYS:O | 11:K:36:ASN:ND2 | 2.46 | 0.49 |
| 14:N:88:DT:H2" | 14:N:89:DA:C8 | 2.48 | 0.49 |
| 26:Z:469:ARG:NH2 | 26:Z:497:GLU:O | 2.46 | 0.49 |
| 28:b:50:ILE:O | 28:b:54:THR:HG23 | 2.13 | 0.49 |
| 1:A:49:GLY:O | 1:A:51:ARG:HD3 | 2.13 | 0.48 |
| 17:Q:816:GLN:HA | 17:Q:819:ASP:OD2 | 2.13 | 0.48 |
| 1:A:367:ILE:HG22 | 1:A:482:PHE:HB2 | 1.95 | 0.48 |
| 1:A:602:CYS:SG | 1:A:603:ILE:N | 2.86 | 0.48 |
| 7:G:107:PHE:HB3 | 26:Z:508:MET:HE1 | 1.95 | 0.48 |
| 17:Q:380:ILE:HD12 | 17:Q:400:HIS:CE1 | 2.48 | 0.48 |
| 17:Q:711:PHE:CE2 | 23:W:233:SER:HB3 | 2.45 | 0.48 |
| 25:Y:42:MET:HE3 | 25:Y:42:MET:HB3 | 1.64 | 0.48 |
| 1:A:693:ILE:HD13 | 1:A:828:LEU:HD21 | 1.96 | 0.48 |
| 2:B:388:TYR:H | 2:B:504:THR:HG21 | 1.77 | 0.48 |
| 7:G:112:SER:HA | 7:G:164:MET:HE3 | 1.94 | 0.48 |
| 8:H:6:PHE:CZ | 8:H:8:ASP:HB3 | 2.47 | 0.48 |
| 18:R:577:LYS:NZ | 22:V:127:VAL:HA | 2.28 | 0.48 |
| 30:d:90:GLU:N | 30:d:90:GLU:OE1 | 2.46 | 0.48 |
| 1:A:873:VAL:HG22 | 1:A:879:VAL:HG22 | 1.95 | 0.48 |
| 2:B:283:ASP:O | 2:B:287:HIS:ND1 | 2.44 | 0.48 |
| 23:W:248:VAL:HG13 | 23:W:282:TYR:OH | 2.12 | 0.48 |
| 25:Y:40:LEU:HB3 | 25:Y:42:MET:CE | 2.44 | 0.48 |
| 27:a:121:PRO:HG2 | 28:b:49:LEU:HD12 | 1.95 | 0.48 |
| 1:A:660:MET:HE3 | 1:A:660:MET:HA | 1.94 | 0.48 |
| 2:B:128:ILE:HD13 | 2:B:431:LEU:HD12 | 1.95 | 0.48 |
| 20:T:-60:DT:H2" | 20:T:-59:DT:C5 | 2.49 | 0.48 |
| 1:A:1173:THR:HG23 | 1:A:1214:VAL:HG22 | 1.94 | 0.48 |
| 1:A:1473:LEU:HD23 | 6:F:104:ILE:HG21 | 1.95 | 0.48 |
| 17:Q:310:TYR:OH | 17:Q:346:GLY:HA3 | 2.13 | 0.48 |
| 17:Q:380:ILE:HB | 17:Q:400:HIS:CE1 | 2.48 | 0.48 |
| 23:W:17:ASP:OD1 | 23:W:18:ALA:N | 2.40 | 0.48 |
| 1:A:969:ILE:HG23 | 1:A:970:PHE:CD1 | 2.49 | 0.48 |
| 1:A:1005:HIS:ND1 | 1:A:1007:ILE:HG22 | 2.29 | 0.48 |
| 4:D:59:GLU:OE1 | 4:D:59:GLU:N | 2.45 | 0.48 |
| 27:e:68:GLN:HE21 | 27:e:72:ARG:HH21 | 1.62 | 0.48 |
| 3:C:82:LEU:HG | 3:C:97:CYS:HA | 1.95 | 0.48 |
| 7:G:98:PHE:CE1 | 26:Z:508:MET:HE3 | 2.48 | 0.48 |
| 17:Q:555:LYS:O | 17:Q:559:GLN:HG2 | 2.14 | 0.48 |
| 29:c:54:VAL:HA | 30:d:110:GLU:OE1 | 2.13 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 28:f:77:LYS:HD3 | 28:f:77:LYS:N | 2.29 | 0.48 |
| 1:A:561:MET:HE2 | 11:K:58:PHE:HA | 1.95 | 0.48 |
| 17:Q:568:TRP:HE1 | 17:Q:591:ILE:HD12 | 1.79 | 0.48 |
| 26:Z:746:ASP:OD1 | 26:Z:747:ARG:N | 2.47 | 0.48 |
| 2:B:223:SER:OG | 2:B:350:HIS:ND1 | 2.43 | 0.48 |
| 2:B:342:VAL:HG23 | 2:B:346:GLU:HG3 | 1.95 | 0.48 |
| 9:I:86:CYS:SG | 9:I:87:GLN:N | 2.87 | 0.48 |
| 17:Q:602:TYR:OH | 22:V:40:PRO:HG2 | 2.13 | 0.48 |
| 17:Q:684:TRP:HE3 | 17:Q:703:MET:HG3 | 1.79 | 0.48 |
| 28:b:75:HIS:HD1 | 28:b:75:HIS:C | 2.21 | 0.48 |
| 28:f:60:VAL:O | 28:f:64:ASN:ND2 | 2.47 | 0.48 |
| 13:M:783:GLY:N | 13:M:797:ALA:O | 2.47 | 0.47 |
| 17:Q:590:ARG:HA | 17:Q:593:LYS:HG3 | 1.95 | 0.47 |
| 23:W:51:ASP:CG | 23:W:51:ASP:O | 2.57 | 0.47 |
| 1:A:702:ILE:HD13 | 1:A:786:ALA:HA | 1.96 | 0.47 |
| 1:A:1416:ARG:HD2 | 1:A:1434:GLU:OE2 | 2.13 | 0.47 |
| 2:B:581:GLU:O | 2:B:585:ASN:ND2 | 2.46 | 0.47 |
| 2:B:891:ASP:OD1 | 2:B:893:SER:OG | 2.21 | 0.47 |
| 27:a:115:LYS:HE2 | 27:a:115:LYS:H | 1.79 | 0.47 |
| 28:b:63:GLU:OE1 | 28:b:63:GLU:HA | 2.14 | 0.47 |
| 1:A:971:PRO:O | 1:A:972:THR:OG1 | 2.29 | 0.47 |
| 8:H:96:VAL:HA | 8:H:116:VAL:HA | 1.96 | 0.47 |
| 26:Z:451:MET:HB2 | 26:Z:460:MET:CG | 2.41 | 0.47 |
| 29:c:29:ARG:HH21 | 29:c:32:ARG:HD3 | 1.78 | 0.47 |
| 27:e:72:ARG:HH12 | 27:e:83:ARG:HH12 | 1.63 | 0.47 |
| 2:B:1080:ARG:HB2 | 2:B:1080:ARG:HH11 | 1.78 | 0.47 |
| 6:F:69:ARG:NE | 6:F:96:GLU:OE1 | 2.46 | 0.47 |
| 7:G:94:LYS:N | 7:G:94:LYS:HE2 | 2.30 | 0.47 |
| 7:G:138:GLN:N | 7:G:138:GLN:OE1 | 2.47 | 0.47 |
| 8:H:48:TYR:CE2 | 8:H:90:TYR:HB2 | 2.50 | 0.47 |
| 9:I:105:GLU:OE1 | 9:I:105:GLU:N | 2.38 | 0.47 |
| 17:Q:285:TYR:HA | 17:Q:288:VAL:HG12 | 1.97 | 0.47 |
| 23:W:191:MET:CG | 23:W:210:ASP:HB2 | 2.44 | 0.47 |
| 26:Z:729:GLU:N | 26:Z:729:GLU:OE1 | 2.47 | 0.47 |
| 1:A:687:ILE:HD13 | 2:B:972:ILE:HB | 1.96 | 0.47 |
| 2:B:992:ASN:O | 10:J:46:ARG:NH1 | 2.48 | 0.47 |
| 3:C:210:GLU:N | 3:C:210:GLU:OE1 | 2.46 | 0.47 |
| 2:B:42:GLN:OE1 | 2:B:42:GLN:N | 2.43 | 0.47 |
| 8:H:12:VAL:C | 8:H:13:LYS:HD2 | 2.40 | 0.47 |
| 23:W:176:ASP:HB2 | 23:W:183:LEU:HD11 | 1.96 | 0.47 |
| 23:W:251:SER:OG | 23:W:253:ASP:OD1 | 2.28 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:Z:588:ASP:OD1 | 26:Z:592:ASN:N | 2.42 | 0.47 |
| 27:e:67:PHE:O | 27:e:71:VAL:HG23 | 2.15 | 0.47 |
| 1:A:551:ARG:HD2 | 8:H:25:VAL:HG21 | 1.97 | 0.47 |
| 1:A:1280:ASP:OD1 | 1:A:1281:ASP:N | 2.48 | 0.47 |
| 2:B:1062:ARG:CZ | 2:B:1074:PRO:HB3 | 2.44 | 0.47 |
| 18:R:560:ILE:HA | 18:R:563:ILE:HG22 | 1.97 | 0.47 |
| 26:Z:338:ARG:HA | 26:Z:338:ARG:NE | 2.29 | 0.47 |
| 2:B:59:VAL:HG11 | 2:B:91:ILE:HG23 | 1.96 | 0.47 |
| 2:B:265:GLN:N | 2:B:265:GLN:OE1 | 2.48 | 0.47 |
| 9:I:27:LYS:N | 9:I:36:LEU:O | 2.43 | 0.47 |
| 23:W:27:ASN:ND2 | 23:W:74:HIS:O | 2.47 | 0.47 |
| 27:a:121:PRO:HB3 | 28:b:53:GLU:OE1 | 2.15 | 0.47 |
| 1:A:685:HIS:NE2 | 1:A:769:MET:SD | 2.73 | 0.47 |
| 5:E:72:MET:HG3 | 5:E:102:ALA:HA | 1.97 | 0.47 |
| 17:Q:406:GLU:HG2 | 17:Q:407:GLN:N | 2.30 | 0.47 |
| 26:Z:424:ASP:HB2 | 26:Z:440:ILE:HD12 | 1.97 | 0.47 |
| 6:F:75:MET:HE1 | 7:G:64:GLY:H | 1.79 | 0.47 |
| 17:Q:329:TYR:O | 17:Q:347:LEU:HD21 | 2.14 | 0.47 |
| 17:Q:768:VAL:HG21 | 17:Q:778:GLU:CG | 2.43 | 0.47 |
| 17:Q:829:ALA:O | 17:Q:833:LYS:HG3 | 2.15 | 0.47 |
| 26:Z:550:ILE:HD13 | 26:Z:558:PHE:HB3 | 1.96 | 0.47 |
| 29:c:118:LYS:HE3 | 29:c:118:LYS:HA | 1.97 | 0.47 |
| 1:A:31:LEU:HA | 1:A:34:MET:HG2 | 1.95 | 0.46 |
| 17:Q:468:GLY:O | 17:Q:472:LYS:HG2 | 2.14 | 0.46 |
| 29:c:19:SER:O | 30:d:117:LYS:NZ | 2.47 | 0.46 |
| 1:A:18:ILE:HB | 1:A:1462:GLN:HE22 | 1.79 | 0.46 |
| 1:A:197:GLU:N | 1:A:197:GLU:OE1 | 2.48 | 0.46 |
| 1:A:467:MET:HB3 | 1:A:491:PRO:HB3 | 1.95 | 0.46 |
| 3:C:256:LEU:HD11 | 11:K:94:LEU:HD23 | 1.96 | 0.46 |
| 17:Q:777:LYS:HD2 | 17:Q:780:LEU:HD12 | 1.97 | 0.46 |
| 26:Z:192:THR:OG1 | 26:Z:244:ASN:ND2 | 2.48 | 0.46 |
| 28:f:50:ILE:O | 28:f:54:THR:HG23 | 2.16 | 0.46 |
| 1:A:231:GLU:OE1 | 1:A:231:GLU:N | 2.46 | 0.46 |
| 1:A:350:VAL:O | 1:A:355:MET:HG2 | 2.16 | 0.46 |
| 11:K:84:GLN:N | 11:K:84:GLN:OE1 | 2.46 | 0.46 |
| 14:N:59:DA:H2" | 14:N:60:DA:N7 | 2.30 | 0.46 |
| 17:Q:277:ASN:HB3 | 17:Q:311:GLN:NE2 | 2.30 | 0.46 |
| 20:T:-77:DC:H2" | 20:T:-76:DG:H8 | 1.81 | 0.46 |
| 25:Y:23:LYS:NZ | 25:Y:32:GLY:O | 2.39 | 0.46 |
| 1:A:340:LYS:O | 1:A:344:LYS:N | 2.48 | 0.46 |
| 2:B:230:ARG:HH12 | 2:B:345:LYS:HB3 | 1.80 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 6:F:69:ARG:NE | 6:F:73:ILE:HD11 | 2.31 | 0.46 |
| 9:I:109:ARG:HH11 | 9:I:124:THR:HG21 | 1.80 | 0.46 |
| 27:e:83:ARG:HH11 | 27:e:84:PHE:H | 1.64 | 0.46 |
| 1:A:695:ASP:O | 1:A:696:SER:OG | 2.29 | 0.46 |
| 2:B:604:ILE:HD13 | 2:B:668:LEU:HG | 1.98 | 0.46 |
| 2:B:697:GLU:HG3 | 2:B:698:ILE:N | 2.31 | 0.46 |
| 5:E:167:GLU:OE1 | 5:E:167:GLU:N | 2.44 | 0.46 |
| 12:L:19:CYS:SG | 12:L:20:GLY:N | 2.89 | 0.46 |
| 27:e:71:VAL:HG13 | 28:f:66:ILE:HD11 | 1.97 | 0.46 |
| 27:e:106:ASP:OD2 | 27:e:131:ARG:NH2 | 2.45 | 0.46 |
| 2:B:939:HIS:NE2 | 2:B:983:GLU:OE1 | 2.44 | 0.46 |
| 17:Q:420:GLN:O | 24:X:229:ARG:NH1 | 2.48 | 0.46 |
| 17:Q:711:PHE:CE2 | 23:W:253:ASP:HB3 | 2.51 | 0.46 |
| 17:Q:803:MET:O | 17:Q:803:MET:HG2 | 2.15 | 0.46 |
| 25:Y:36:CYS:O | 25:Y:42:MET:HE1 | 2.16 | 0.46 |
| 1:A:566:PHE:HB3 | 1:A:674:THR:HG22 | 1.97 | 0.46 |
| 16:P:8:U:O2' | 16:P:9:U:OP1 | 2.30 | 0.46 |
| 27:a:82:LEU:HD12 | 27:a:83:ARG:H | 1.80 | 0.46 |
| 28:b:92:ARG:NH2 | 30:d:97:LEU:HB3 | 2.30 | 0.46 |
| 29:c:115:LEU:HD11 | 27:e:108:ASN:HD21 | 1.80 | 0.46 |
| 2:B:305:LEU:HD23 | 9:I:23:MET:HE1 | 1.98 | 0.46 |
| 7:G:116:GLU:N | 7:G:116:GLU:OE1 | 2.45 | 0.46 |
| 8:H:18:GLU:N | 8:H:18:GLU:OE1 | 2.49 | 0.46 |
| 17:Q:476:ALA:O | 17:Q:480:ARG:HG2 | 2.16 | 0.46 |
| 17:Q:720:VAL:HG21 | 17:Q:743:ALA:HB2 | 1.98 | 0.46 |
| 24:X:247:LYS:HD3 | 24:X:248:ASN:H | 1.80 | 0.46 |
| 1:A:687:ILE:HD11 | 1:A:766:PHE:CZ | 2.51 | 0.46 |
| 1:A:945:ASN:OD1 | 1:A:947:HIS:N | 2.48 | 0.46 |
| 3:C:91:GLU:N | 3:C:91:GLU:OE1 | 2.48 | 0.46 |
| 20:T:-21:DG:H2' | 20:T:-20:DA:C8 | 2.51 | 0.46 |
| 25:Y:48:MET:SD | 25:Y:48:MET:C | 2.98 | 0.46 |
| 1:A:327:ARG:NE | 1:A:335:PRO:HB3 | 2.31 | 0.46 |
| 1:A:763:TYR:OH | 8:H:23:ASP:OD2 | 2.21 | 0.46 |
| 1:A:837:PHE:O | 1:A:841:MET:HG3 | 2.15 | 0.46 |
| 14:N:90:DA:H4' | 27:a:63:ARG:NH1 | 2.31 | 0.46 |
| 14:N:142:DT:H2" | 14:N:143:DG:H8 | 1.81 | 0.46 |
| 23:W:14:ALA:N | 23:W:296:GLN:O | 2.46 | 0.46 |
| 26:Z:462:GLU:N | 26:Z:462:GLU:OE1 | 2.49 | 0.46 |
| 1:A:461:GLN:HE21 | 20:T:-25:DG:H4' | 1.80 | 0.45 |
| 1:A:1372:GLU:HG2 | 5:E:146:PRO:HG3 | 1.98 | 0.45 |
| 14:N:114:DC:C4 | 14:N:115:DA:N6 | 2.84 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:Q:400:HIS:O | 17:Q:404:VAL:HG13 | 2.15 | 0.45 |
| 17:Q:716:ASN:HB3 | 17:Q:719:VAL:HG22 | 1.98 | 0.45 |
| 18:R:490:GLN:OE1 | 18:R:493:GLU:HB2 | 2.16 | 0.45 |
| 25:Y:64:MET:HE2 | 26:Z:212:ILE:O | 2.16 | 0.45 |
| 1:A:1177:TYR:CE1 | 9:I:53:ILE:HG13 | 2.51 | 0.45 |
| 2:B:783:ALA:HB2 | 2:B:1041:ILE:HG23 | 1.97 | 0.45 |
| 14:N:95:DT:H2' | 14:N:96:DG:H8 | 1.81 | 0.45 |
| 14:N:128:DC:H2" | 14:N:129:DG:C8 | 2.51 | 0.45 |
