

wwPDB EM Validation Summary Report (i)

Mar 19, 2024 – 07:27 PM JST

| PDB ID | : | 6J4X |
|--------------|---|--|
| EMDB ID | : | EMD-0672 |
| Title | : | RNA polymerase II elongation complex bound with Elf1 and Spt $4/5$, stalled |
| | | at SHL(-1) of the nucleosome $(+1A)$ |
| Authors | : | Ehara, H.; Kujirai, T.; Fujino, Y.; Shirouzu, M.; Kurumizaka, H.; Sekine, S. |
| Deposited on | : | 2019-01-10 |
| Resolution | : | 4.30 Å(reported) |
| | | |

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

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

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

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

| EMDB validation analysis | : | 0.0.1.dev70 |
|--------------------------------|---|--|
| MolProbity | : | 4.02b-467 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

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 4.30 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 | $egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$ | ${f EM} {f structures} \ (\#{f Entries})$ |
|-----------------------|--|---|
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |
| RNA backbone | 4643 | 859 |

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 | А | 1743 | 8% 80% • | 19% |
| 2 | В | 1227 | 92% | • 6% |
| 3 | С | 304 | 8 5% | • 13% |
| 4 | D | 186 | 87% | •• 10% |
| 5 | Е | 214 | 98% | • |
| 6 | F | 155 | 5 4% 46% | |
| 7 | G | 171 | 55% 99% | · |
| 8 | Н | 145 | 90% | • 8% |

Continued on next page...



| Mol | Chain | Length | Quality of cha | in |
|-----|-------|--------|-----------------|--------|
| | | | 50% | |
| 9 | Ι | 115 | 94% | • • |
| 10 | J | 72 | ⊷ 90% | • 8% |
| | | | 9% | |
| 11 | K | 118 | 96% | • |
| 12 | L | 72 | 60% | • 38% |
| 13 | Р | 16 | 19% | 50% 6% |
| 14 | Т | 198 | 6 2% | • 36% |
| 15 | N | 198 | 8% 57% 5% | 38% |
| 16 | М | 113 | 52% | 43% |
| 17 | V | 108 | 79% | • 6% |
| | | | 27% | |
| 18 | W | 911 | 29% • | 70% |
| 19 | a | 139 | 68% | • 30% |
| 19 | е | 139 | 68% | • 30% |
| 20 | b | 106 | 74% | • 25% |
| | c | 100 | 30% | |
| 20 | İ | 106 | 73% | • 26% |
| 21 | с | 133 | 77% | 23% |
| 21 | g | 133 | 70% | • 21% |
| 22 | d | 129 | 21% | • 26% |
| 22 | h | 129 | 50% | • 29% |

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2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 46185 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 |
|-----|-------|----------|----------------|-----------|-----------|-----------|---------|---------|-------|
| 1 | А | 1411 | Total 11116 | C 7009 | N 1937 | O 2100 | S 70 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|-----------|-----------|---------|---------|-------|
| 2 | В | 1157 | Total 9228 | C 5816 | N 1630 | 0 1724 | S 58 | 0 | 0 |

• Molecule 3 is a protein called RNA polymerase II third largest subunit B44, part of central core.

| Mol | Chain | Residues | | At | | AltConf | Trace | | |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---|---|
| 3 | С | 263 | Total 2098 | C 1319 | N 354 | 0 413 | S 12 | 0 | 0 |

• Molecule 4 is a protein called RNA polymerase II subunit B32.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---|---------|-------|
| 4 | D | 168 | Total 1314 | C 812 | N 237 | O 263 | $\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$ | 0 | 0 |

• Molecule 5 is a protein called RNA polymerase subunit ABC27, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 5 | Е | 213 | Total 1740 | C 1094 | N 312 | 0 324 | S 10 | 0 | 0 |

• Molecule 6 is a protein called RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III.



| Mol | Chain | Residues | | At | oms | | AltConf | Trace | |
|-----|-------|----------|--------------|----------|----------|----------|-----------------|-------|---|
| 6 | F | 84 | Total 677 | C 429 | N 114 | 0 131 | ${ m S} { m 3}$ | 0 | 0 |

• Molecule 7 is a protein called RNA polymerase II subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|----------------|---------|-------|
| 7 | G | 171 | Total 1324 | C 858 | N 214 | O 247 | ${ m S}{ m 5}$ | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|----------|----------|----------|---------------|---------|-------|
| 8 | Н | 133 | Total 1052 | С 671 | N 169 | O 208 | ${S \atop 4}$ | 0 | 0 |

