



wwPDB EM Validation Summary Report ⓘ

Dec 10, 2022 – 08:43 am GMT

PDB ID : 5A9Q
EMDB ID : EMD-3103
Title : Human nuclear pore complex
Authors : von Appen, A.; Kosinski, J.; Sparks, L.; Ori, A.; DiGuilio, A.; Vollmer, B.; Mackmull, M.; Banterle, N.; Parca, L.; Kastritis, P.; Buczak, K.; Mosalaganti, S.; Hagen, W.; Andres-Pons, A.; Lemke, E.A.; Bork, P.; Antonin, W.; Glavy, J.S.; Bui, K.H.; Beck, M.
Deposited on : 2015-07-22
Resolution : 23.00 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 ⓘ 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:

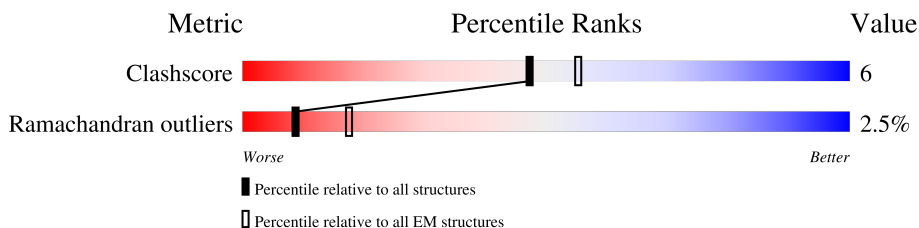
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 23.00 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 | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |

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 $\leq 5\%$. 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 | 0 | 380 | 8% 82% 17% |
| 1 | 9 | 380 | 8% 82% 17% |
| 1 | I | 380 | 8% 82% 17% |
| 1 | R | 380 | 8% 82% 17% |
| 2 | 1 | 1436 | 14% 65% 5% 30% |
| 2 | J | 1436 | 8% 65% 5% 30% |
| 2 | S | 1436 | 8% 65% 5% 30% |
| 2 | a | 1436 | 8% 68% 5% 30% |
| 3 | 2 | 326 | 15% 84% 11% 2% |





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | K | 326 | 84% 11% .. |
| 3 | T | 326 | 84% 11% .. |
| 3 | b | 326 | 7% 90% 6% .. |
| 4 | 3 | 1156 | 6% 40% 5% . 54% |
| 4 | C | 1156 | 8% 41% . . 54% |
| 4 | L | 1156 | 41% . . 54% |
| 4 | U | 1156 | 10% 41% . . 54% |
| 5 | 4 | 925 | 70% . 29% |
| 5 | D | 925 | 69% . 29% |
| 5 | M | 925 | 70% . 29% |
| 5 | V | 925 | 5% 69% . 29% |
| 6 | 5 | 937 | 42% . 55% |
| 6 | E | 937 | 42% . 55% |
| 6 | N | 937 | 42% . 55% |
| 6 | W | 937 | 42% . 55% |
| 7 | 6 | 322 | 76% 12% . 11% |
| 7 | F | 322 | 75% 12% . 11% |
| 7 | O | 322 | 76% 12% . 11% |
| 7 | X | 322 | 7% 76% 12% . 11% |
| 8 | 7 | 360 | 79% 8% . 11% |
| 8 | G | 360 | 79% 8% . 11% |
| 8 | P | 360 | 79% 8% . 11% |
| 8 | Y | 360 | 79% 8% . 11% |
| 9 | 8 | 656 | 63% . 34% |
| 9 | H | 656 | 63% . 34% |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 9 | Q | 656 |  63% 34% |
| 9 | Z | 656 |  63% 34% |
| 10 | A | 1391 |  16% 74% 21% |
| 10 | B | 1391 |  10% 72% 6% 21% |

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 95884 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 NUCLEOPORIN NUP43.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 1 | 0 | 316 | 1562 | 930 | 316 | 316 | 0 | 0 |
| 1 | 9 | 316 | 1562 | 930 | 316 | 316 | 0 | 0 |
| 1 | I | 316 | 1562 | 930 | 316 | 316 | 0 | 0 |
| 1 | R | 316 | 1562 | 930 | 316 | 316 | 0 | 0 |

- Molecule 2 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP160.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| | | | Total | C | N | O | | |
| 2 | 1 | 1009 | 4997 | 2979 | 1009 | 1009 | 0 | 0 |
| 2 | J | 1009 | 4997 | 2979 | 1009 | 1009 | 0 | 0 |
| 2 | S | 1009 | 4997 | 2979 | 1009 | 1009 | 0 | 0 |
| 2 | a | 1009 | 4997 | 2979 | 1009 | 1009 | 0 | 0 |

- Molecule 3 is a protein called NUCLEOPORIN NUP37.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 3 | 2 | 318 | 1566 | 930 | 318 | 318 | 0 | 0 |
| 3 | K | 318 | 1566 | 930 | 318 | 318 | 0 | 0 |
| 3 | T | 318 | 1566 | 930 | 318 | 318 | 0 | 0 |
| 3 | b | 318 | 1566 | 930 | 318 | 318 | 0 | 0 |

- Molecule 4 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP133.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 4 | 3 | 528 | Total | C | N | O | 0 | 0 |
| | | | 2629 | 1573 | 528 | 528 | | |
| 4 | C | 528 | Total | C | N | O | 0 | 0 |
| | | | 2629 | 1573 | 528 | 528 | | |
| 4 | L | 528 | Total | C | N | O | 0 | 0 |
| | | | 2629 | 1573 | 528 | 528 | | |
| 4 | U | 528 | Total | C | N | O | 0 | 0 |
| | | | 2629 | 1573 | 528 | 528 | | |

- Molecule 5 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP107.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 5 | 4 | 660 | Total | C | N | O | 0 | 0 |
| | | | 3278 | 1958 | 660 | 660 | | |
| 5 | D | 660 | Total | C | N | O | 0 | 0 |
| | | | 3278 | 1958 | 660 | 660 | | |
| 5 | M | 660 | Total | C | N | O | 0 | 0 |
| | | | 3278 | 1958 | 660 | 660 | | |
| 5 | V | 660 | Total | C | N | O | 0 | 0 |
| | | | 3278 | 1958 | 660 | 660 | | |

- Molecule 6 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP96.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| 6 | 5 | 417 | Total | C | N | O | 0 | 0 |
| | | | 2073 | 1239 | 417 | 417 | | |
| 6 | E | 417 | Total | C | N | O | 0 | 0 |
| | | | 2073 | 1239 | 417 | 417 | | |
| 6 | N | 417 | Total | C | N | O | 0 | 0 |
| | | | 2073 | 1239 | 417 | 417 | | |
| 6 | W | 417 | Total | C | N | O | 0 | 0 |
| | | | 2073 | 1239 | 417 | 417 | | |

- Molecule 7 is a protein called PROTEIN SEC13 HOMOLOG.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| 7 | 6 | 285 | Total | C | N | O | 0 | 0 |
| | | | 1402 | 832 | 285 | 285 | | |
| 7 | F | 285 | Total | C | N | O | 0 | 0 |
| | | | 1402 | 832 | 285 | 285 | | |
| 7 | O | 285 | Total | C | N | O | 0 | 0 |
| | | | 1402 | 832 | 285 | 285 | | |

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| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 7 | X | 285 | 1402 | 832 | 285 | 285 | 0 | 0 |

- Molecule 8 is a protein called NUCLEOPORIN SEH1.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 8 | 7 | 322 | 1593 | 949 | 322 | 322 | 0 | 0 |
| 8 | G | 322 | 1593 | 949 | 322 | 322 | 0 | 0 |
| 8 | P | 322 | 1593 | 949 | 322 | 322 | 0 | 0 |
| 8 | Y | 322 | 1593 | 949 | 322 | 322 | 0 | 0 |

- Molecule 9 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP85.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---------|-------|
| | | | Total | C | N | O | | |
| 9 | 8 | 434 | 2153 | 1285 | 434 | 434 | 0 | 0 |
| 9 | H | 434 | 2153 | 1285 | 434 | 434 | 0 | 0 |
| 9 | Q | 434 | 2153 | 1285 | 434 | 434 | 0 | 0 |
| 9 | Z | 434 | 2153 | 1285 | 434 | 434 | 0 | 0 |


- Molecule 10 is a protein called NUCLEAR PORE COMPLEX PROTEIN NUP155.