| 18:R:504:LYS:CE | 18:R:507:PRO:HG2 | 2.44 | 0.45 |
| 20:T:-68:DC:H1' | 20:T:-67:DC:H5" | 1.98 | 0.45 |
| 27:a:100:LEU:HD11 | 28:b:37:LEU:HD22 | 1.99 | 0.45 |
| 30:d:36:ILE:O | 30:d:40:LYS:HG2 | 2.15 | 0.45 |
| 5:E:148:HIS:CD2 | 5:E:179:VAL:HG11 | 2.51 | 0.45 |
| 7:G:41:LYS:O | 7:G:78:ARG:NH1 | 2.50 | 0.45 |
| 17:Q:378:MET:HA | 17:Q:381:LEU:HB3 | 1.97 | 0.45 |
| 17:Q:847:GLN:O | 17:Q:851:LEU:HG | 2.17 | 0.45 |
| 1:A:614:ASP:OD1 | 1:A:615:SER:N | 2.49 | 0.45 |
| 3:C:154:ARG:NH1 | 10:J:60:LEU:O | 2.37 | 0.45 |
| 8:H:87:GLN:N | 8:H:87:GLN:OE1 | 2.49 | 0.45 |
| 8:H:112:LEU:HB2 | 8:H:132:LEU:HD12 | 1.99 | 0.45 |
| 17:Q:777:LYS:HA | 17:Q:780:LEU:HD12 | 1.97 | 0.45 |
| 23:W:237:ASN:HB3 | 23:W:280:VAL:HG22 | 1.99 | 0.45 |
| 25:Y:33:CYS:H | 25:Y:42:MET:HG3 | 1.81 | 0.45 |
| 28:f:79:LYS:HE3 | 28:f:79:LYS:HA | 1.98 | 0.45 |
| 1:A:266:MET:HB3 | 1:A:266:MET:HE3 | 1.72 | 0.45 |
| 1:A:459:ASN:OD1 | 1:A:460:ARG:N | 2.50 | 0.45 |
| 27:a:107:THR:OG1 | 27:a:124:ILE:HG12 | 2.17 | 0.45 |
| 27:e:79:LYS:HD2 | 28:f:79:LYS:HZ2 | 1.81 | 0.45 |
| 17:Q:454:LEU:HA | 17:Q:457:VAL:HG12 | 1.99 | 0.45 |
| 17:Q:581:TRP:O | 17:Q:585:GLN:HB2 | 2.17 | 0.45 |
| 18:R:392:GLY:HA3 | 26:Z:777:MET:HE3 | 1.99 | 0.45 |
| 1:A:99:PHE:CD2 | 1:A:248:MET:HG2 | 2.51 | 0.45 |
| 1:A:519:ALA:O | 1:A:520:MET:HE2 | 2.15 | 0.45 |
| 2:B:139:GLN:OE1 | 2:B:139:GLN:N | 2.50 | 0.45 |
| 17:Q:366:LYS:CG | 17:Q:369:LYS:HZ3 | 2.30 | 0.45 |
| 20:T:-59:DT:H6 | 20:T:-59:DT:H2' | 1.58 | 0.45 |
| 29:c:51:LEU:O | 29:c:55:LEU:HG | 2.17 | 0.45 |
| 28:f:84:MET:SD | 28:f:84:MET:N | 2.81 | 0.45 |
| 1:A:467:MET:HG3 | 1:A:534:VAL:HG21 | 1.98 | 0.45 |
| 7:G:99:THR:OG1 | 7:G:100:GLU:N | 2.50 | 0.45 |
| 17:Q:849:LYS:O | 17:Q:852:LEU:HG | 2.16 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:W:81:SER:HB3 | 23:W:91:TRP:NE1 | 2.30 | 0.45 |
| 1:A:34:MET:HE3 | 1:A:34:MET:HB2 | 1.77 | 0.45 |
| 17:Q:344:PHE:CE1 | 17:Q:366:LYS:HD2 | 2.52 | 0.45 |
| 17:Q:516:ALA:HB3 | 17:Q:540:MET:HE1 | 1.99 | 0.45 |
| 20:T:-119:DC:H4' | 30:d:30:ARG:HH11 | 1.82 | 0.45 |
| 20:T:-24:DC:H2' | 20:T:-23:DA:H8 | 1.82 | 0.45 |
| 29:c:37:GLY:HA3 | 29:c:39:TYR:CE2 | 2.52 | 0.45 |
| 1:A:1318:LYS:NZ | 19:S:292:ASN:O | 2.50 | 0.45 |
| 2:B:230:ARG:NH1 | 2:B:345:LYS:O | 2.51 | 0.45 |
| 8:H:17:PRO:HD2 | 8:H:18:GLU:OE1 | 2.16 | 0.45 |
| 9:I:17:CYS:SG | 9:I:18:GLN:N | 2.90 | 0.45 |
| 14:N:115:DA:C2 | 20:T:-114:DG:N1 | 2.84 | 0.45 |
| 17:Q:711:PHE:CZ | 23:W:232:ALA:HB3 | 2.52 | 0.45 |
| 2:B:309:PHE:CE1 | 9:I:25:TYR:CE1 | 3.03 | 0.44 |
| 2:B:395:LEU:HD21 | 2:B:532:ILE:HG21 | 1.98 | 0.44 |
| 2:B:592:ARG:NH2 | 2:B:663:GLU:OE1 | 2.47 | 0.44 |
| 27:a:129:ARG:HB3 | 27:a:129:ARG:NH1 | 2.32 | 0.44 |
| 27:e:116:ARG:CZ | 27:e:120:MET:HE2 | 2.47 | 0.44 |
| 1:A:520:MET:HG3 | 1:A:522:PRO:HD2 | 1.98 | 0.44 |
| 8:H:50:VAL:HG12 | 8:H:147:LYS:HZ1 | 1.82 | 0.44 |
| 12:L:15:MET:HB3 | 12:L:28:ILE:O | 2.17 | 0.44 |
| 14:N:85:DG:H2' | 14:N:86:DT:H71 | 2.00 | 0.44 |
| 17:Q:768:VAL:HG13 | 17:Q:769:LEU:HG | 1.98 | 0.44 |
| 28:b:49:LEU:HD13 | 28:b:49:LEU:O | 2.16 | 0.44 |
| 7:G:162:SER:HB2 | 7:G:164:MET:SD | 2.57 | 0.44 |
| 13:M:1086:ALA:O | 13:M:1090:GLU:N | 2.46 | 0.44 |
| 17:Q:343:PRO:O | 17:Q:347:LEU:HD23 | 2.18 | 0.44 |
| 17:Q:448:ASP:OD1 | 17:Q:449:VAL:N | 2.50 | 0.44 |
| 17:Q:802:LYS:HE2 | 17:Q:807:LEU:HB2 | 1.99 | 0.44 |
| 17:Q:855:LYS:O | 17:Q:858:LYS:HG3 | 2.18 | 0.44 |
| 20:T:-116:DT:OP2 | 29:c:17:ARG:NH2 | 2.50 | 0.44 |
| 28:b:73:THR:HG21 | 28:b:81:VAL:HA | 1.98 | 0.44 |
| 3:C:40:ALA:O | 3:C:170:GLY:N | 2.50 | 0.44 |
| 8:H:41:LEU:HD21 | 8:H:145:MET:HE1 | 1.99 | 0.44 |
| 8:H:48:TYR:CD2 | 8:H:90:TYR:HB2 | 2.52 | 0.44 |
| 17:Q:373:ASN:O | 17:Q:377:THR:HG23 | 2.18 | 0.44 |
| 17:Q:382:GLY:CA | 22:V:53:PHE:HE2 | 2.30 | 0.44 |
| 23:W:53:ARG:HB3 | 23:W:53:ARG:NH1 | 2.32 | 0.44 |
| 17:Q:325:ALA:HB3 | 17:Q:350:MET:HE2 | 1.99 | 0.44 |
| 23:W:9:PHE:HE2 | 23:W:11:GLN:HB2 | 1.83 | 0.44 |
| 2:B:471:ASN:HD21 | 2:B:473:LEU:HB3 | 1.83 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:D:24:LYS:H | 4:D:24:LYS:HD2 | 1.82 | 0.44 |
| 9:I:56:ASN:HD22 | 9:I:56:ASN:C | 2.26 | 0.44 |
| 26:Z:197:MET:HE2 | 26:Z:201:ILE:HD11 | 1.98 | 0.44 |
| 1:A:487:SER:OG | 1:A:673:GLN:OE1 | 2.25 | 0.44 |
| 1:A:1370:GLY:O | 1:A:1374:VAL:HG23 | 2.18 | 0.44 |
| 2:B:438:ARG:HD2 | 2:B:438:ARG:N | 2.33 | 0.44 |
| 17:Q:384:LEU:HG | 17:Q:386:ALA:H | 1.82 | 0.44 |
| 17:Q:720:VAL:HG21 | 17:Q:743:ALA:CB | 2.48 | 0.44 |
| 17:Q:737:LYS:HZ3 | 17:Q:761:LEU:HA | 1.82 | 0.44 |
| 17:Q:838:GLU:HA | 17:Q:841:LEU:CD2 | 2.48 | 0.44 |
| 27:a:63:ARG:HG2 | 27:a:63:ARG:NH1 | 2.33 | 0.44 |
| 17:Q:527:HIS:CE1 | 17:Q:529:ASN:HB2 | 2.53 | 0.44 |
| 20:T:-58:DT:H2" | 20:T:-57:DA:C5 | 2.53 | 0.44 |
| 28:b:43:VAL:C | 28:b:44:LYS:HE2 | 2.43 | 0.44 |
| 22:V:61:TYR:N | 22:V:62:LYS:HA | 2.33 | 0.44 |
| 27:e:64:LYS:HZ2 | 27:e:89:VAL:CG1 | 2.27 | 0.44 |
| 2:B:175:ASN:HB3 | 2:B:742:VAL:HG11 | 1.99 | 0.43 |
| 7:G:151:ARG:HB3 | 7:G:158:PHE:O | 2.18 | 0.43 |
| 17:Q:296:PHE:CD2 | 17:Q:308:SER:HB2 | 2.54 | 0.43 |
| 23:W:233:SER:HB2 | 23:W:252:SER:HB2 | 1.99 | 0.43 |
| 26:Z:428:VAL:HG13 | 26:Z:467:GLU:HG2 | 1.98 | 0.43 |
| 1:A:26:LEU:HD11 | 2:B:1163:MET:HG3 | 2.01 | 0.43 |
| 1:A:1180:ASN:OD1 | 1:A:1182:GLN:HG3 | 2.18 | 0.43 |
| 2:B:629:GLU:HG2 | 2:B:634:LEU:HD21 | 2.00 | 0.43 |
| 2:B:780:VAL:HG22 | 2:B:965:ILE:HB | 2.00 | 0.43 |
| 14:N:55:DG:H2" | 14:N:56:DT:O5' | 2.18 | 0.43 |
| 16:P:18:U:O2' | 16:P:19:C:OP1 | 2.30 | 0.43 |
| 17:Q:335:PHE:N | 17:Q:335:PHE:CD1 | 2.84 | 0.43 |
| 17:Q:602:TYR:CE1 | 24:X:234:ARG:HB3 | 2.53 | 0.43 |
| 17:Q:631:ARG:O | 17:Q:635:ILE:HG12 | 2.18 | 0.43 |
| 18:R:554:THR:O | 18:R:558:SER:OG | 2.35 | 0.43 |
| 23:W:191:MET:N | 23:W:191:MET:HE2 | 2.32 | 0.43 |
| 1:A:359:VAL:HG11 | 2:B:1106:ARG:NE | 2.33 | 0.43 |
| 20:T:-60:DT:H6 | 20:T:-60:DT:H2' | 1.68 | 0.43 |
| 30:d:52:SER:C | 30:d:56:MET:HE3 | 2.43 | 0.43 |
| 1:A:84:HIS:O | 1:A:257:PRO:HB3 | 2.18 | 0.43 |
| 1:A:104:MET:HE2 | 1:A:104:MET:HB2 | 1.93 | 0.43 |
| 1:A:469:MET:HG3 | 2:B:1093:CYS:SG | 2.58 | 0.43 |
| 1:A:764:ASN:OD1 | 1:A:765:ASN:N | 2.52 | 0.43 |
| 1:A:997:ASN:O | 1:A:999:ARG:N | 2.46 | 0.43 |
| 3:C:37:VAL:HG12 | 3:C:248:ALA:HB1 | 2.00 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:146:ASP:HB2 | 10:J:19:GLU:OE2 | 2.18 | 0.43 |
| 17:Q:852:LEU:O | 17:Q:855:LYS:HE3 | 2.18 | 0.43 |
| 26:Z:452:PRO:O | 26:Z:460:MET:HG3 | 2.19 | 0.43 |
| 1:A:386:ALA:O | 1:A:449:HIS:ND1 | 2.52 | 0.43 |
| 2:B:388:TYR:CD1 | 2:B:391:LYS:HD2 | 2.54 | 0.43 |
| 17:Q:586:LYS:O | 17:Q:590:ARG:HG3 | 2.18 | 0.43 |
| 1:A:364:ARG:HG2 | 1:A:500:GLU:OE2 | 2.19 | 0.43 |
| 1:A:1180:ASN:HB3 | 1:A:1183:SER:HB3 | 2.00 | 0.43 |
| 8:H:15:ILE:HG12 | 8:H:28:LEU:HD13 | 1.99 | 0.43 |
| 17:Q:611:TRP:HE1 | 17:Q:628:HIS:HA | 1.84 | 0.43 |
| 17:Q:761:LEU:HD22 | 17:Q:785:GLU:HB3 | 1.99 | 0.43 |
| 27:a:120:MET:HG2 | 27:a:121:PRO:HD2 | 2.00 | 0.43 |
| 1:A:479:TRP:HB2 | 1:A:483:ARG:NH2 | 2.33 | 0.43 |
| 1:A:1180:ASN:O | 1:A:1183:SER:OG | 2.34 | 0.43 |
| 4:D:70:ARG:NH1 | 7:G:88:VAL:HG21 | 2.34 | 0.43 |
| 5:E:44:PHE:HB3 | 5:E:53:PRO:HB3 | 2.01 | 0.43 |
| 17:Q:714:HIS:CE1 | 23:W:276:GLN:HG3 | 2.54 | 0.43 |
| 17:Q:821:LEU:O | 17:Q:825:GLN:HG2 | 2.18 | 0.43 |
| 27:a:129:ARG:HB3 | 27:a:129:ARG:CZ | 2.49 | 0.43 |
| 29:c:50:TYR:O | 29:c:54:VAL:HG23 | 2.18 | 0.43 |
| 1:A:117:LEU:HG | 1:A:232:GLU:OE2 | 2.18 | 0.43 |
| 1:A:461:GLN:HB3 | 20:T:-26:DG:H21 | 1.84 | 0.43 |
| 2:B:269:ILE:HG21 | 2:B:369:VAL:HG21 | 2.00 | 0.43 |
| 2:B:285:LEU:HD11 | 2:B:305:LEU:CD2 | 2.47 | 0.43 |
| 2:B:351:VAL:HA | 2:B:572:CYS:SG | 2.58 | 0.43 |
| 17:Q:535:LEU:HD23 | 22:V:44:PHE:HZ | 1.84 | 0.43 |
| 17:Q:869:GLU:OE2 | 17:Q:873:LYS:HG3 | 2.18 | 0.43 |
| 1:A:663:ASP:OD1 | 1:A:664:ILE:N | 2.52 | 0.43 |
| 2:B:21:LEU:HD22 | 18:R:579:LEU:HB3 | 2.00 | 0.43 |
| 2:B:746:THR:HG22 | 2:B:747:LEU:HG | 2.00 | 0.43 |
| 3:C:190:ASN:ND2 | 3:C:195:THR:O | 2.52 | 0.43 |
| 6:F:82:GLU:HA | 6:F:82:GLU:OE1 | 2.19 | 0.43 |
| 28:f:78:ARG:NH1 | 28:f:80:THR:O | 2.51 | 0.43 |
| 1:A:467:MET:HG3 | 1:A:534:VAL:HG11 | 2.01 | 0.43 |
| 1:A:476:ILE:O | 1:A:476:ILE:HD12 | 2.19 | 0.43 |
| 1:A:868:MET:HE1 | 1:A:1091:ALA:HB3 | 2.00 | 0.43 |
| 2:B:993:LYS:HG2 | 2:B:1018:TYR:OH | 2.19 | 0.43 |
| 5:E:80:PRO:HA | 5:E:107:GLN:HB2 | 2.01 | 0.43 |
| 6:F:119:GLY:O | 6:F:123:LEU:HD23 | 2.19 | 0.43 |
| 8:H:76:ASN:N | 8:H:76:ASN:OD1 | 2.51 | 0.43 |
| 14:N:112:DA:OP2 | 29:c:35:ARG:NH2 | 2.52 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 27:a:96:SER:O | 27:a:100:LEU:HG | 2.18 | 0.43 |
| 1:A:457:ILE:HD11 | 1:A:469:MET:HB3 | 2.01 | 0.42 |
| 1:A:890:ARG:CZ | 1:A:1023:VAL:HG22 | 2.49 | 0.42 |
| 20:T:-83:DC:N3 | 20:T:-82:DA:N6 | 2.67 | 0.42 |
| 23:W:237:ASN:HB3 | 23:W:250:SER:HB3 | 2.01 | 0.42 |
| 27:e:64:LYS:HA | 27:e:64:LYS:HE2 | 2.00 | 0.42 |
| 2:B:903:ILE:HD12 | 3:C:62:GLU:OE2 | 2.19 | 0.42 |
| 3:C:86:ARG:NH2 | 3:C:172:GLU:OE2 | 2.51 | 0.42 |
| 17:Q:373:ASN:HB3 | 17:Q:375:TYR:CE2 | 2.54 | 0.42 |
| 17:Q:459:ALA:HB1 | 22:V:46:PRO:HB2 | 2.00 | 0.42 |
| 17:Q:682:ASP:OD1 | 17:Q:683:VAL:N | 2.52 | 0.42 |
| 18:R:570:TRP:HA | 18:R:573:VAL:HG22 | 2.01 | 0.42 |
| 23:W:76:LEU:HD12 | 23:W:77:PRO:HD2 | 2.00 | 0.42 |