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

| Mol | Chain | Residues | | \mathbf{A}^{\dagger} | AltConf | Trace | | | |
|-----|-------|----------|--------------|------------------------|----------|----------|---------|---|---|
| 9 | Ι | 111 | Total 917 | C 565 | N 161 | 0 180 | S 11 | 0 | 0 |

• Molecule 10 is a protein called RNA polymerase subunit ABC10-beta, common to RNA polymerases I, II, and III.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|----------|---------|---------|--------|---------|-------|
| 10 | J | 66 | Total | C 240 | N 05 | 0 05 | S 6 | 0 | 0 |
| | | | 545 | 349 | 95 | 95 | 0 | | |

• Molecule 11 is a protein called RNA polymerase II subunit B12.5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|--------|---------|-------|
| 11 | K | 113 | Total 932 | C 599 | N 160 | O 169 | S 4 | 0 | 0 |

• Molecule 12 is a protein called RNA polymerase subunit ABC10-alpha.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|----------------|---------|-------|
| 12 | L | 45 | Total 359 | C 221 | N 72 | O 61 | ${ m S}{ m 5}$ | 0 | 0 |

• Molecule 13 is a RNA chain called RNA (5'-R(P*CP*CP*UP*GP*GP*UP*GP*UP*CP*U P*UP*GP*GP*UP*G)-3').



| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|----------|---------|---------|-------|
| 13 | Р | 16 | Total 341 | C 151 | N 56 | O 118 | Р 16 | 0 | 0 |

• Molecule 14 is a DNA chain called DNA (198-MER).

| Mol | Chain | Residues | | At | AltConf | Trace | | | |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---|---|
| 14 | Т | 127 | Total 2589 | C 1227 | N 486 | O 750 | Р 126 | 0 | 0 |

• Molecule 15 is a DNA chain called DNA (198-MER).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|----------|---------|-------|
| 15 | Ν | 122 | Total 2509 | C 1188 | N 459 | O 740 | Р 122 | 0 | 0 |

• Molecule 16 is a protein called Transcription elongation factor 1 homolog.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|---------|---------|--------|---------|-------|
| 16 | М | 64 | Total 505 | C 318 | N 82 | O 99 | S 6 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| М | -2 | GLY | - | expression tag | UNP C4QZ45 |
| М | -1 | PRO | - | expression tag | UNP C4QZ45 |
| М | 0 | GLY | - | expression tag | UNP C4QZ45 |

• Molecule 17 is a protein called Transcription elongation factor SPT4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|--------------|----------|----------|----------|------------|---------|-------|
| 17 | V | 102 | Total 792 | C 492 | N 143 | O 150 | ${ m S} 7$ | 0 | 0 |

There is a discrepancy between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| V | 7 | MET | - | initiating methionine | UNP C4R0E6 |

• Molecule 18 is a protein called Protein that forms a complex with Spt4p.



| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|-------|
| 18 | W | 275 | Total 2226 | C 1425 | N 397 | O 403 | S 1 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| W | -2 | GLY | - | expression tag | UNP C4R370 |
| W | -1 | PRO | - | expression tag | UNP C4R370 |
| W | 0 | GLY | - | expression tag | UNP C4R370 |

• Molecule 19 is a protein called Histone H3.3.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|------|-------|----------|-------|-----|-----|---|---------|-------|---|
| 10 | 10 | 07 | Total | С | Ν | 0 | S | 0 | 0 |
| 19 a | 91 | 797 | 503 | 155 | 137 | 2 | 0 | U | |
| 10 | 10 | 07 | Total | С | Ν | 0 | S | 0 | 0 |
| 19 e | 97 | 796 | 501 | 155 | 138 | 2 | 0 | 0 | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| a | -3 | GLY | - | expression tag | UNP P84243 |
| a | -2 | SER | - | expression tag | UNP P84243 |
| a | -1 | HIS | - | expression tag | UNP P84243 |
| e | -3 | GLY | - | expression tag | UNP P84243 |
| e | -2 | SER | - | expression tag | UNP P84243 |
| е | -1 | HIS | - | expression tag | UNP P84243 |