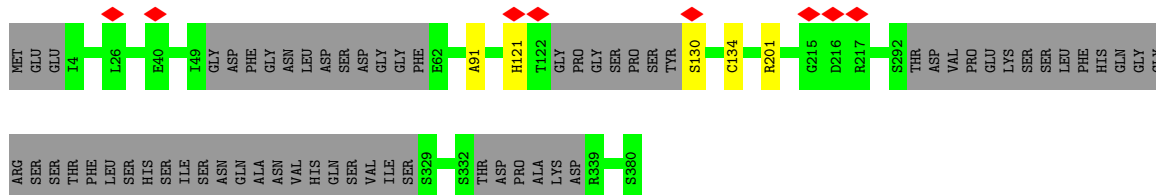
| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|---------|-------|
| | | | Total | C | N | O | | |
| 10 | A | 1097 | 5436 | 3242 | 1097 | 1097 | 0 | 0 |
| 10 | B | 1097 | 5436 | 3242 | 1097 | 1097 | 0 | 0 |

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

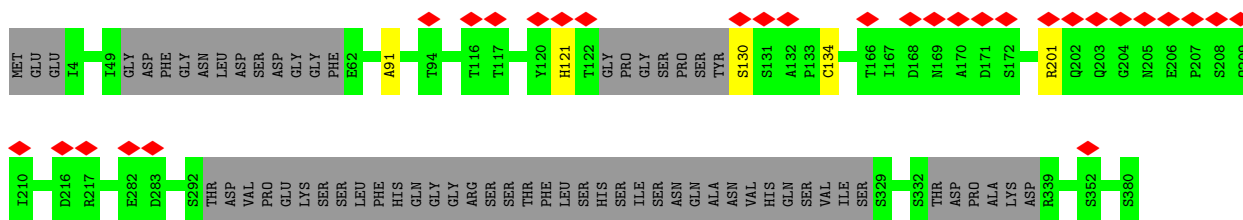
- Molecule 1: NUCLEOPORIN NUP43

Chain 0: 




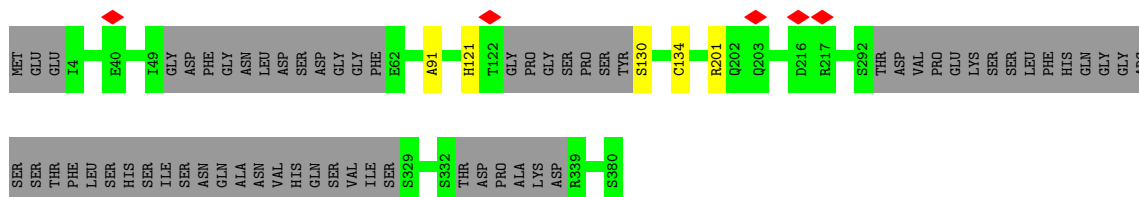
- Molecule 1: NUCLEOPORIN NUP43

Chain 9: 




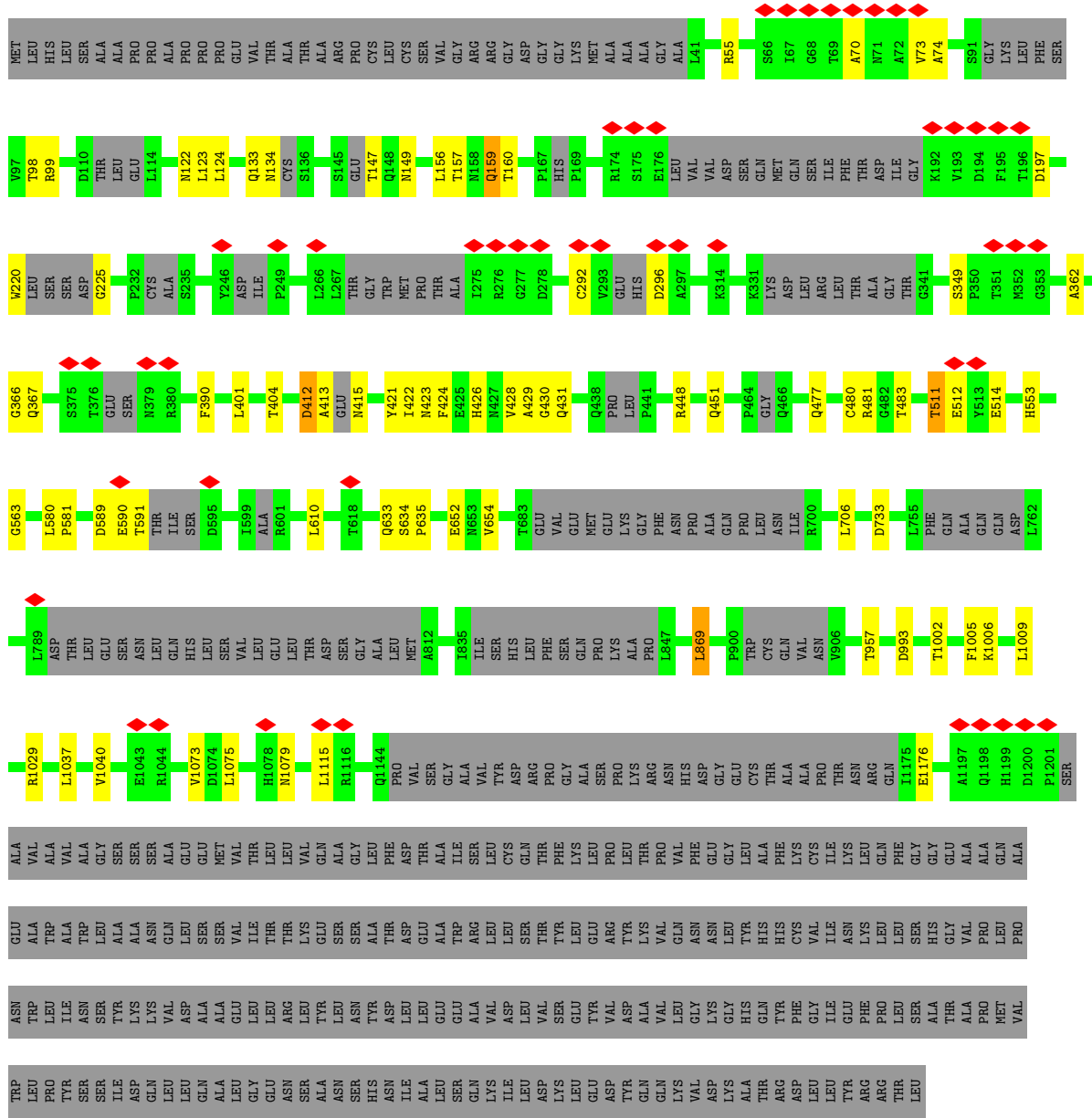
- Molecule 1: NUCLEOPORIN NUP43

Chain I: 