| 23:W:88:ILE:O | 23:W:102:ILE:N | 2.46 | 0.42 |
| 27:a:108:ASN:O | 27:a:112:ILE:HD13 | 2.19 | 0.42 |
| 2:B:403:LEU:HD13 | 2:B:407:MET:SD | 2.59 | 0.42 |
| 2:B:1090:GLU:OE1 | 2:B:1090:GLU:N | 2.47 | 0.42 |
| 6:F:79:VAL:HG21 | 6:F:83:LEU:HD21 | 2.00 | 0.42 |
| 7:G:139:GLN:OE1 | 7:G:139:GLN:N | 2.46 | 0.42 |
| 14:N:126:DC:C6 | 14:N:127:DT:H72 | 2.54 | 0.42 |
| 20:T:-24:DC:H2' | 20:T:-23:DA:C8 | 2.54 | 0.42 |
| 27:a:90:MET:HE2 | 27:a:94:GLU:HG2 | 2.02 | 0.42 |
| 1:A:94:VAL:HG13 | 1:A:250:VAL:HG23 | 2.01 | 0.42 |
| 23:W:231:HIS:NE2 | 23:W:257:LYS:HB2 | 2.35 | 0.42 |
| 25:Y:40:LEU:HB3 | 25:Y:42:MET:HE1 | 2.01 | 0.42 |
| 29:c:102:ILE:HG23 | 30:d:58:ILE:HD13 | 2.02 | 0.42 |
| 27:e:60:LEU:HD13 | 27:e:93:GLN:HG2 | 2.01 | 0.42 |
| 1:A:561:MET:HE1 | 11:K:57:LEU:O | 2.20 | 0.42 |
| 1:A:1178:ASP:OD1 | 1:A:1185:VAL:HG13 | 2.19 | 0.42 |
| 14:N:145:DT:H2" | 14:N:146:DA:C8 | 2.55 | 0.42 |
| 23:W:110:TRP:CD1 | 23:W:111:THR:HG22 | 2.54 | 0.42 |
| 1:A:376:ASP:HB3 | 1:A:522:PRO:HD3 | 2.00 | 0.42 |
| 1:A:469:MET:HB3 | 1:A:469:MET:HE2 | 1.89 | 0.42 |
| 1:A:752:THR:HB | 1:A:786:ALA:HB1 | 2.00 | 0.42 |
| 1:A:1024:ASN:O | 5:E:162:ARG:NH2 | 2.52 | 0.42 |
| 14:N:34:DT:H2" | 14:N:35:DA:H8 | 1.84 | 0.42 |
| 14:N:108:DT:H2" | 14:N:109:DA:N7 | 2.34 | 0.42 |
| 17:Q:340:PHE:CE2 | 22:V:66:LEU:HD21 | 2.53 | 0.42 |
| 17:Q:474:PHE:HB2 | 17:Q:503:LEU:HD13 | 2.02 | 0.42 |
| 17:Q:743:ALA:O | 17:Q:746:VAL:HG22 | 2.20 | 0.42 |
| 22:V:96:PRO:HA | 22:V:97:ASN:HA | 1.71 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:1038:THR:HA | 3:C:195:THR:HA | 2.02 | 0.42 |
| 7:G:13:LEU:HD21 | 7:G:17:TYR:HB2 | 2.02 | 0.42 |
| 19:S:158:TYR:O | 19:S:162:GLY:N | 2.51 | 0.42 |
| 23:W:289:ILE:N | 23:W:301:TYR:O | 2.51 | 0.42 |
| 26:Z:451:MET:O | 26:Z:451:MET:HG2 | 2.20 | 0.42 |
| 17:Q:375:TYR:OH | 22:V:66:LEU:HD12 | 2.20 | 0.42 |
| 21:U:522:THR:O | 21:U:524:LYS:N | 2.53 | 0.42 |
| 29:c:20:ARG:O | 30:d:117:LYS:HD3 | 2.19 | 0.42 |
| 1:A:465:HIS:NE2 | 1:A:467:MET:HB2 | 2.35 | 0.42 |
| 1:A:841:MET:HE2 | 1:A:841:MET:HB3 | 1.82 | 0.42 |
| 2:B:529:MET:HG3 | 2:B:624:PRO:HD2 | 2.02 | 0.42 |
| 17:Q:305:GLN:HG3 | 17:Q:335:PHE:HD2 | 1.85 | 0.42 |
| 27:a:74:ILE:HD13 | 28:b:62:LEU:HB3 | 2.02 | 0.42 |
| 1:A:962:ASP:HB3 | 1:A:1043:ILE:HG23 | 2.01 | 0.42 |
| 17:Q:741:LEU:HD23 | 17:Q:741:LEU:HA | 1.91 | 0.42 |
| 23:W:44:VAL:HB | 23:W:60:LEU:HB2 | 2.02 | 0.42 |
| 24:X:243:LYS:HD2 | 24:X:243:LYS:C | 2.45 | 0.42 |
| 1:A:488:VAL:O | 1:A:491:PRO:HD2 | 2.20 | 0.41 |
| 1:A:841:MET:HE3 | 2:B:501:LEU:O | 2.20 | 0.41 |
| 1:A:930:LEU:HD13 | 1:A:934:LEU:HD13 | 2.02 | 0.41 |
| 2:B:139:GLN:O | 2:B:140:LEU:HD13 | 2.19 | 0.41 |
| 2:B:1007:ASN:HB3 | 18:R:594:PHE:CE1 | 2.55 | 0.41 |
| 3:C:49:TRP:NE1 | 26:Z:719:GLY:O | 2.51 | 0.41 |
| 14:N:41:DT:H2' | 14:N:42:DA:C8 | 2.55 | 0.41 |
| 14:N:52:DG:C4 | 14:N:53:DC:C5 | 3.08 | 0.41 |
| 17:Q:754:MET:HE1 | 17:Q:796:LEU:HB3 | 2.02 | 0.41 |
| 1:A:47:THR:OG1 | 1:A:51:ARG:O | 2.27 | 0.41 |
| 1:A:370:ASP:HA | 2:B:788:TYR:CE2 | 2.55 | 0.41 |
| 1:A:457:ILE:CG2 | 1:A:504:HIS:HB2 | 2.49 | 0.41 |
| 2:B:161:CYS:SG | 2:B:162:LEU:N | 2.92 | 0.41 |
| 2:B:544:PHE:O | 2:B:547:GLU:HG3 | 2.20 | 0.41 |
| 2:B:859:ARG:HA | 2:B:859:ARG:CZ | 2.48 | 0.41 |
| 10:J:30:THR:OG1 | 10:J:31:GLU:OE1 | 2.37 | 0.41 |
| 14:N:33:DC:H2' | 14:N:34:DT:C6 | 2.55 | 0.41 |
| 23:W:216:ILE:HB | 23:W:264:ARG:HH22 | 1.85 | 0.41 |
| 26:Z:180:TRP:HB2 | 26:Z:227:VAL:HG13 | 2.02 | 0.41 |
| 1:A:1133:LYS:HB2 | 1:A:1133:LYS:HE3 | 1.75 | 0.41 |
| 2:B:584:MET:HE2 | 2:B:584:MET:HA | 2.02 | 0.41 |
| 2:B:1066:PRO:HB2 | 2:B:1075:MET:HE2 | 2.01 | 0.41 |
| 2:B:1123:GLY:HA3 | 2:B:1171:MET:N | 2.35 | 0.41 |
| 7:G:152:VAL:HG22 | 7:G:157:ILE:HG22 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:7:GLU:HG2 | 8:H:59:VAL:HG22 | 2.02 | 0.41 |
| 9:I:106:ASP:N | 9:I:106:ASP:OD1 | 2.51 | 0.41 |
| 17:Q:342:LEU:HD11 | 22:V:67:GLU:HG2 | 2.01 | 0.41 |
| 17:Q:527:HIS:CD2 | 17:Q:530:TYR:HB2 | 2.55 | 0.41 |
| 26:Z:478:VAL:HB | 26:Z:518:LEU:HD11 | 2.02 | 0.41 |
| 26:Z:486:GLU:OE2 | 26:Z:555:ARG:NH2 | 2.53 | 0.41 |
| 28:b:72:TYR:OH | 28:b:92:ARG:HD3 | 2.20 | 0.41 |
| 27:e:72:ARG:NH1 | 27:e:83:ARG:HH12 | 2.17 | 0.41 |
| 28:f:26:ILE:H | 28:f:26:ILE:CD1 | 2.30 | 0.41 |
| 2:B:27:TRP:CD1 | 2:B:762:ARG:HE | 2.37 | 0.41 |
| 8:H:91:VAL:HG22 | 8:H:144:LEU:HD23 | 2.02 | 0.41 |
| 17:Q:424:GLN:HB2 | 24:X:231:TRP:CE3 | 2.56 | 0.41 |
| 17:Q:500:SER:OG | 17:Q:523:ILE:HD11 | 2.20 | 0.41 |
| 18:R:507:PRO:HA | 18:R:508:ASN:HA | 1.54 | 0.41 |
| 29:c:29:ARG:HE | 29:c:29:ARG:HA | 1.85 | 0.41 |
| 1:A:627:LYS:O | 1:A:629:VAL:HG23 | 2.21 | 0.41 |
| 1:A:880:ARG:CZ | 5:E:165:LEU:HD12 | 2.51 | 0.41 |
| 2:B:309:PHE:O | 2:B:309:PHE:CD2 | 2.70 | 0.41 |
| 5:E:140:THR:OG1 | 5:E:141:GLU:OE1 | 2.33 | 0.41 |
| 10:J:31:GLU:OE1 | 10:J:31:GLU:N | 2.40 | 0.41 |
| 14:N:95:DT:H2' | 14:N:96:DG:C8 | 2.56 | 0.41 |
| 17:Q:751:THR:HA | 17:Q:754:MET:HG3 | 2.02 | 0.41 |
| 18:R:505:ALA:N | 18:R:506:PRO:HD2 | 2.35 | 0.41 |
| 28:b:59:LYS:HA | 28:b:59:LYS:HD2 | 1.93 | 0.41 |
| 1:A:350:VAL:HG23 | 1:A:351:ARG:H | 1.86 | 0.41 |
| 2:B:543:GLU:HA | 2:B:543:GLU:OE2 | 2.21 | 0.41 |
| 3:C:56:SER:OG | 3:C:158:GLU:N | 2.46 | 0.41 |
| 4:D:76:ASN:HD21 | 4:D:78:GLU:HB2 | 1.85 | 0.41 |
| 17:Q:650:ALA:HA | 17:Q:653:ILE:HG12 | 2.02 | 0.41 |
| 17:Q:810:ALA:HA | 17:Q:813:GLU:OE1 | 2.21 | 0.41 |
| 20:T:-59:DT:H2" | 20:T:-58:DT:C6 | 2.55 | 0.41 |
| 26:Z:505:ASP:N | 26:Z:505:ASP:OD1 | 2.53 | 0.41 |
| 29:c:41:GLU:HG2 | 29:c:42:ARG:HG2 | 2.03 | 0.41 |
| 1:A:196:LEU:HD23 | 1:A:311:GLN:HG3 | 2.02 | 0.41 |
| 1:A:1416:ARG:HB3 | 1:A:1432:PHE:HE2 | 1.85 | 0.41 |
| 7:G:13:LEU:HG | 7:G:17:TYR:HD2 | 1.85 | 0.41 |
| 14:N:58:DA:H1' | 14:N:59:DA:O4' | 2.19 | 0.41 |
| 17:Q:386:ALA:HB2 | 17:Q:393:LYS:HB3 | 2.03 | 0.41 |
| 20:T:-63:DC:H2" | 20:T:-62:DG:C8 | 2.56 | 0.41 |
| 29:c:25:PHE:HZ | 29:c:59:THR:HG21 | 1.84 | 0.41 |
| 30:d:36:ILE:HG13 | 30:d:37:TYR:N | 2.36 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:961:GLU:O | 1:A:965:VAL:HG23 | 2.20 | 0.41 |
| 1:A:1177:TYR:CE2 | 1:A:1210:TRP:HE3 | 2.39 | 0.41 |
| 1:A:1451:MET:SD | 1:A:1456:GLU:HB3 | 2.61 | 0.41 |
| 2:B:529:MET:HE3 | 2:B:702:MET:HG2 | 2.03 | 0.41 |
| 1:A:404:GLU:OE1 | 1:A:407:ARG:NH1 | 2.54 | 0.41 |
| 1:A:863:ARG:NH2 | 1:A:1129:ASN:HD21 | 2.19 | 0.41 |
| 1:A:1093:GLN:HE22 | 2:B:1093:CYS:HA | 1.85 | 0.41 |
| 6:F:124:ILE:HD12 | 6:F:124:ILE:N | 2.33 | 0.41 |
| 7:G:1:MET:HG3 | 7:G:3:TYR:HE1 | 1.86 | 0.41 |
| 17:Q:713:LYS:HA | 17:Q:713:LYS:HE2 | 2.02 | 0.41 |
| 23:W:214:ILE:N | 23:W:228:LEU:O | 2.52 | 0.41 |
| 23:W:248:VAL:HG13 | 23:W:282:TYR:CZ | 2.56 | 0.41 |
| 26:Z:206:THR:OG1 | 26:Z:207:ASP:N | 2.54 | 0.41 |
| 26:Z:478:VAL:HG21 | 26:Z:502:LEU:HD22 | 2.02 | 0.41 |
| 27:a:62:ILE:CG1 | 28:b:37:LEU:HD11 | 2.50 | 0.41 |
| 29:c:50:TYR:HB3 | 30:d:91:ILE:CD1 | 2.46 | 0.41 |
| 1:A:51:ARG:HD3 | 1:A:51:ARG:N | 2.24 | 0.41 |
| 1:A:794:GLU:N | 1:A:845:GLU:OE2 | 2.45 | 0.41 |
| 1:A:901:VAL:HB | 1:A:978:VAL:HG12 | 2.03 | 0.41 |
| 2:B:20:ASP:OD2 | 18:R:586:MET:HE1 | 2.19 | 0.41 |
| 8:H:63:THR:HG21 | 8:H:68:GLY:HA2 | 2.03 | 0.41 |
| 17:Q:345:PHE:HE1 | 17:Q:379:LYS:HE2 | 1.86 | 0.41 |
| 17:Q:816:GLN:HG3 | 17:Q:820:LEU:HD11 | 2.02 | 0.41 |
| 27:e:64:LYS:HD3 | 27:e:64:LYS:C | 2.46 | 0.41 |
| 1:A:354:LEU:HA | 1:A:357:LYS:HE2 | 2.03 | 0.40 |
| 1:A:1307:VAL:HG22 | 1:A:1338:THR:HG22 | 2.02 | 0.40 |
| 8:H:84:ARG:HD2 | 8:H:144:LEU:HD13 | 2.02 | 0.40 |
| 9:I:75:ASP:O | 9:I:80:ARG:NH2 | 2.50 | 0.40 |
| 17:Q:819:ASP:O | 17:Q:822:SER:OG | 2.33 | 0.40 |
| 17:Q:866:ARG:HH12 | 17:Q:870:GLU:CB | 2.18 | 0.40 |
| 18:R:574:GLU:HG2 | 18:R:577:LYS:HE3 | 2.03 | 0.40 |
| 20:T:-77:DC:H2" | 20:T:-76:DG:C8 | 2.57 | 0.40 |
| 20:T:-17:DC:H4' | 20:T:-16:DA:O5' | 2.20 | 0.40 |
| 22:V:53:PHE:CD1 | 22:V:54:ASP:N | 2.89 | 0.40 |
| 6:F:102:ILE:N | 6:F:102:ILE:HD12 | 2.36 | 0.40 |
| 9:I:80:ARG:HD3 | 9:I:93:GLU:OE1 | 2.20 | 0.40 |
| 17:Q:314:ARG:HH12 | 17:Q:349:GLN:HE22 | 1.69 | 0.40 |
| 20:T:-75:DC:H2" | 20:T:-74:DG:H8 | 1.85 | 0.40 |
| 1:A:1026:ASP:O | 1:A:1026:ASP:OD1 | 2.40 | 0.40 |
| 5:E:18:MET:HE1 | 5:E:60:VAL:HG21 | 2.03 | 0.40 |
| 8:H:37:MET:CG | 8:H:127:GLY:HA3 | 2.39 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:H:97:TYR:CZ | 8:H:115:TYR:HB3 | 2.56 | 0.40 |
| 17:Q:855:LYS:HG2 | 17:Q:858:LYS:HE3 | 2.03 | 0.40 |
| 20:T:-114:DG:N1 | 20:T:-113:DG:C6 | 2.89 | 0.40 |
| 1:A:288:ASN:HA | 1:A:291:ARG:HH12 | 1.86 | 0.40 |
| 1:A:809:HIS:HE1 | 2:B:506:TRP:CZ2 | 2.38 | 0.40 |
| 1:A:868:MET:HB2 | 1:A:868:MET:HE2 | 1.88 | 0.40 |
| 1:A:1366:PHE:HB2 | 1:A:1374:VAL:HG21 | 2.03 | 0.40 |
| 17:Q:534:TYR:HD2 | 17:Q:557:ALA:HB2 | 1.85 | 0.40 |
| 17:Q:636:TYR:HA | 17:Q:639:VAL:HG22 | 2.03 | 0.40 |
| 20:T:-75:DC:C2 | 20:T:-74:DG:N7 | 2.90 | 0.40 |
| 23:W:110:TRP:CG | 23:W:111:THR:H | 2.39 | 0.40 |
| 28:f:68:ASP:OD2 | 28:f:93:GLN:NE2 | 2.51 | 0.40 |
| 1:A:291:ARG:NH1 | 1:A:291:ARG:HB3 | 2.37 | 0.40 |
| 1:A:1286:ARG:O | 1:A:1289:GLU:HG3 | 2.22 | 0.40 |
| 4:D:76:ASN:ND2 | 4:D:78:GLU:HB2 | 2.37 | 0.40 |
| 23:W:176:ASP:O | 23:W:180:GLY:N | 2.44 | 0.40 |
| 23:W:191:MET:HG2 | 23:W:210:ASP:HB2 | 2.04 | 0.40 |
| 26:Z:474:MET:HA | 26:Z:474:MET:CE | 2.52 | 0.40 |