• Molecule 20 is a protein called Histone H4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|---|
| 20 | b | 80 | Total 638 | C 401 | N 125 | 0 111 | S 1 | 0 | 0 |
| 20 | f | 78 | Total 619 | C 391 | N 120 | O 107 | S 1 | 0 | 0 |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| b | -3 | GLY | - | expression tag | UNP P62805 |
| b | -2 | SER | - | expression tag | UNP P62805 |
| b | -1 | HIS | - | expression tag | UNP P62805 |

Continued on next page...



| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| f | -3 | GLY | - | expression tag | UNP P62805 |
| f | -2 | SER | - | expression tag | UNP P62805 |
| f | -1 | HIS | - | expression tag | UNP P62805 |

Continued from previous page...

• Molecule 21 is a protein called Histone H2A type 1-B/E.

| Mol | Chain | Residues | Atoms | | | AltConf | Trace | | |
|------|-------|----------|-------|-----|-----|---------|-------|---|--|
| 91 | 0 | 103 | Total | С | Ν | Ο | 0 | 0 | |
| | C | 105 | 796 | 502 | 155 | 139 | 0 | 0 | |
| 91 | C. | 105 | Total | С | Ν | Ο | 0 | 0 | |
| 21 g | g | 105 | 810 | 511 | 158 | 141 | | 0 | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| с | -3 | GLY | - | expression tag | UNP P04908 |
| с | -2 | SER | - | expression tag | UNP P04908 |
| с | -1 | HIS | - | expression tag | UNP P04908 |
| g | -3 | GLY | - | expression tag | UNP P04908 |
| g | -2 | SER | - | expression tag | UNP P04908 |
| g | -1 | HIS | - | expression tag | UNP P04908 |

• Molecule 22 is a protein called Histone H2B type 1-J.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace | |
|-----|-------|----------|-------|-----|-----|---|---------|-------|---|
| 22 | d | 05 | Total | С | Ν | Ο | S | 0 | 0 |
| | 90 | 746 | 468 | 136 | 140 | 2 | 0 | 0 | |
| | h | 01 | Total | С | Ν | 0 | S | 0 | 0 |
| | 91 | 708 | 447 | 125 | 134 | 2 | 0 | 0 | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| d | -6 | GLY | - | expression tag | UNP P06899 |
| d | -5 | SER | - | expression tag | UNP P06899 |
| d | -4 | HIS | - | expression tag | UNP P06899 |
| h | -6 | GLY | - | expression tag | UNP P06899 |
| h | -5 | SER | - | expression tag | UNP P06899 |
| h | -4 | HIS | - | expression tag | UNP P06899 |

• Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 23 | А | 2 | Total Zn 2 2 | 0 |
| 23 | В | 1 | Total Zn 1 1 | 0 |
| 23 | С | 1 | Total Zn 1 1 | 0 |
| 23 | Ι | 2 | Total Zn 2 2 | 0 |
| 23 | J | 1 | Total Zn 1 1 | 0 |
| 23 | L | 1 | Total Zn 1 1 | 0 |
| 23 | М | 1 | Total Zn 1 1 | 0 |
| 23 | V | 1 | Total Zn 1 1 | 0 |

• Molecule 24 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 24 | А | 1 | Total Mg 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



• Molecule 2: DNA-directed RNA polymerase subunit beta





• Molecule 6: RNA polymerase subunit ABC23, common to RNA polymerases I, II, and III