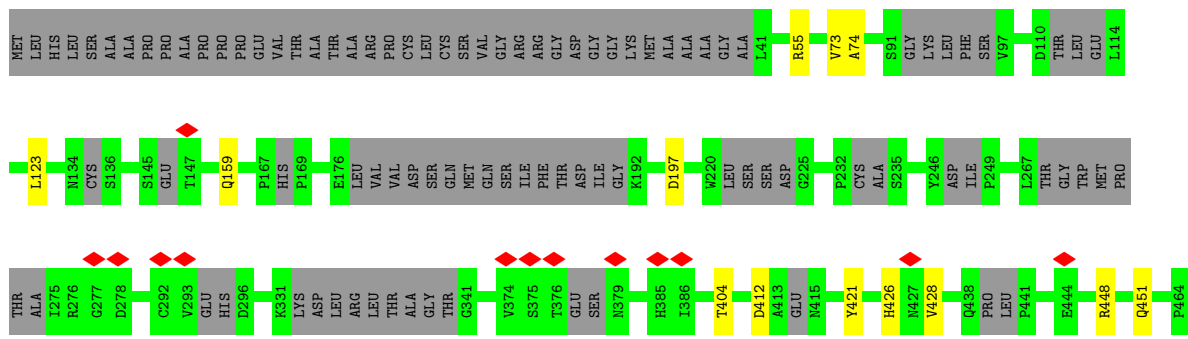


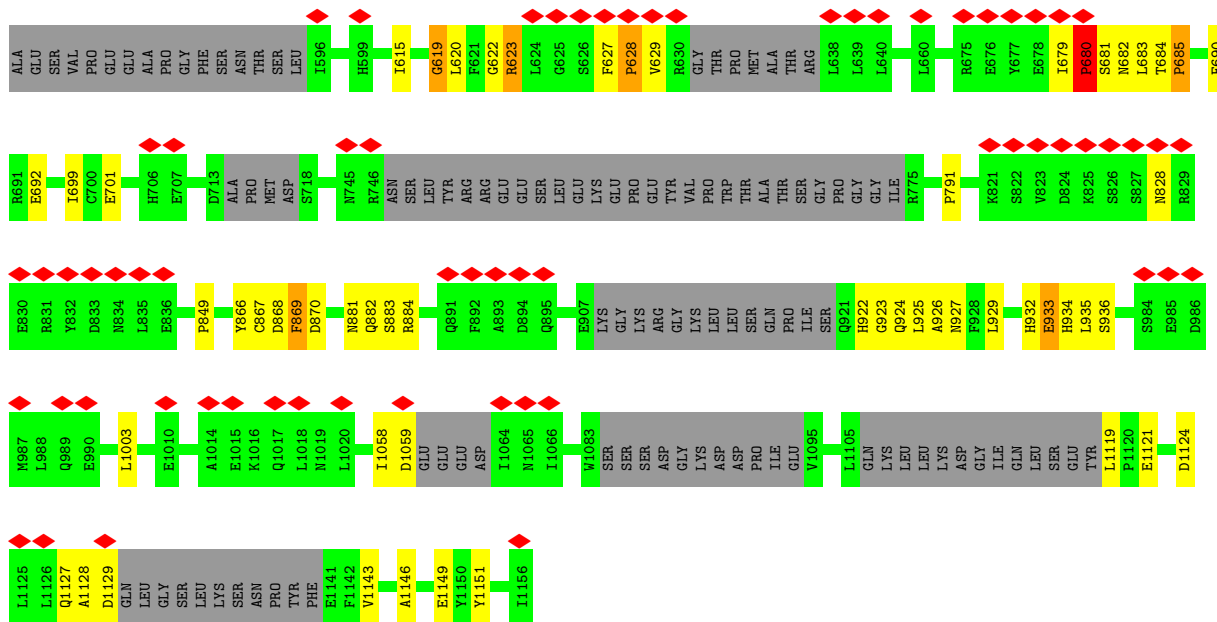
- Molecule 1: NUCLEOPORIN NUP43

Chain R: 

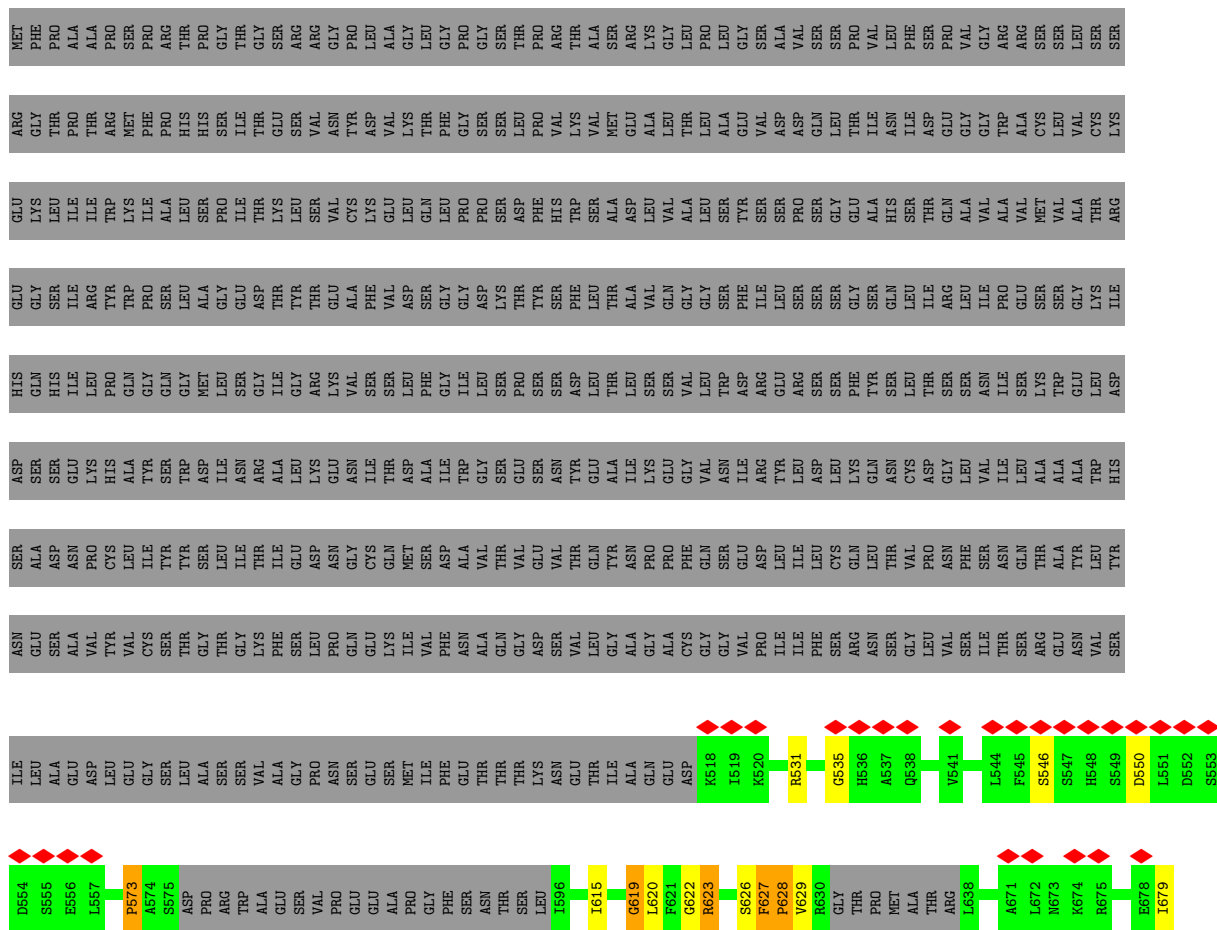
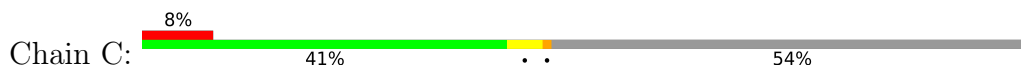