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 PDB entries followed by that with respect to all EM entries.

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 | 1408/1984 (71%) | 1330 (94%) | 76 (5%) | 2 (0%) | 48 77 |
| 2 | B | 1112/1251 (89%) | 1042 (94%) | 70 (6%) | 0 | 100 100 |
| 3 | C | 254/275 (92%) | 236 (93%) | 18 (7%) | 0 | 100 100 |
| 4 | D | 124/142 (87%) | 120 (97%) | 4 (3%) | 0 | 100 100 |
| 5 | E | 207/210 (99%) | 200 (97%) | 7 (3%) | 0 | 100 100 |
| 6 | F | 76/127 (60%) | 74 (97%) | 2 (3%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 7 | G | 169/172 (98%) | 162 (96%) | 7 (4%) | 0 | 100 | 100 |
| 8 | H | 147/150 (98%) | 137 (93%) | 10 (7%) | 0 | 100 | 100 |
| 9 | I | 114/125 (91%) | 104 (91%) | 10 (9%) | 0 | 100 | 100 |
| 10 | J | 64/67 (96%) | 58 (91%) | 6 (9%) | 0 | 100 | 100 |
| 11 | K | 113/117 (97%) | 111 (98%) | 2 (2%) | 0 | 100 | 100 |
| 12 | L | 45/58 (78%) | 39 (87%) | 5 (11%) | 1 (2%) | 5 | 21 |
| 13 | M | 976/1729 (56%) | 935 (96%) | 40 (4%) | 1 (0%) | 48 | 77 |
| 15 | O | 130/821 (16%) | 127 (98%) | 3 (2%) | 0 | 100 | 100 |
| 17 | Q | 888/1179 (75%) | 863 (97%) | 25 (3%) | 0 | 100 | 100 |
| 18 | R | 240/713 (34%) | 230 (96%) | 10 (4%) | 0 | 100 | 100 |
| 19 | S | 157/304 (52%) | 156 (99%) | 1 (1%) | 0 | 100 | 100 |
| 21 | U | 117/666 (18%) | 104 (89%) | 12 (10%) | 1 (1%) | 14 | 43 |
| 22 | V | 234/531 (44%) | 220 (94%) | 14 (6%) | 0 | 100 | 100 |
| 23 | W | 298/305 (98%) | 282 (95%) | 16 (5%) | 0 | 100 | 100 |
| 24 | X | 41/531 (8%) | 40 (98%) | 1 (2%) | 0 | 100 | 100 |
| 25 | Y | 114/121 (94%) | 106 (93%) | 8 (7%) | 0 | 100 | 100 |
| 26 | Z | 497/1087 (46%) | 477 (96%) | 19 (4%) | 1 (0%) | 44 | 73 |
| 27 | a | 75/136 (55%) | 75 (100%) | 0 | 0 | 100 | 100 |
| 27 | e | 95/136 (70%) | 95 (100%) | 0 | 0 | 100 | 100 |
| 28 | b | 81/103 (79%) | 79 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | f | 76/103 (74%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 29 | c | 101/130 (78%) | 100 (99%) | 1 (1%) | 0 | 100 | 100 |
| 30 | d | 93/123 (76%) | 90 (97%) | 3 (3%) | 0 | 100 | 100 |
| All | All | 8046/13396 (60%) | 7666 (95%) | 374 (5%) | 6 (0%) | 50 | 77 |