| Chain F: | 54% | 46% | |
|--|--|---|--|
| MET SER CLU CLU CLU CLU ASN CLU CLU CLU ASN PHE CLU ASN PHE CLU CLU CLU | ASP GLU HIS PHE SER SER ASP ASP CLU CLU CLU ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU | CLU CLU TYR TYR ALA CLY CLY CLY ALA ALA ASP CLY CLY CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN | GLU VAL ASN GLSN CLSN THR THR |
| ILE LYS ALA ALA ARG ARG ARG SER ARG SER LYS SER LYS CY1 LYS LYS SER ARG SER ARG SER ARG SER ARG SER ARG ARG ARG ARG ARG ARG ARG ARA ARA AR | | | |
| • Molecule 7: RNA poly | merase II subunit | | |
| Chain G: | 55% 99% | | • |
| M1 K5 K5 C34 C36 C36 C36 C40 C41 C41 C42 C43 C43 C43 C43 C43 C43 C43 C43 C43 C43 | M52 N53 K83 K83 K83 K83 C84 C84 V87 V87 A89 D88 A89 V91 | 892 N94 N94 S95 P96 F100 F100 A101 D102 C104 C103 F105 C106 N107 N107 | <pre>F109 F109 F109 F112 F112 F114 F115 F115 F116 F116 F116 V120 V120 V120 V121 V122 F123 F123</pre> |
| S124 N125 S126 P127 P128 A129 Y130 Y133 S132 N133 L135 L135 | T138 K139 G140 G140 S141 K142 K144 K146 K146 K146 K146 K148 C149 | T150 R151 T152 D153 V164 C155 E156 T157 T157 T157 C161 C161 C161 C161 C161 C161 C161 C16 | |
| • Molecule 8: DNA-direc | cted RNA polymerases | s I, II, and III subunit RPA | BC3 |
| Chain H: | 90% | • 8% | |
| MET SER SER SER ASP GLV GLV GLV GLV GLV ASN ASN ASN ASN ASN SER SER SER SER SER | E108 | | |
| • Molecule 9: DNA-direc | cted RNA polymerase | subunit | |
| Chain I: | 0% 94% | | |
| MET ALLA S 3 S 3 F 4 F 4 B 15 F 4 F 4 F 4 F 4 F 4 F 4 F 4 F 4 F 4 F 4 | B33 L37 L37 A38 B40 B40 L48 148 NS1 S51 S52 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C47 C48 C48 C48 C48 C48 C48 C48 C48 | 653 E54 E54 E54 E54 G67 G67 E50 D60 D61 E52 C63 C63 C63 C63 C64 C64 C63 C63 C63 C63 C63 C63 C63 C63 C63 C63 | K73 E74 775 775 775 775 877 881 881 881 882 7884 7885 7885 |
| Q89 Q80 Q91 R91 R91 R92 R93 D94 L103 L105 K107 K108 K108 K109 T109 | E113 SER GLU | | |
| • Molecule 10: RNA po III | lymerase subunit AB | C10-beta, common to RNA | polymerases I, II, and |
| Chain J: | 90% | • 8% | |
| M1 P64 E66 E66 E86 LYS LYS ASP PHE ASP PHE SER | | | |
| • Molecule 11: RNA pol | ymerase II subunit B1 | 2.5 | |
| Chain K: | 96% | | - |
| | W O PROTI | R L D W I D E PDB IN DATA BANK | |













| • •••• | ** *** ******** | ******* | • ••••• |
|---|---|--|--|
| N60 561 F62 V63 N64 D65 F67 F67 F67 E68 R69 R69 A71 | 575 177 177 177 177 177 178 188 188 186 186 186 186 186 186 187 187 187 187 187 187 187 187 187 187 | R96 L97 L98 L98 P100 G101 E102 L103 | A107 V108 S109 E110 G111 T112 A114 V115 T116 K117 Y118 T119 S120 A121 S120 |



4 Experimental information (i)

| Property | Value | Source |
|------------------------------------|---------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 35691 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | NONE | Depositor |
| Microscope | FEI TECNAI ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose $(e^-/\text{\AA}^2)$ | 50.0 | Depositor |
| Minimum defocus (nm) | Not provided | |
| Maximum defocus (nm) | Not provided | |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k x 4k) | Depositor |
| Maximum map value | 0.061 | Depositor |
| Minimum map value | -0.020 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.003 | Depositor |
| Recommended contour level | 0.016 | Depositor |
| Map size (Å) | 357.6, 357.6, 357.6 | wwPDB |
| Map dimensions | 240, 240, 240 | wwPDB |
| Map angles $(^{\circ})$ | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.49, 1.49, 1.49 | Depositor |



5 Model quality (i)

5.1 Standard geometry (i)

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

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).