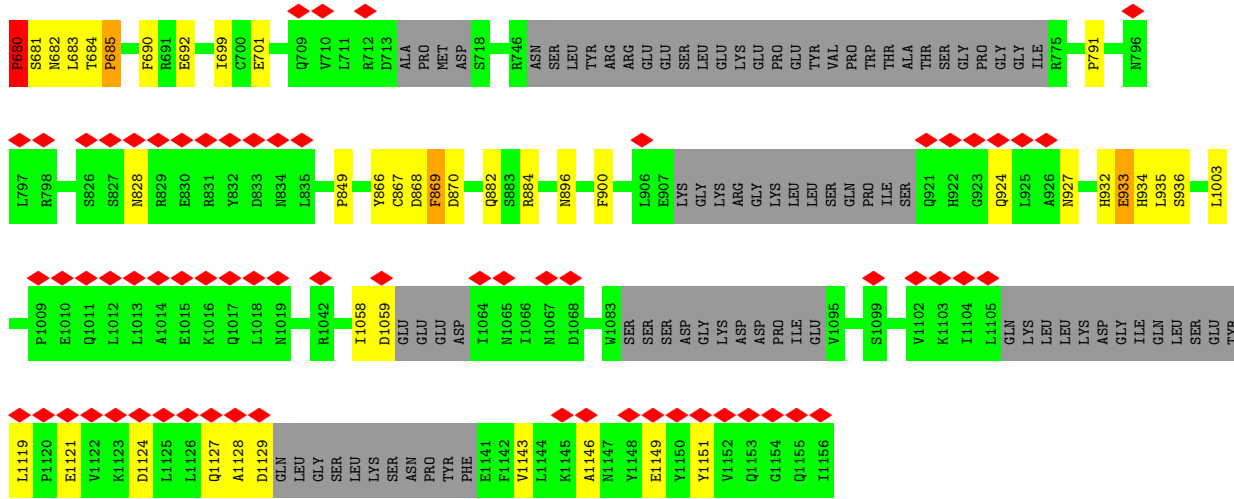
● Molecule 2: NUCLEAR PORE COMPLEX PROTEIN NUP160



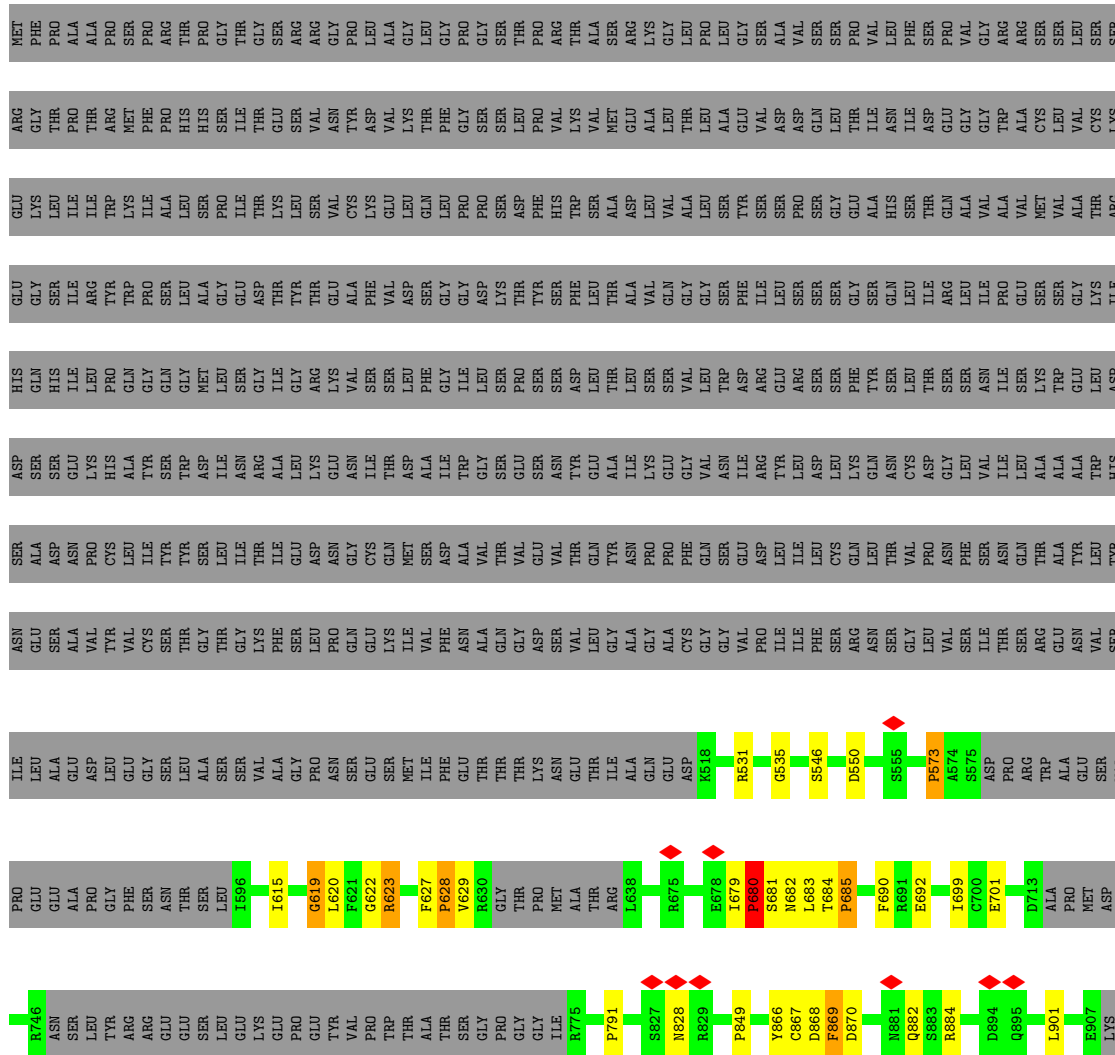


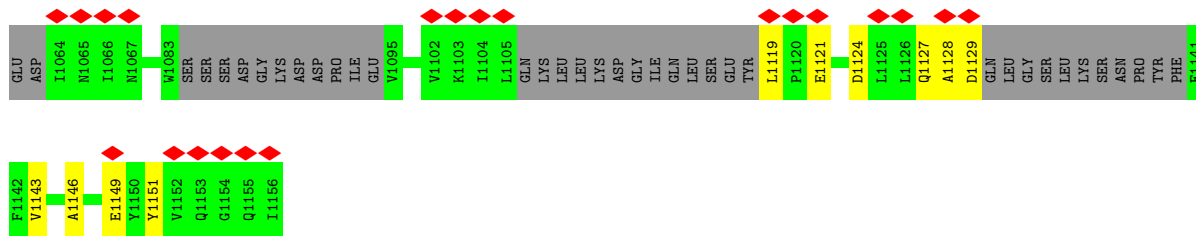
● Molecule 4: NUCLEAR PORE COMPLEX PROTEIN NUP133