All (6) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 1343 | LEU |
| 12 | L | 39 | CYS |
| 13 | M | 700 | HIS |
| 21 | U | 510 | LYS |
| 26 | Z | 774 | GLN |
| 1 | A | 433 | PRO |

### 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 PDB entries followed by that with respect to all EM entries.

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 | 1229/1761 (70%) | 1225 (100%) | 4 (0%) | 91 97 |
| 2 | B | 986/1084 (91%) | 980 (99%) | 6 (1%) | 84 95 |
| 3 | C | 235/252 (93%) | 235 (100%) | 0 | 100 100 |
| 4 | D | 109/126 (86%) | 109 (100%) | 0 | 100 100 |
| 5 | E | 191/192 (100%) | 190 (100%) | 1 (0%) | 86 96 |
| 6 | F | 68/111 (61%) | 68 (100%) | 0 | 100 100 |
| 7 | G | 146/153 (95%) | 146 (100%) | 0 | 100 100 |
| 8 | H | 130/131 (99%) | 126 (97%) | 4 (3%) | 35 70 |
| 9 | I | 104/112 (93%) | 103 (99%) | 1 (1%) | 73 91 |
| 10 | J | 55/56 (98%) | 55 (100%) | 0 | 100 100 |
| 11 | K | 104/106 (98%) | 104 (100%) | 0 | 100 100 |
| 12 | L | 44/55 (80%) | 43 (98%) | 1 (2%) | 45 77 |
| 13 | M | 41/1524 (3%) | 41 (100%) | 0 | 100 100 |
| 17 | Q | 533/1011 (53%) | 529 (99%) | 4 (1%) | 79 93 |
| 18 | R | 57/625 (9%) | 56 (98%) | 1 (2%) | 54 82 |
| 19 | S | 4/268 (2%) | 4 (100%) | 0 | 100 100 |
| 22 | V | 46/462 (10%) | 46 (100%) | 0 | 100 100 |
| 23 | W | 255/260 (98%) | 255 (100%) | 0 | 100 100 |
| 24 | X | 40/467 (9%) | 40 (100%) | 0 | 100 100 |
| 25 | Y | 102/105 (97%) | 100 (98%) | 2 (2%) | 50 79 |
| 26 | Z | 435/939 (46%) | 434 (100%) | 1 (0%) | 92 98 |
| 27 | a | 67/111 (60%) | 66 (98%) | 1 (2%) | 60 85 |
| 27 | e | 84/111 (76%) | 84 (100%) | 0 | 100 100 |
| 28 | b | 68/79 (86%) | 68 (100%) | 0 | 100 100 |
| 28 | f | 63/79 (80%) | 63 (100%) | 0 | 100 100 |
| 29 | c | 82/102 (80%) | 82 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 30 | d | 81/103 (79%) | 79 (98%) | 2 (2%) | 42 75 |
| All | All | 5359/10385 (52%) | 5331 (100%) | 28 (0%) | 85 96 |