| Mal | Chain | Bond lengths | | Bond angles | | |
|-----|---------|--------------|-------------------------------|-------------|-------------------------------|--|
| MOI | Ullalli | RMSZ | # Z > 5 | RMSZ | # Z > 5 | |
| 1 | А | 0.44 | 0/11322 | 0.67 | 6/15300~(0.0%) | |
| 2 | В | 0.48 | 0/9407 | 0.71 | 6/12685~(0.0%) | |
| 3 | С | 0.46 | 0/2139 | 0.72 | 1/2895~(0.0%) | |
| 4 | D | 0.32 | 0/1326 | 0.68 | 1/1788~(0.1%) | |
| 5 | Е | 0.42 | 0/1772 | 0.64 | 0/2385 | |
| 6 | F | 0.45 | 0/687 | 0.64 | 0/931 | |
| 7 | G | 0.36 | 0/1353 | 0.71 | 0/1837 | |
| 8 | Н | 0.42 | 0/1069 | 0.67 | 0/1444 | |
| 9 | Ι | 0.35 | 0/934 | 0.80 | 2/1257~(0.2%) | |
| 10 | J | 0.57 | 0/554 | 0.75 | 0/742 | |
| 11 | Κ | 0.44 | 0/953 | 0.65 | 0/1291 | |
| 12 | L | 0.46 | 0/365 | 0.76 | 0/484 | |
| 13 | Р | 1.11 | 3/379~(0.8%) | 1.29 | 4/589~(0.7%) | |
| 14 | Т | 1.07 | 2/2905~(0.1%) | 1.08 | 3/4477~(0.1%) | |
| 15 | Ν | 1.13 | 10/2812~(0.4%) | 1.09 | 0/4339 | |
| 16 | М | 0.26 | 0/513 | 0.45 | 0/693 | |
| 17 | V | 0.46 | 0/808 | 0.60 | 0/1097 | |
| 18 | W | 0.40 | 0/2267 | 0.68 | 4/3048~(0.1%) | |
| 19 | a | 0.42 | 0/809 | 0.62 | 0/1085 | |
| 19 | е | 0.45 | 0/807 | 0.55 | 0/1081 | |
| 20 | b | 0.44 | 0/645 | 0.64 | 0/862 | |
| 20 | f | 0.43 | 0/626 | 0.61 | 0/837 | |
| 21 | с | 0.40 | 0/806 | 0.58 | 0/1089 | |
| 21 | g | 0.36 | 0/820 | 0.55 | 0/1107 | |
| 22 | d | 0.46 | 0/757 | 0.56 | 0/1015 | |
| 22 | h | 0.41 | 0/719 | 0.56 | 0/968 | |
| All | All | 0.57 | $15/\overline{47554}~(0.0\%)$ | 0.75 | $27/\overline{65326}~(0.0\%)$ | |

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



| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | В | 0 | 1 |
| 19 | a | 0 | 2 |
| 19 | е | 0 | 1 |
| All | All | 0 | 4 |

sidechain that are expected to be planar.

The worst 5 of 15 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 13 | Р | -2 | G | C1'-N9 | -7.33 | 1.36 | 1.46 |
| 13 | Р | -1 | G | C1'-N9 | -7.31 | 1.36 | 1.46 |
| 15 | Ν | -37 | DG | C1'-N9 | -6.94 | 1.37 | 1.47 |
| 13 | Р | 4 | U | C1'-N1 | 6.65 | 1.58 | 1.48 |
| 15 | Ν | -19 | DG | C1'-N9 | -6.59 | 1.38 | 1.47 |

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

| Mol | Chain | Res | Type | Atoms | | $Observed(^{o})$ | $Ideal(^{o})$ |
|-----|-------|-----|------|-------------|-------|------------------|---------------|
| 18 | W | 389 | PRO | CA-N-CD | -8.57 | 99.51 | 111.50 |
| 1 | А | 473 | LEU | CA-CB-CG | -8.22 | 96.40 | 115.30 |
| 2 | В | 63 | GLN | N-CA-CB | -7.67 | 96.80 | 110.60 |
| 2 | В | 63 | GLN | N-CA-C | -6.91 | 92.33 | 111.00 |
| 14 | Т | -26 | DT | O4'-C4'-C3' | -6.71 | 101.81 | 104.50 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | \mathbf{Res} | Type | Group |
|-----|-------|----------------|------|-----------|
| 2 | В | 336 | ILE | Mainchain |
| 19 | а | 42 | ARG | Peptide |
| 19 | a | 63 | ARG | Peptide |
| 19 | е | 63 | ARG | Peptide |

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.