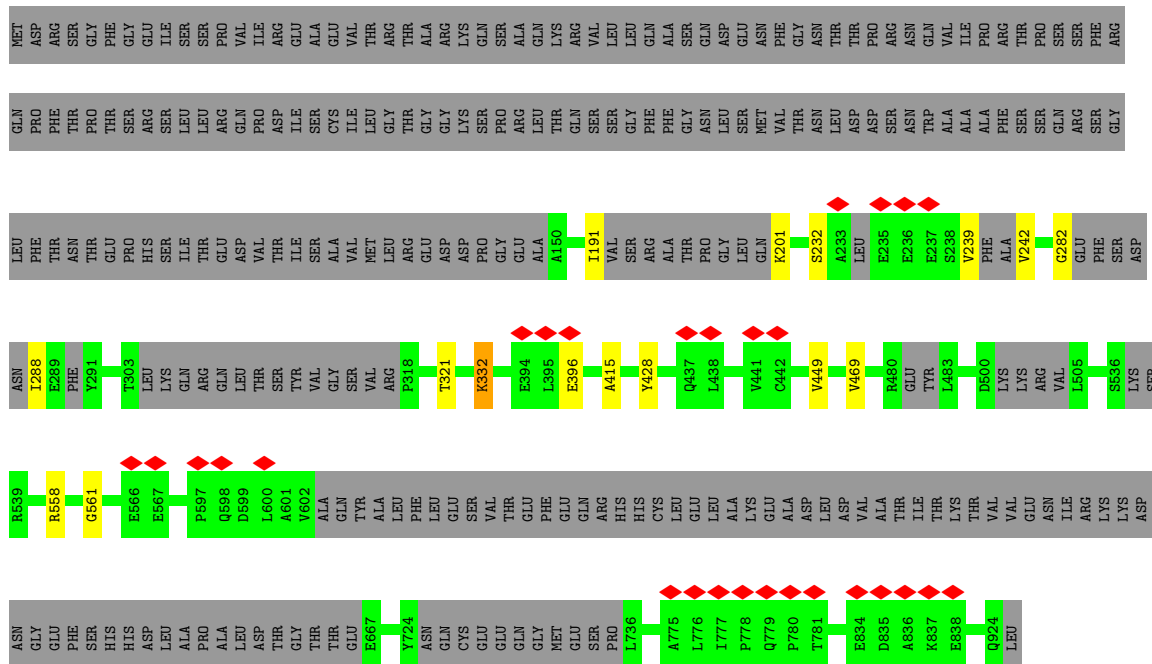


● Molecule 4: NUCLEAR PORE COMPLEX PROTEIN NUP133

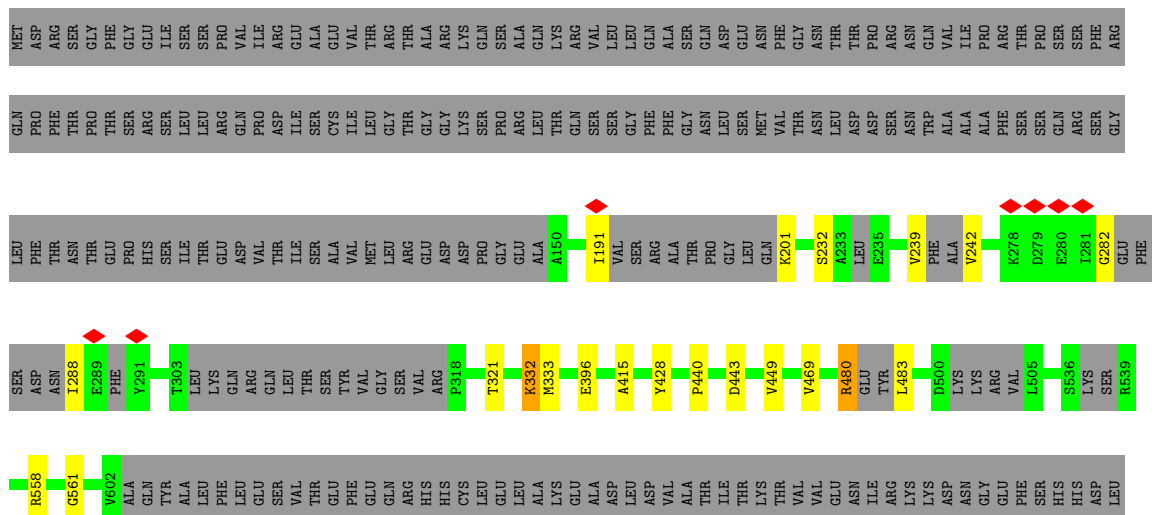


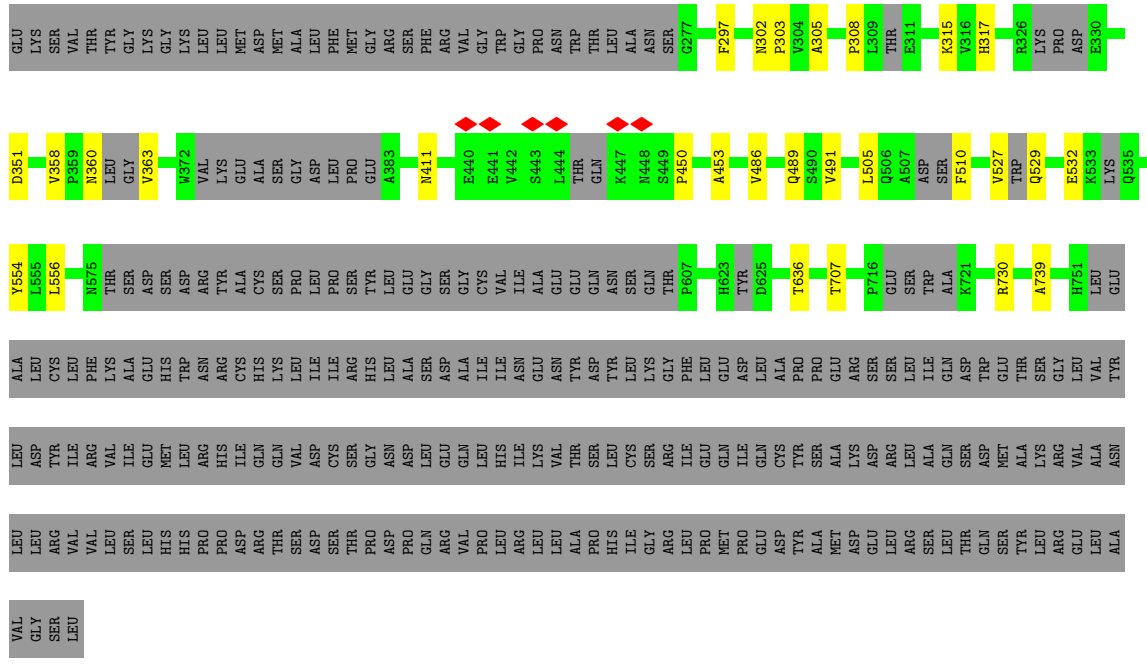


• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107

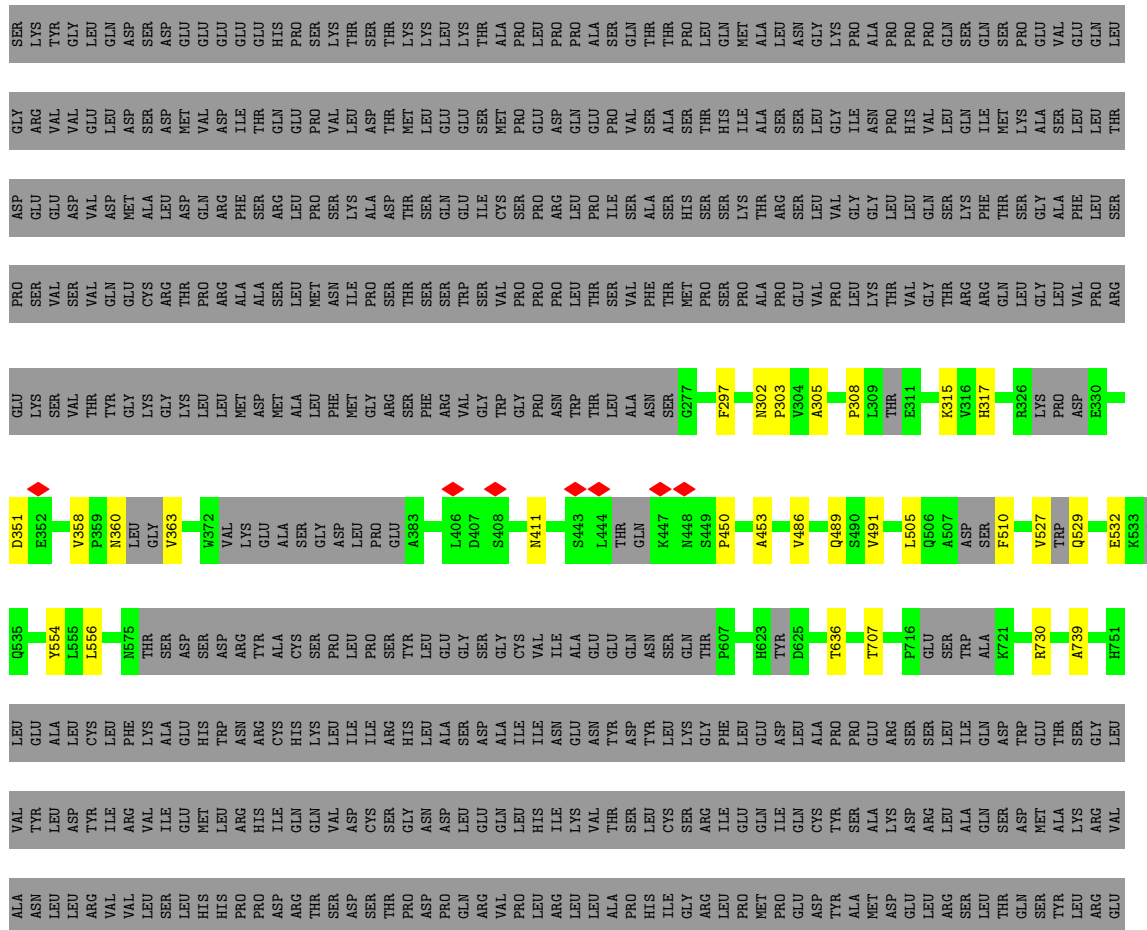


• Molecule 5: NUCLEAR PORE COMPLEX PROTEIN NUP107



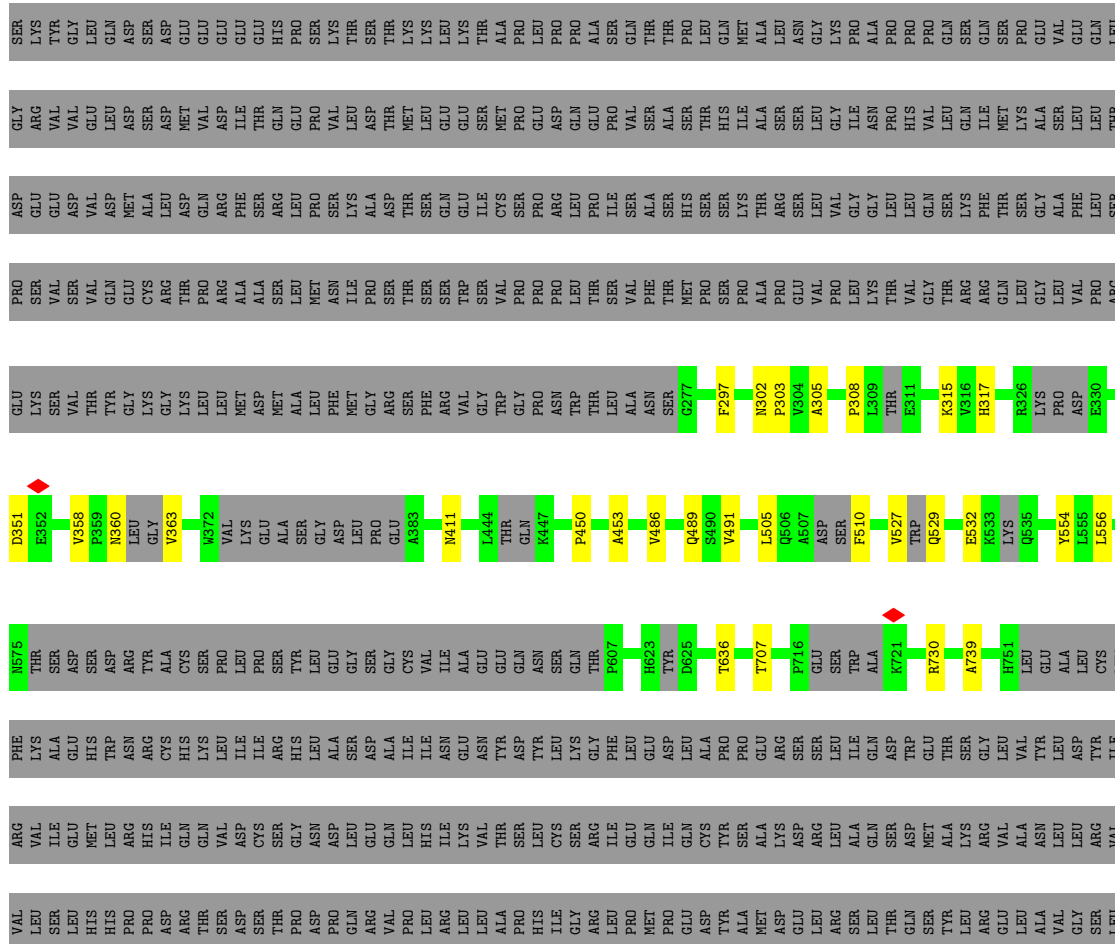


● Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96

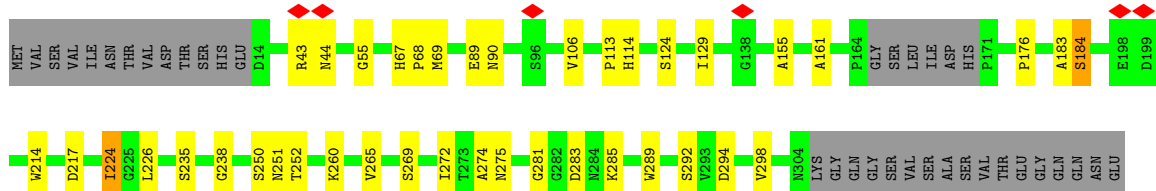
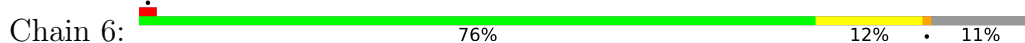


LEU
ALA
VAL
GLY
SER
LEU

• Molecule 6: NUCLEAR PORE COMPLEX PROTEIN NUP96



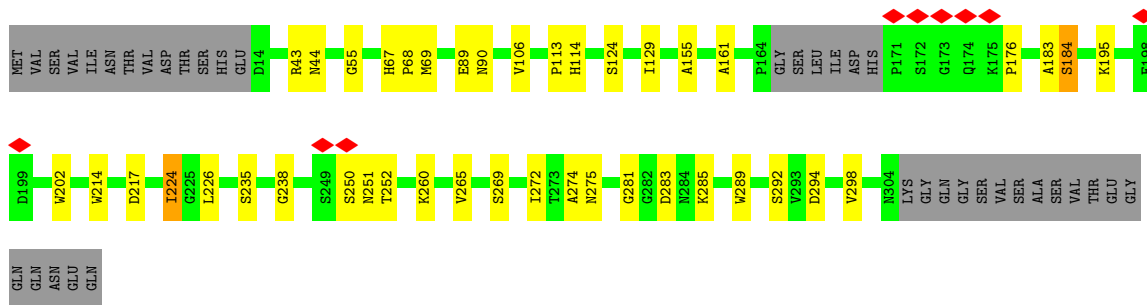
• Molecule 7: PROTEIN SEC13 HOMOLOG



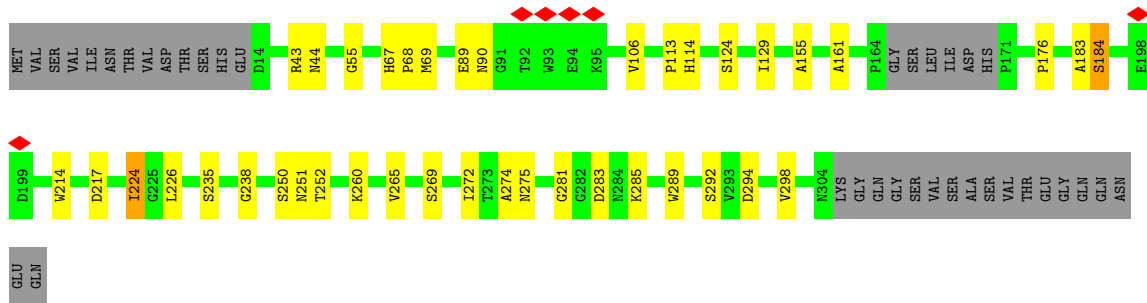
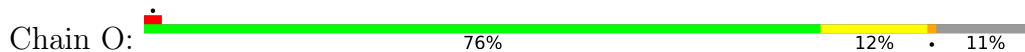
GLN