All (28) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 238 | MET |
| 1 | A | 510 | GLU |
| 1 | A | 524 | MET |
| 1 | A | 561 | MET |
| 2 | B | 84 | TYR |
| 2 | B | 155 | MET |
| 2 | B | 297 | MET |
| 2 | B | 388 | TYR |
| 2 | B | 604 | ILE |
| 2 | B | 1163 | MET |
| 5 | E | 29 | THR |
| 8 | H | 51 | ASP |
| 8 | H | 70 | LEU |
| 8 | H | 123 | MET |
| 8 | H | 145 | MET |
| 9 | I | 83 | ASP |
| 12 | L | 34 | ILE |
| 17 | Q | 310 | TYR |
| 17 | Q | 707 | CYS |
| 17 | Q | 718 | GLU |
| 17 | Q | 837 | GLU |
| 18 | R | 500 | GLU |
| 25 | Y | 48 | MET |
| 25 | Y | 64 | MET |
| 26 | Z | 429 | CYS |
| 27 | a | 120 | MET |
| 30 | d | 85 | THR |
| 30 | d | 103 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 96 | HIS |
| 1 | A | 122 | ASN |
| 1 | A | 188 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 273 | GLN |
| 1 | A | 288 | ASN |
| 1 | A | 320 | ASN |
| 1 | A | 372 | ASN |
| 1 | A | 539 | GLN |
| 1 | A | 700 | GLN |
| 1 | A | 711 | GLN |
| 1 | A | 790 | GLN |
| 1 | A | 791 | GLN |
| 1 | A | 804 | HIS |
| 1 | A | 991 | GLN |
| 1 | A | 1036 | ASN |
| 1 | A | 1044 | HIS |
| 1 | A | 1129 | ASN |
| 1 | A | 1172 | ASN |
| 1 | A | 1332 | GLN |
| 1 | A | 1417 | HIS |
| 1 | A | 1457 | ASN |
| 1 | A | 1462 | GLN |
| 2 | B | 197 | GLN |
| 2 | B | 227 | ASN |
| 2 | B | 387 | HIS |
| 2 | B | 582 | GLN |
| 2 | B | 731 | GLN |
| 2 | B | 1142 | ASN |
| 2 | B | 1160 | GLN |
| 3 | C | 111 | GLN |
| 3 | C | 145 | GLN |
| 5 | E | 30 | GLN |
| 5 | E | 132 | GLN |
| 5 | E | 169 | GLN |
| 7 | G | 9 | HIS |
| 8 | H | 29 | HIS |
| 9 | I | 32 | ASN |
| 9 | I | 56 | ASN |
| 9 | I | 91 | HIS |
| 9 | I | 98 | GLN |
| 17 | Q | 273 | ASN |
| 17 | Q | 311 | GLN |
| 17 | Q | 324 | GLN |
| 17 | Q | 373 | ASN |
| 17 | Q | 391 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 17 | Q | 424 | GLN |
| 17 | Q | 527 | HIS |
| 17 | Q | 559 | GLN |
| 17 | Q | 564 | HIS |
| 17 | Q | 616 | HIS |
| 17 | Q | 714 | HIS |
| 17 | Q | 816 | GLN |
| 17 | Q | 860 | GLN |
| 17 | Q | 877 | GLN |
| 22 | V | 56 | ASN |
| 22 | V | 69 | GLN |
| 22 | V | 72 | HIS |
| 23 | W | 27 | ASN |
| 23 | W | 57 | GLN |
| 23 | W | 131 | ASN |
| 23 | W | 268 | HIS |
| 23 | W | 273 | HIS |
| 25 | Y | 12 | HIS |
| 26 | Z | 244 | ASN |
| 26 | Z | 272 | ASN |
| 26 | Z | 446 | ASN |
| 26 | Z | 519 | GLN |
| 28 | b | 93 | GLN |
| 29 | c | 112 | GLN |
| 30 | d | 64 | ASN |
| 27 | e | 68 | GLN |
| 27 | e | 108 | ASN |

### 5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|---|---|---|---|---|
| 16 | P | 20/21 (95%) | 7 (35%) | 3 (15%) |

All (7) RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 8 | U |
| 16 | P | 9 | U |
| 16 | P | 10 | U |
| 16 | P | 11 | U |
| 16 | P | 16 | U |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 17 | G |
| 16 | P | 19 | C |

All (3) RNA pucker outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | P | 8 | U |
| 16 | P | 16 | U |
| 16 | P | 18 | U |

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

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 1 | SEP | A | 1547 | 1 | 8,9,10 | 1.62 | 1 (12%) | 7,12,14 | 1.29 | 1 (14%) |
| 26 | TPO | Z | 775 | 26 | 8,10,11 | 1.12 | 0 | 10,14,16 | 1.97 | 1 (10%) |
| 1 | TPO | A | 1525 | 1 | 8,10,11 | 1.11 | 0 | 10,14,16 | 2.14 | 1 (10%) |

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 |
|---|---|---|---|---|---|---|---|
| 1 | SEP | A | 1547 | 1 | - | 0/6/8/10 | - |
| 26 | TPO | Z | 775 | 26 | - | 2/9/11/13 | - |
| 1 | TPO | A | 1525 | 1 | - | 0/9/11/13 | - |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1547 | SEP | P-O1P | 3.53 | 1.61 | 1.50 |

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 1525 | TPO | P-OG1-CB | -6.14 | 106.65 | 123.33 |
| 26 | Z | 775 | TPO | P-OG1-CB | -5.70 | 107.84 | 123.33 |
| 1 | A | 1547 | SEP | OG-CB-CA | 2.81 | 110.88 | 108.14 |

There are no chirality outliers.

All (2) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 26 | Z | 775 | TPO | C-CA-CB-CG2 |
| 26 | Z | 775 | TPO | CB-OG1-P-O2P |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

| Mol | Chain | Number of breaks |
|---|---|---|
| 21 | U | 1 |
| 22 | V | 1 |
| 13 | M | 1 |

All chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|---|---|---|---|---|---|---|
| 1 | U | 497:ASP | C | 505:SER | N | 27.06 |
| 1 | V | 299:GLU | C | 310:ASN | N | 12.67 |
| 1 | M | 1334:ASN | C | 1338:ILE | N | 5.50 |

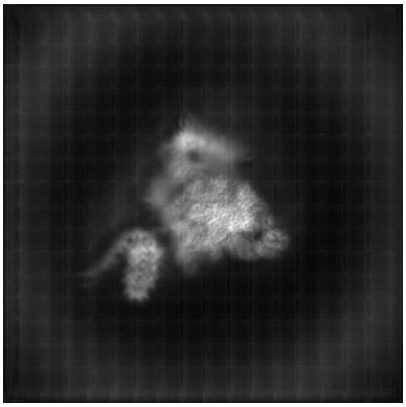
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-48039. These allow visual inspection of the internal detail of the map and identification of artifacts.

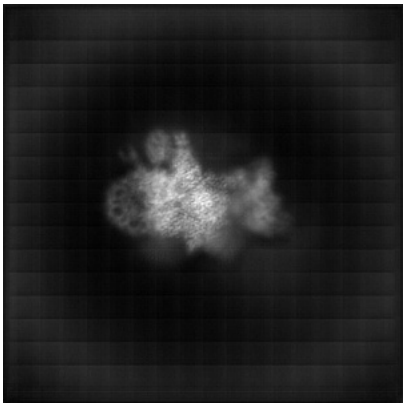
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

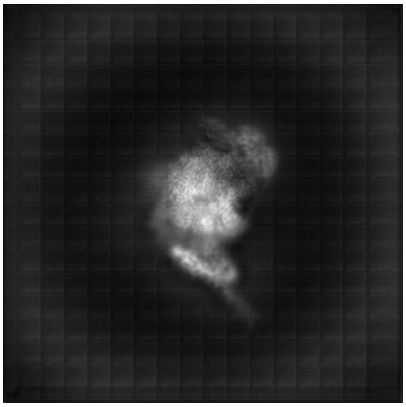
### 6.1.1 Primary map



X



Y

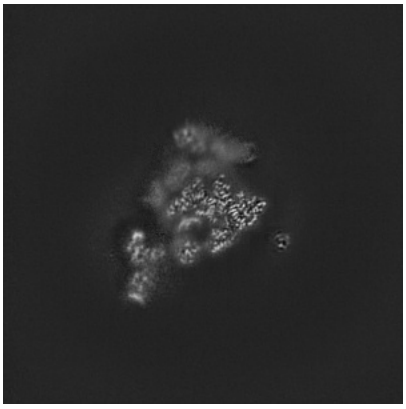


Z

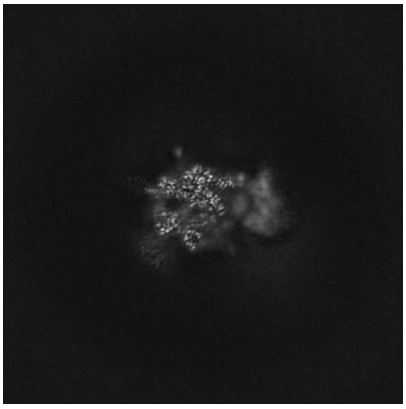
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

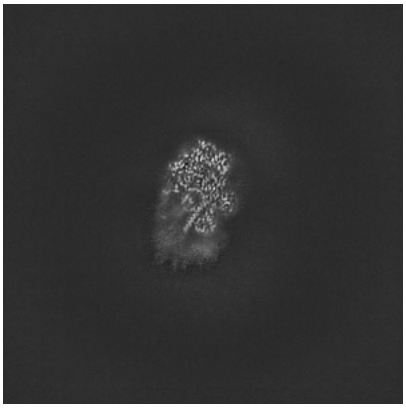
### 6.2.1 Primary map



X Index: 250



Y Index: 250

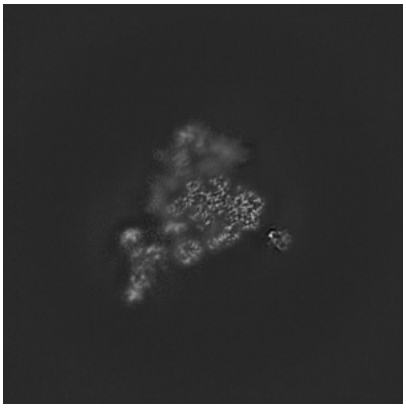


Z Index: 250

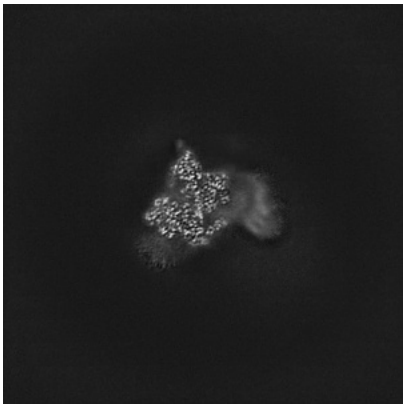
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

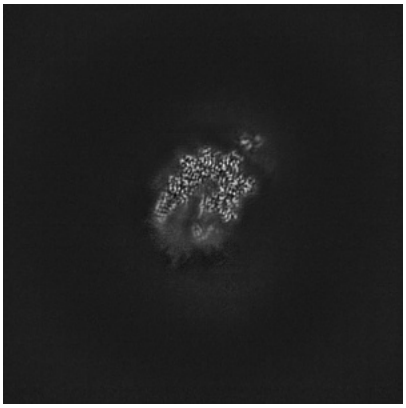
### 6.3.1 Primary map



X Index: 257



Y Index: 264

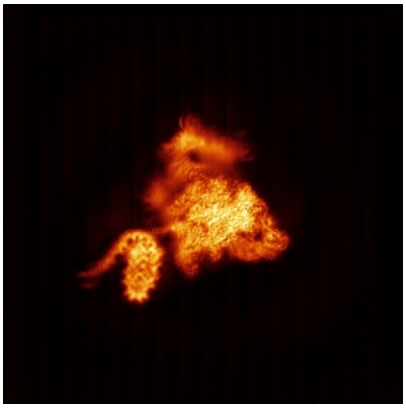


Z Index: 236

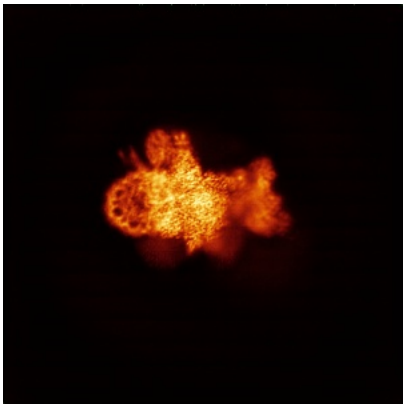
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) (i)