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 | А | 1399/1743~(80%) | 1342 (96%) | 47 (3%) | 10 (1%) | 22 62 |
| 2 | В | 1145/1227~(93%) | 1082~(94%) | 55~(5%) | 8 (1%) | 22 62 |
| 3 | С | 261/304~(86%) | 253~(97%) | 6(2%) | 2(1%) | 19 60 |
| 4 | D | 162/186~(87%) | 149~(92%) | 9~(6%) | 4(2%) | 5 35 |
| 5 | Ε | 211/214~(99%) | 207~(98%) | 4(2%) | 0 | 100 100 |
| 6 | F | 82/155~(53%) | 80~(98%) | 2(2%) | 0 | 100 100 |
| 7 | G | 169/171~(99%) | 159 (94%) | 8 (5%) | 2(1%) | 13 50 |
| 8 | Н | 129/145~(89%) | 125~(97%) | 2(2%) | 2(2%) | 9 45 |
| 9 | Ι | 109/115~(95%) | 102 (94%) | 6~(6%) | 1 (1%) | 17 56 |
| 10 | J | 64/72~(89%) | 61 (95%) | 2(3%) | 1 (2%) | 9 45 |
| 11 | Κ | 111/118 (94%) | 110 (99%) | 1 (1%) | 0 | 100 100 |
| 12 | L | 43/72~(60%) | 42 (98%) | 0 | 1 (2%) | 6 37 |
| 16 | М | 62/113~(55%) | 58 (94%) | 4~(6%) | 0 | 100 100 |
| 17 | V | 100/108~(93%) | 97~(97%) | 3~(3%) | 0 | 100 100 |
| 18 | W | 265/911~(29%) | 246~(93%) | 17~(6%) | 2(1%) | 19 60 |
| 19 | a | 95/139~(68%) | 85~(90%) | 10 (10%) | 0 | 100 100 |
| 19 | е | 95/139~(68%) | 89 (94%) | 6~(6%) | 0 | 100 100 |
| 20 | b | 78/106~(74%) | 74 (95%) | 4 (5%) | 0 | 100 100 |
| 20 | f | 76/106~(72%) | 69 (91%) | 7 (9%) | 0 | 100 100 |
| 21 | с | 101/133~(76%) | 92 (91%) | 9~(9%) | 0 | 100 100 |
| 21 | g | 103/133~(77%) | 94 (91%) | 9 (9%) | 0 | 100 100 |
| 22 | d | 93/129~(72%) | 91 (98%) | 2(2%) | 0 | 100 100 |
| 22 | h | 89/129~(69%) | 87~(98%) | 2(2%) | 0 | 100 100 |
| All | All | $50\overline{42/6668}\ (76\%)$ | 4794 (95%) | 215 (4%) | 33 (1%) | 26 62 |



5 of 33 Ramachandran outliers are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 1 | А | 255 | GLU |
| 1 | А | 287 | GLN |
| 1 | А | 960 | VAL |
| 1 | А | 1109 | VAL |
| 2 | В | 155 | LYS |

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 | Perce | ntiles |
|-----|-------|-----------------|------------|----------|-------|--------|
| 1 | А | 1224/1528~(80%) | 1217~(99%) | 7(1%) | 86 | 92 |
| 2 | В | 1012/1077~(94%) | 1001 (99%) | 11 (1%) | 73 | 85 |
| 3 | С | 236/264~(89%) | 235 (100%) | 1 (0%) | 91 | 94 |
| 4 | D | 143/160~(89%) | 140 (98%) | 3(2%) | 53 | 72 |
| 5 | Ε | 196/197~(100%) | 193~(98%) | 3~(2%) | 65 | 80 |
| 6 | F | 75/137~(55%) | 75 (100%) | 0 | 100 | 100 |
| 7 | G | 148/148 (100%) | 148 (100%) | 0 | 100 | 100 |
| 8 | Н | 120/130~(92%) | 120 (100%) | 0 | 100 | 100 |
| 9 | Ι | 106/109~(97%) | 105 (99%) | 1 (1%) | 78 | 88 |
| 10 | J | 60/66~(91%) | 60 (100%) | 0 | 100 | 100 |
| 11 | Κ | 104/109~(95%) | 104 (100%) | 0 | 100 | 100 |
| 12 | L | 38/56~(68%) | 37~(97%) | 1 (3%) | 46 | 67 |
| 16 | М | 61/99~(62%) | 61 (100%) | 0 | 100 | 100 |
| 17 | V | 86/92~(94%) | 85 (99%) | 1 (1%) | 71 | 84 |
| 18 | W | 241/796~(30%) | 239~(99%) | 2(1%) | 81 | 89 |
| 19 | a | 83/112~(74%) | 82~(99%) | 1 (1%) | 71 | 84 |
| 19 | е | 82/112~(73%) | 81 (99%) | 1 (1%) | 71 | 84 |
| 20 | b | 65/81~(80%) | 63~(97%) | 2(3%) | 40 | 63 |
| 20 | f | 63/81~(78%) | 62 (98%) | 1 (2%) | 62 | 79 |