• Molecule 7: PROTEIN SEC13 HOMOLOG

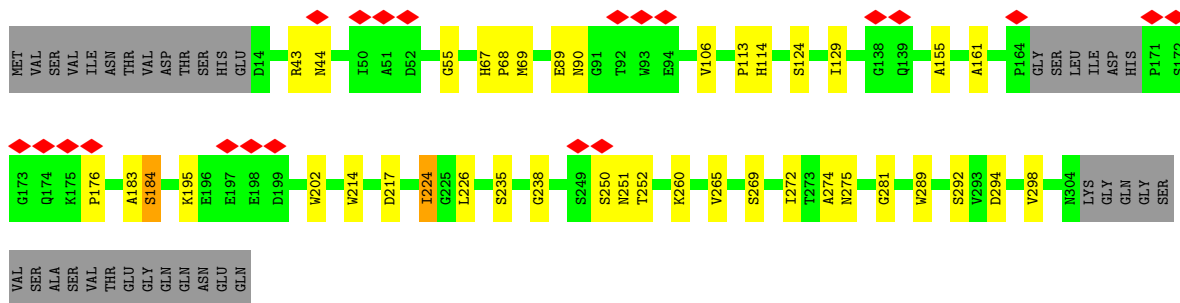
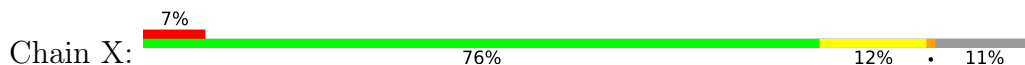




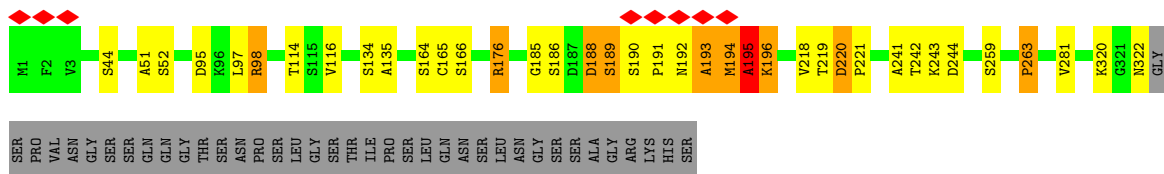
• Molecule 7: PROTEIN SEC13 HOMOLOG



• Molecule 7: PROTEIN SEC13 HOMOLOG



• Molecule 8: NUCLEOPORIN SEH1



• Molecule 8: NUCLEOPORIN SEH1



4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------------|-----------|
| EM reconstruction method | TOMOGRAPHY | Depositor |
| Imposed symmetry | POINT, C8 | Depositor |
| Number of tilted images used | Not provided | |
| Resolution determination method | Not provided | |
| CTF correction method | PHASE FLIPPING OF TILT SERIES | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 110 | Depositor |
| Minimum defocus (nm) | 2000 | Depositor |
| Maximum defocus (nm) | 4000 | Depositor |
| Magnification | 42000 | Depositor |
| Image detector | GATAN K2 (4k x 4k) | Depositor |
| Maximum voxel value | 15.038 | Depositor |
| Minimum voxel value | -7.184 | Depositor |
| Average voxel value | -0.000 | Depositor |
| Voxel value standard deviation | 1.629 | Depositor |
| Recommended contour level | 3.5 | Depositor |
| Tomogram size (\AA) | 1422.72, 1422.72, 1422.72 | wwPDB |
| Tomogram dimensions | 208, 208, 208 | wwPDB |
| Tomogram angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Grid spacing (\AA) | 6.8399997, 6.8399997, 6.8399997 | Depositor |

5 Model quality i

5.1 Standard geometry i

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 | 0 | 0.79 | 0/1557 | 0.76 | 0/2161 |
| 1 | 9 | 0.79 | 0/1557 | 0.76 | 0/2161 |
| 1 | I | 0.79 | 0/1557 | 0.76 | 0/2161 |
| 1 | R | 0.79 | 0/1557 | 0.76 | 0/2161 |
| 2 | 1 | 0.94 | 0/4972 | 1.15 | 8/6892 (0.1%) |
| 2 | J | 0.94 | 0/4971 | 1.15 | 7/6889 (0.1%) |
| 2 | S | 0.94 | 0/4971 | 1.15 | 7/6889 (0.1%) |
| 2 | a | 0.94 | 0/4971 | 1.15 | 7/6889 (0.1%) |
| 3 | 2 | 0.93 | 0/1565 | 1.28 | 7/2175 (0.3%) |
| 3 | K | 0.93 | 0/1565 | 1.28 | 7/2175 (0.3%) |
| 3 | T | 0.93 | 0/1565 | 1.28 | 7/2175 (0.3%) |
| 3 | b | 0.93 | 0/1565 | 1.28 | 7/2175 (0.3%) |
| 4 | 3 | 0.26 | 0/2619 | 0.54 | 6/3644 (0.2%) |
| 4 | C | 0.26 | 0/2619 | 0.54 | 6/3644 (0.2%) |
| 4 | L | 0.26 | 0/2619 | 0.54 | 6/3644 (0.2%) |
| 4 | U | 0.26 | 0/2619 | 0.54 | 6/3644 (0.2%) |
| 5 | 4 | 0.73 | 0/3266 | 0.87 | 2/4540 (0.0%) |
| 5 | D | 0.72 | 1/3268 (0.0%) | 0.88 | 4/4546 (0.1%) |
| 5 | M | 0.73 | 0/3266 | 0.88 | 2/4540 (0.0%) |
| 5 | V | 0.72 | 1/3268 (0.0%) | 0.88 | 4/4546 (0.1%) |
| 6 | 5 | 0.91 | 0/2061 | 1.09 | 3/2859 (0.1%) |
| 6 | E | 0.91 | 0/2061 | 1.09 | 3/2859 (0.1%) |
| 6 | N | 0.91 | 0/2061 | 1.09 | 3/2859 (0.1%) |
| 6 | W | 0.91 | 0/2061 | 1.09 | 3/2859 (0.1%) |
| 7 | 6 | 0.46 | 0/1400 | 0.79 | 1/1943 (0.1%) |
| 7 | F | 0.46 | 0/1400 | 0.82 | 1/1943 (0.1%) |
| 7 | O | 0.46 | 0/1400 | 0.79 | 1/1943 (0.1%) |
| 7 | X | 0.46 | 0/1400 | 0.82 | 1/1943 (0.1%) |
| 8 | 7 | 0.99 | 0/1592 | 1.28 | 6/2217 (0.3%) |
| 8 | G | 0.99 | 0/1592 | 1.28 | 6/2217 (0.3%) |
| 8 | P | 0.99 | 0/1592 | 1.28 | 6/2217 (0.3%) |
| 8 | Y | 0.99 | 0/1592 | 1.28 | 6/2217 (0.3%) |
| 9 | 8 | 1.03 | 1/2145 (0.0%) | 1.04 | 0/2980 |
| 9 | H | 1.03 | 1/2145 (0.0%) | 1.04 | 0/2980 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 9 | Q | 1.03 | 1/2145 (0.0%) | 1.04 | 0/2980 |
| 9 | Z | 1.03 | 1/2145 (0.0%) | 1.04 | 0/2980 |
| 10 | A | 0.93 | 0/5409 | 1.18 | 10/7500 (0.1%) |
| 10 | B | 0.93 | 0/5409 | 1.18 | 10/7500 (0.1%) |
| All | All | 0.84 | 6/95527 (0.0%) | 1.03 | 153/132647 (0.1%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 2 | 1 | 0 | 1 |
| 2 | J | 0 | 1 |
| 2 | S | 0 | 1 |
| 2 | a | 0 | 1 |
| 3 | 2 | 0 | 1 |
| 3 | K | 0 | 1 |
| 3 | T | 0 | 1 |
| 3 | b | 0 | 1 |
| 5 | D | 0 | 1 |
| 5 | V | 0 | 1 |
| 10 | A | 0 | 1 |
| 10 | B | 0 | 1 |
| All | All | 0 | 12 |

The worst 5 of 6 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9 | 8 | 64 | TYR | C-N | 24.26 | 1.89 | 1.34 |
| 9 | Q | 64 | TYR | C-N | 24.23 | 1.89 | 1.34 |
| 9 | Z | 64 | TYR | C-N | 24.20 | 1.89 | 1.34 |
| 9 | H | 64 | TYR | C-N | 24.18 | 1.89 | 1.34 |
| 5 | V | 483 | LEU | C-N | -5.78 | 1.22 | 1.33 |