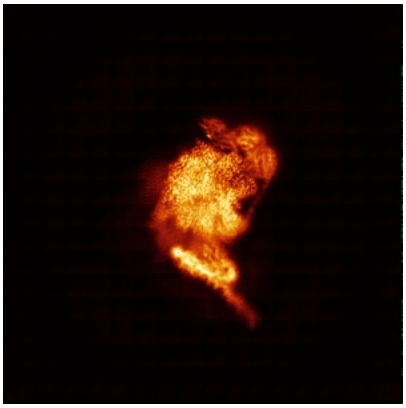
### 6.4.1 Primary map



X



Y

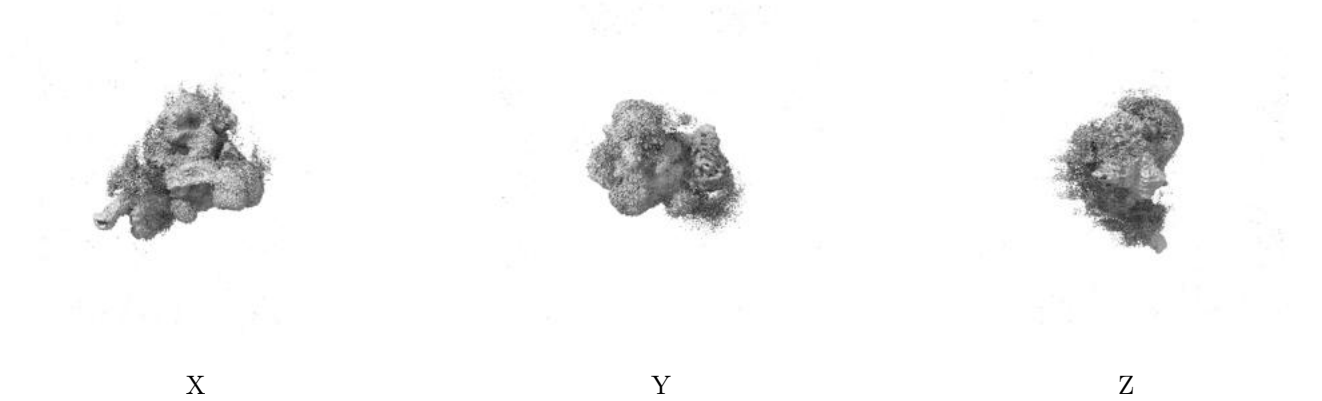


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

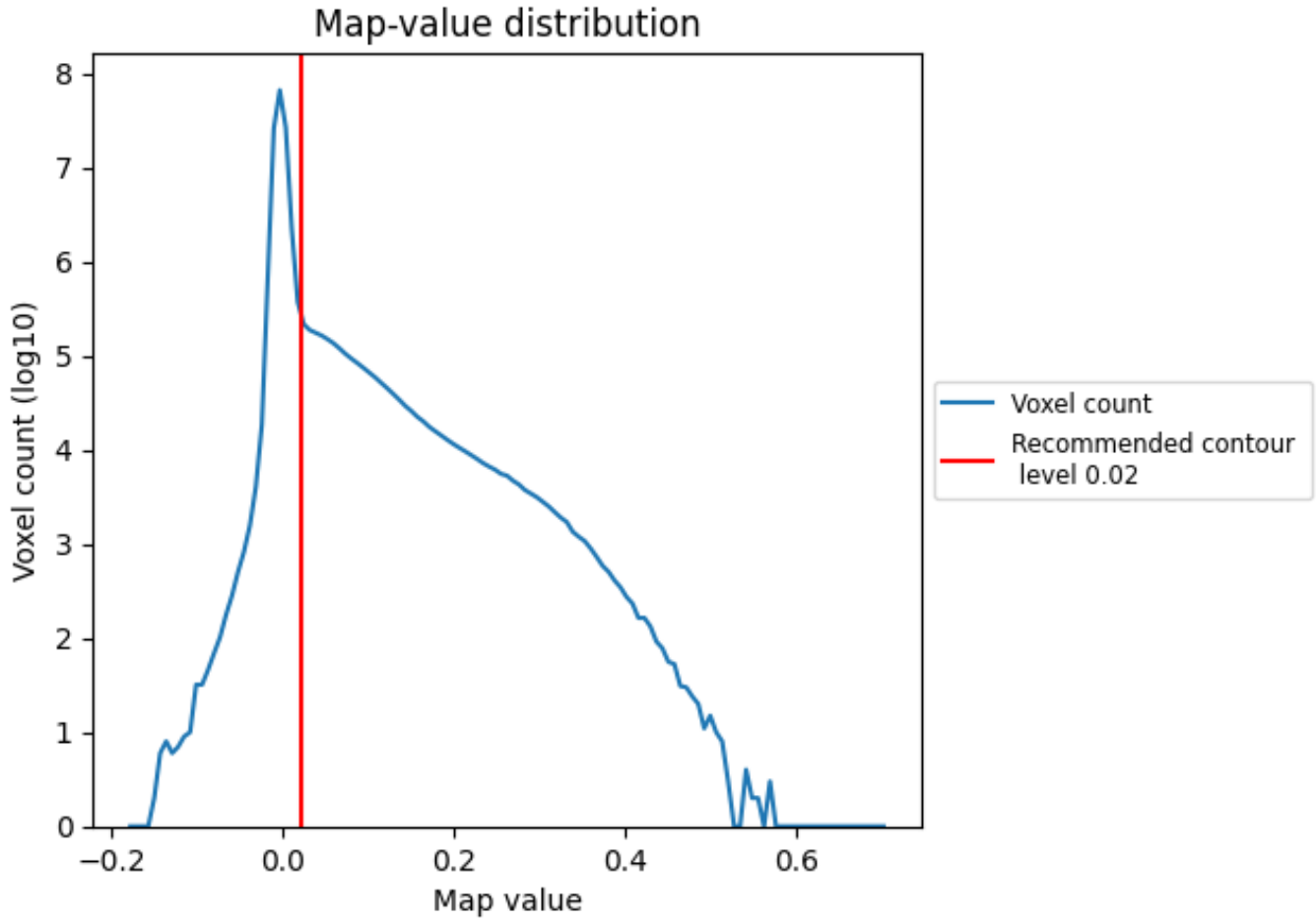
## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

# 7 Map analysis

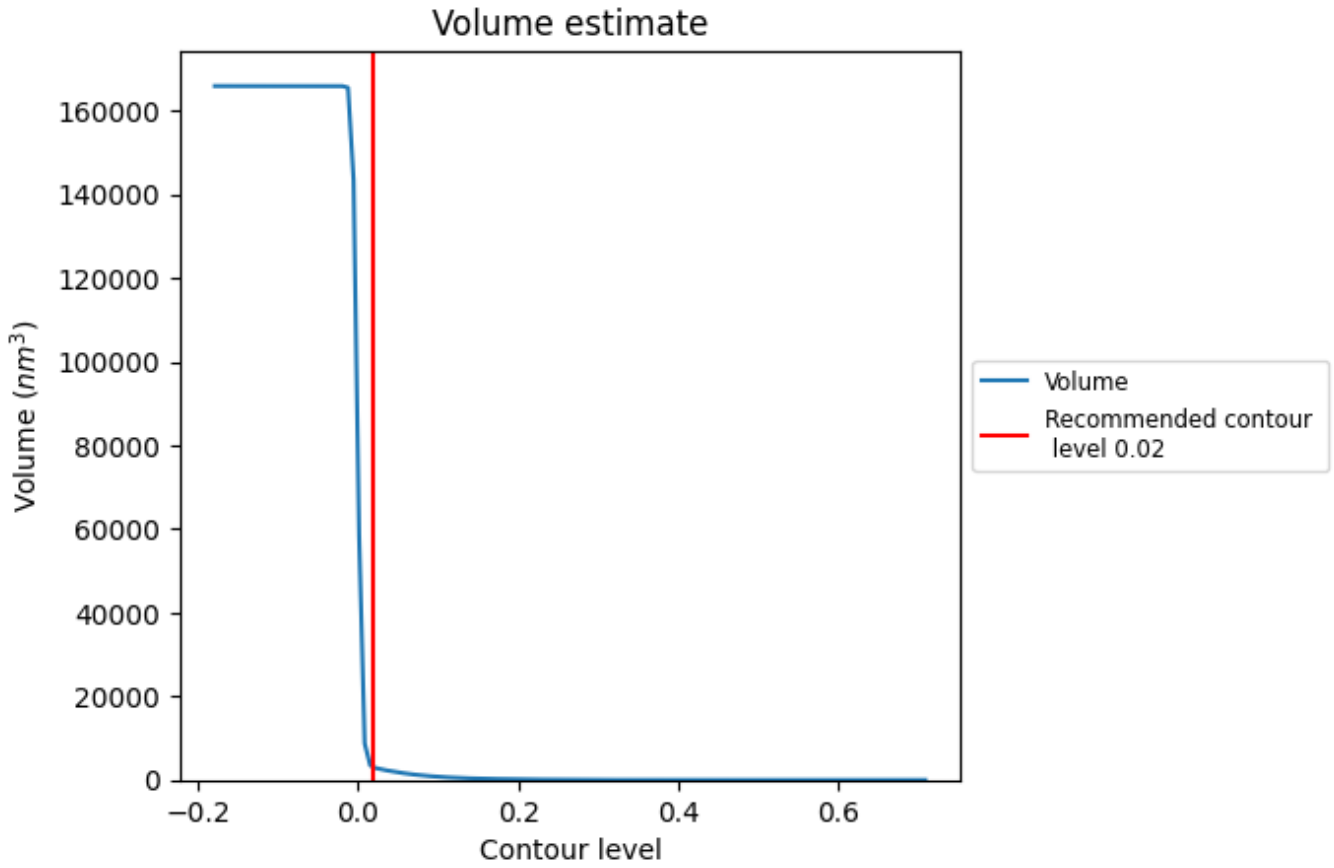
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

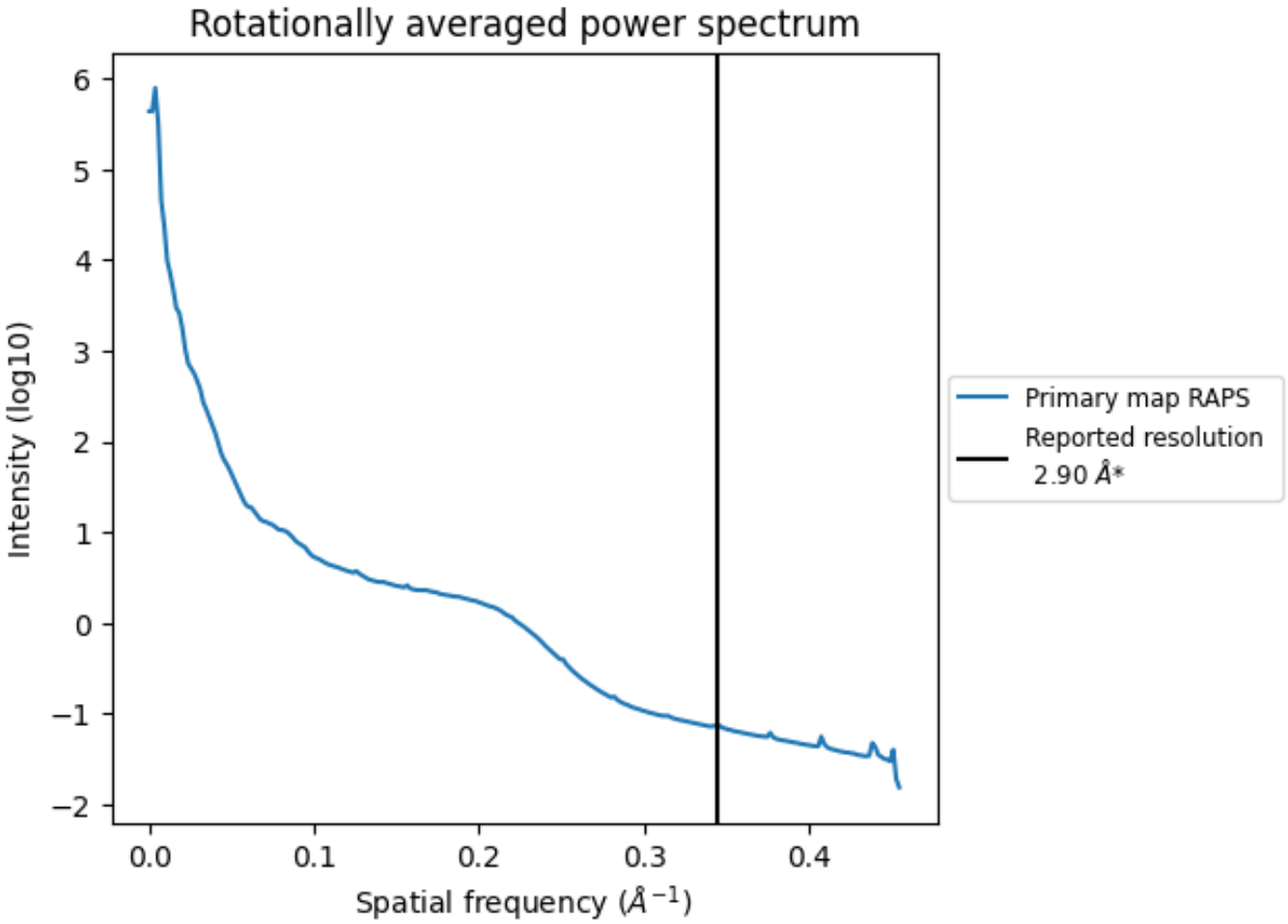
## 7.2 Volume estimate




The volume at the recommended contour level is 3060 $nm^3$; this corresponds to an approximate mass of 2764 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