Continued on next page...



| Mol | Chain | Analysed | Rotameric | Outliers | Perce | ntiles |
|-----|-------|-----------------|------------|----------|-------|--------|
| 21 | с | 82/102~(80%) | 82 (100%) | 0 | 100 | 100 |
| 21 | g | 83/102 (81%) | 82~(99%) | 1 (1%) | 71 | 84 |
| 22 | d | 81/107~(76%) | 79~(98%) | 2(2%) | 47 | 68 |
| 22 | h | 77/107~(72%) | 75~(97%) | 2(3%) | 46 | 67 |
| All | All | 4466/5772 (77%) | 4426 (99%) | 40 (1%) | 79 | 88 |

Continued from previous page...

5 of 40 residues with a non-rotameric side chain are listed below:

| Mol | Chain | \mathbf{Res} | Type |
|-----|-------|----------------|------|
| 18 | W | 264 | GLN |
| 19 | е | 53 | ARG |
| 18 | W | 313 | VAL |
| 20 | b | 92 | ARG |
| 21 | g | 71 | ARG |

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|----------------------|------|
| 21 | g | 31 | HIS |
| 21 | g | 110 | ASN |
| 5 | Е | 4 | ASN |
| 3 | С | 242 | GLN |
| 21 | g | 112 | GLN |

5.3.3 RNA (i)

| Mol | Chain | Analysed | Backbone Outliers | Pucker Outliers |
|-----|-------|-------------|-------------------|-----------------|
| 13 | Р | 15/16~(93%) | 6 (40%) | 0 |

5 of 6 RNA backbone outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 13 | Р | -4 | С |
| 13 | Р | -3 | U |
| 13 | Р | -1 | G |
| 13 | Р | 0 | U |
| 13 | Р | 1 | G |



There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0672. 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 (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 120



Y Index: 120



Z Index: 120



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: 125

Y Index: 121

Z Index: 132

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



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



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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 (i)

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

7.1 Map-value distribution (i)



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 (i)



The volume at the recommended contour level is 428 nm^3 ; this corresponds to an approximate mass of 387 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 0.233 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}



8.2 Resolution estimates (i)

| $\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$ | Estimation criterion (FSC cut-off) | | |
|---|------------------------------------|------|----------|
| Resolution estimate (A) | 0.143 | 0.5 | Half-bit |
| Reported by author | 4.30 | - | - |
| Author-provided FSC curve | 4.23 | 7.32 | 4.40 |
| Unmasked-calculated* | - | - | _ |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0672 and PDB model 6J4X. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.016 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)



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)



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 (0.016).



9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.016) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|----------------|---------|
| All | 0.6170 | 0.2330 |
| А | 0.6980 | 0.3030 |
| В | 0.7270 | 0.3140 |
| С | 0.8100 | 0.3350 |
| D | 0.1460 | 0.0970 |
| Ε | 0.7700 | 0.2820 |
| F | 0.7740 | 0.3200 |
| G | 0.3540 | 0.1600 |
| Н | 0.8450 | 0.3240 |
| Ι | 0.4320 | 0.1430 |
| J | 0.8000 | 0.3250 |
| К | 0.7540 | 0.3270 |
| L | 0.7160 | 0.2720 |
| М | 0.0890 | 0.1220 |
| Ν | 0.7290 | 0.1300 |
| Р | 0.7770 | 0.2300 |
| Т | 0.7490 | 0.1470 |
| V | 0.1560 | 0.0210 |
| W | 0.1070 | 0.0840 |
| a | 0.5180 | 0.1150 |
| b | 0.5960 | 0.1050 |
| с | 0.5640 | 0.0990 |
| d | 0.5790 | 0.0960 |
| e | 0.5420 | 0.1580 |
| f | 0.4810 | 0.1320 |
| g | 0.1080 | 0.0620 |
| h | 0.2320 | 0.0980 |