## 7.3 Rotationally averaged power spectrum (i)




*Reported resolution corresponds to spatial frequency of 0.345 Å$^{-1}$

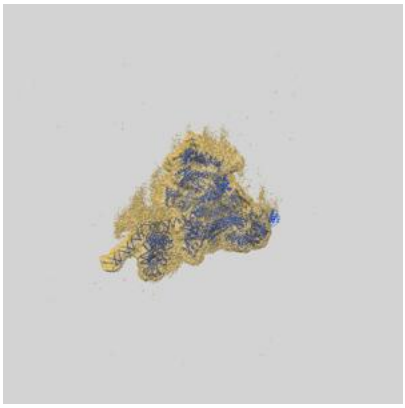
# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

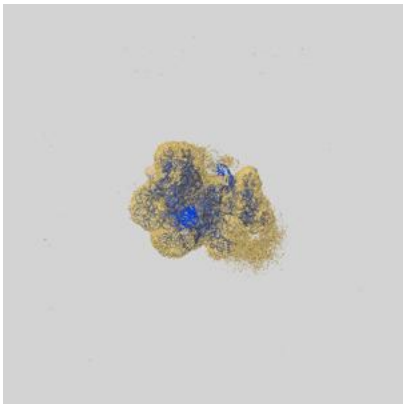
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-48039 and PDB model 9EGX. Per-residue inclusion information can be found in section 3 on page 11.

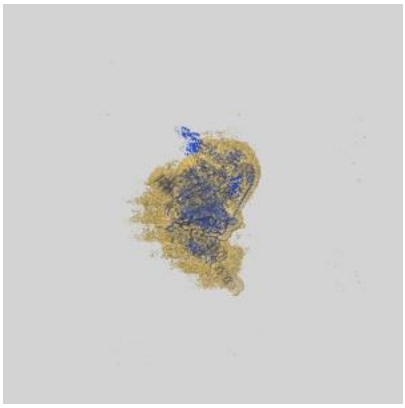
## 9.1 Map-model overlay



X



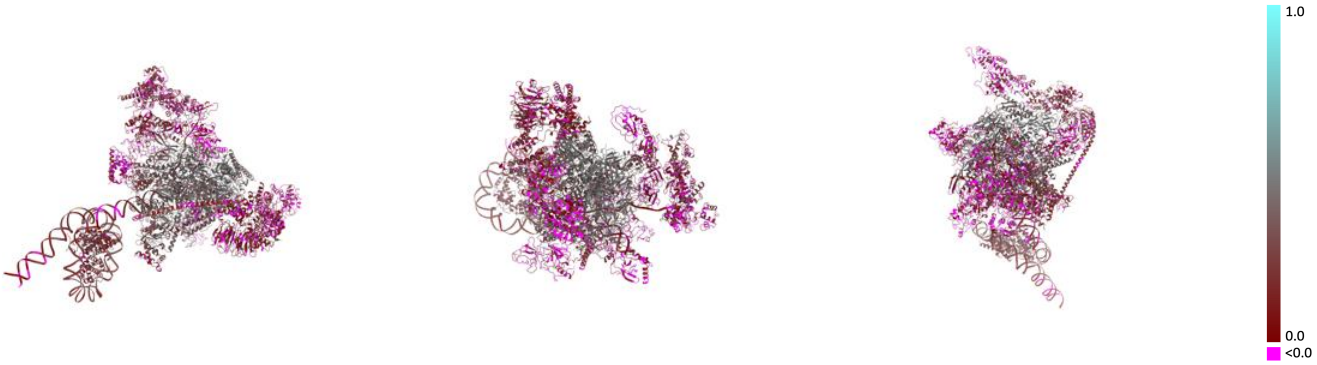
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

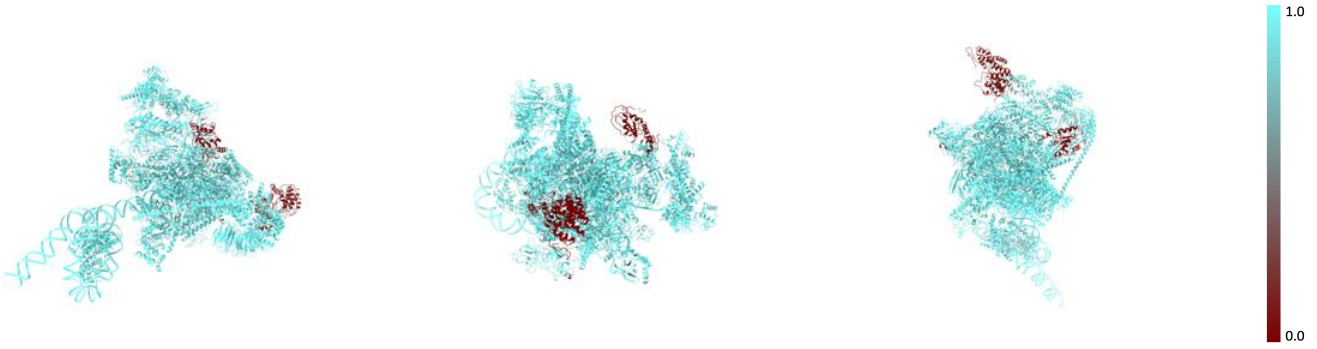
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

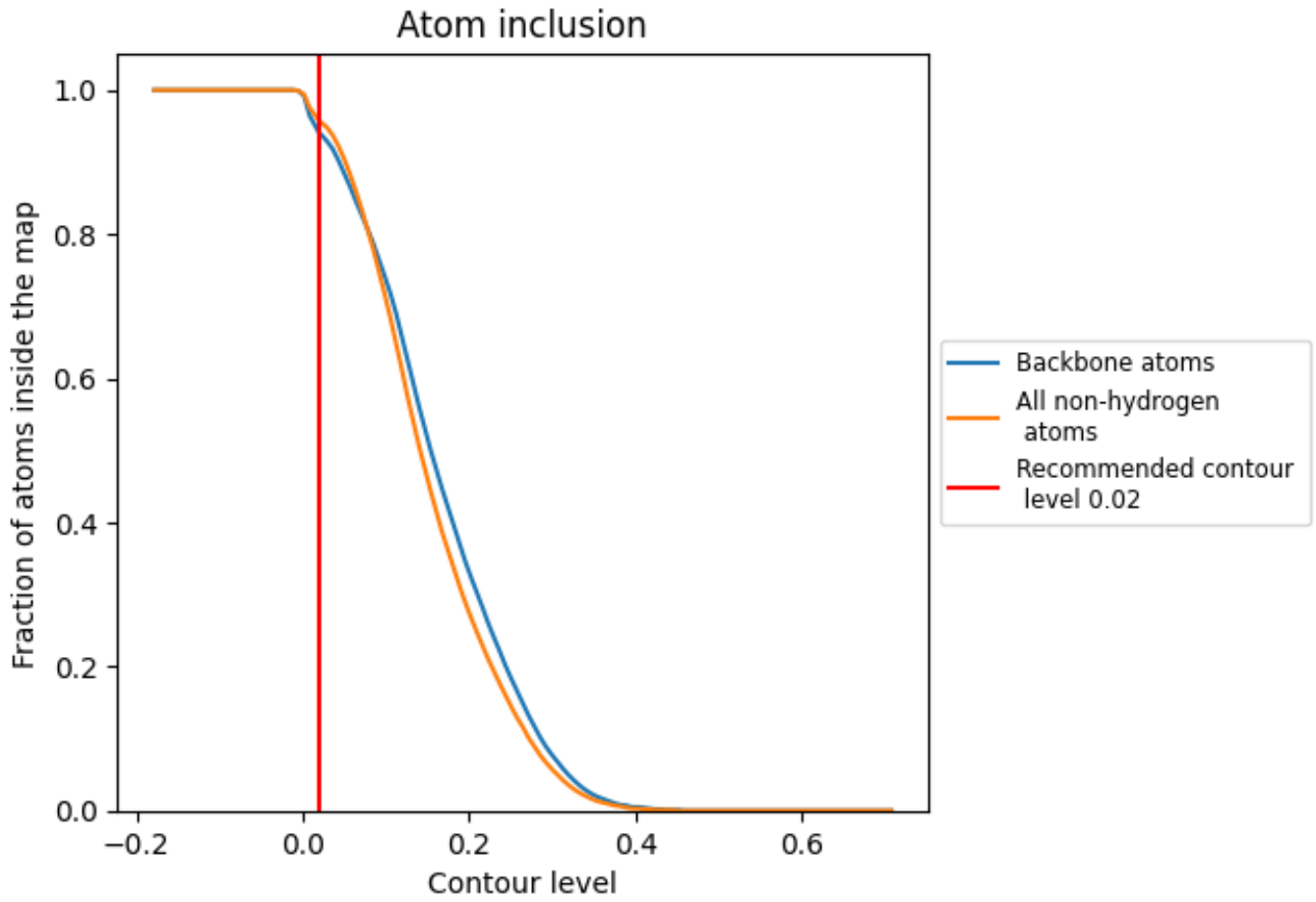
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

## 9.4 Atom inclusion (i)




At the recommended contour level, 94% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9570 | 0.2500 |
| A | 0.9920 | 0.3920 |
| B | 1.0000 | 0.4050 |
| C | 1.0000 | 0.4320 |
| D | 1.0000 | 0.1870 |
| E | 1.0000 | 0.3770 |
| F | 1.0000 | 0.4380 |
| G | 1.0000 | 0.2100 |
| H | 0.9970 | 0.4250 |
| I | 1.0000 | 0.3720 |
| J | 1.0000 | 0.4090 |
| K | 1.0000 | 0.4370 |
| L | 1.0000 | 0.3950 |
| M | 0.8420 | 0.0920 |
| N | 0.9940 | 0.1820 |
| O | 1.0000 | -0.0080 |
| P | 1.0000 | 0.1930 |
| Q | 0.7640 | 0.0960 |
| R | 0.9150 | 0.0610 |
| S | 1.0000 | 0.1990 |
| T | 0.9910 | 0.1850 |
| U | 0.9810 | 0.0890 |
| V | 0.7960 | 0.0690 |
| W | 1.0000 | 0.1390 |
| X | 1.0000 | 0.1580 |
| Y | 1.0000 | 0.0350 |
| Z | 0.9920 | 0.0850 |
| a | 1.0000 | 0.2060 |
| b | 1.0000 | 0.2210 |
| c | 1.0000 | 0.2240 |
| d | 0.9990 | 0.2280 |
| e | 1.0000 | 0.2110 |
| f | 1.0000 | 0.2160 |