The worst 5 of 153 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 10 | B | 276 | ASP | O-C-N | 21.68 | 157.40 | 122.70 |
| 10 | A | 276 | ASP | O-C-N | 21.65 | 157.34 | 122.70 |
| 10 | A | 276 | ASP | CA-C-N | -18.34 | 76.86 | 117.20 |
| 10 | B | 276 | ASP | CA-C-N | -18.33 | 76.86 | 117.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 5 | D | 480 | ARG | CA-C-N | -11.75 | 91.35 | 117.20 |

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 2 | 1 | 511 | THR | Peptide |
| 3 | 2 | 286 | GLY | Peptide |
| 10 | A | 259 | SER | Mainchain |
| 10 | B | 259 | SER | Mainchain |
| 5 | D | 480 | ARG | Mainchain |

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 | 0 | 1562 | 0 | 681 | 6 | 0 |
| 1 | 9 | 1562 | 0 | 681 | 6 | 0 |
| 1 | I | 1562 | 0 | 681 | 6 | 0 |
| 1 | R | 1562 | 0 | 681 | 5 | 0 |
| 2 | 1 | 4997 | 0 | 2175 | 30 | 0 |
| 2 | J | 4997 | 0 | 2174 | 26 | 0 |
| 2 | S | 4997 | 0 | 2174 | 57 | 0 |
| 2 | a | 4997 | 0 | 2174 | 0 | 0 |
| 3 | 2 | 1566 | 0 | 702 | 19 | 0 |
| 3 | K | 1566 | 0 | 702 | 19 | 0 |
| 3 | T | 1566 | 0 | 702 | 18 | 0 |
| 3 | b | 1566 | 0 | 702 | 0 | 0 |
| 4 | 3 | 2629 | 0 | 1167 | 53 | 0 |
| 4 | C | 2629 | 0 | 1167 | 33 | 0 |
| 4 | L | 2629 | 0 | 1167 | 32 | 0 |
| 4 | U | 2629 | 0 | 1167 | 34 | 0 |
| 5 | 4 | 3278 | 0 | 1440 | 8 | 0 |
| 5 | D | 3278 | 0 | 1442 | 9 | 0 |
| 5 | M | 3278 | 0 | 1440 | 8 | 0 |
| 5 | V | 3278 | 0 | 1442 | 8 | 0 |
| 6 | 5 | 2073 | 0 | 907 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6 | E | 2073 | 0 | 907 | 12 | 0 |
| 6 | N | 2073 | 0 | 907 | 12 | 0 |
| 6 | W | 2073 | 0 | 907 | 12 | 0 |
| 7 | 6 | 1402 | 0 | 648 | 19 | 0 |
| 7 | F | 1402 | 0 | 648 | 20 | 0 |
| 7 | O | 1402 | 0 | 648 | 20 | 0 |
| 7 | X | 1402 | 0 | 648 | 20 | 0 |
| 8 | 7 | 1593 | 0 | 731 | 43 | 0 |
| 8 | G | 1593 | 0 | 731 | 43 | 0 |
| 8 | P | 1593 | 0 | 731 | 42 | 0 |
| 8 | Y | 1593 | 0 | 731 | 43 | 0 |
| 9 | 8 | 2153 | 0 | 938 | 15 | 0 |
| 9 | H | 2153 | 0 | 938 | 15 | 0 |
| 9 | Q | 2153 | 0 | 938 | 15 | 0 |
| 9 | Z | 2153 | 0 | 938 | 15 | 0 |
| 10 | A | 5436 | 0 | 2392 | 58 | 0 |
| 10 | B | 5436 | 0 | 2384 | 117 | 0 |
| All | All | 95884 | 0 | 42333 | 825 | 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 6.

The worst 5 of 825 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) |
|-----------------|-----------------|--------------------------|-------------------|
| 4:3:883:SER:CB | 4:3:926:ALA:CA | 1.90 | 1.49 |
| 10:B:844:CYS:C | 10:B:885:ARG:CB | 1.81 | 1.48 |
| 10:B:845:TYR:CB | 10:B:886:GLN:HA | 1.42 | 1.47 |
| 10:B:843:ASN:CB | 10:B:919:GLN:CB | 1.92 | 1.46 |
| 10:B:860:GLN:N | 10:B:874:CYS:N | 1.65 | 1.44 |

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 | 0 | 306/380 (80%) | 296 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | 9 | 306/380 (80%) | 296 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | I | 306/380 (80%) | 296 (97%) | 10 (3%) | 0 | 100 | 100 |
| 1 | R | 306/380 (80%) | 296 (97%) | 10 (3%) | 0 | 100 | 100 |
| 2 | 1 | 959/1436 (67%) | 873 (91%) | 63 (7%) | 23 (2%) | 6 | 33 |
| 2 | J | 957/1436 (67%) | 873 (91%) | 62 (6%) | 22 (2%) | 6 | 34 |
| 2 | S | 957/1436 (67%) | 873 (91%) | 62 (6%) | 22 (2%) | 6 | 34 |
| 2 | a | 957/1436 (67%) | 873 (91%) | 62 (6%) | 22 (2%) | 6 | 34 |
| 3 | 2 | 316/326 (97%) | 280 (89%) | 15 (5%) | 21 (7%) | 1 | 16 |
| 3 | K | 316/326 (97%) | 279 (88%) | 16 (5%) | 21 (7%) | 1 | 16 |
| 3 | T | 316/326 (97%) | 280 (89%) | 15 (5%) | 21 (7%) | 1 | 16 |
| 3 | b | 316/326 (97%) | 279 (88%) | 16 (5%) | 21 (7%) | 1 | 16 |
| 4 | 3 | 508/1156 (44%) | 437 (86%) | 55 (11%) | 16 (3%) | 4 | 27 |
| 4 | C | 508/1156 (44%) | 437 (86%) | 56 (11%) | 15 (3%) | 4 | 28 |
| 4 | L | 508/1156 (44%) | 437 (86%) | 56 (11%) | 15 (3%) | 4 | 28 |
| 4 | U | 508/1156 (44%) | 437 (86%) | 56 (11%) | 15 (3%) | 4 | 28 |
| 5 | 4 | 636/925 (69%) | 607 (95%) | 25 (4%) | 4 (1%) | 25 | 66 |
| 5 | D | 640/925 (69%) | 607 (95%) | 28 (4%) | 5 (1%) | 19 | 60 |
| 5 | M | 636/925 (69%) | 608 (96%) | 24 (4%) | 4 (1%) | 25 | 66 |
| 5 | V | 640/925 (69%) | 607 (95%) | 27 (4%) | 6 (1%) | 17 | 57 |
| 6 | 5 | 393/937 (42%) | 363 (92%) | 19 (5%) | 11 (3%) | 5 | 30 |
| 6 | E | 393/937 (42%) | 363 (92%) | 19 (5%) | 11 (3%) | 5 | 30 |
| 6 | N | 393/937 (42%) | 363 (92%) | 19 (5%) | 11 (3%) | 5 | 30 |
| 6 | W | 393/937 (42%) | 363 (92%) | 19 (5%) | 11 (3%) | 5 | 30 |
| 7 | 6 | 281/322 (87%) | 235 (84%) | 38 (14%) | 8 (3%) | 5 | 30 |
| 7 | F | 281/322 (87%) | 231 (82%) | 42 (15%) | 8 (3%) | 5 | 30 |
| 7 | O | 281/322 (87%) | 235 (84%) | 38 (14%) | 8 (3%) | 5 | 30 |
| 7 | X | 281/322 (87%) | 230 (82%) | 43 (15%) | 8 (3%) | 5 | 30 |
| 8 | 7 | 320/360 (89%) | 288 (90%) | 21 (7%) | 11 (3%) | 3 | 26 |
| 8 | G | 320/360 (89%) | 288 (90%) | 21 (7%) | 11 (3%) | 3 | 26 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|----|
| 8 | P | 320/360 (89%) | 288 (90%) | 21 (7%) | 11 (3%) | 3 | 26 |
| 8 | Y | 320/360 (89%) | 288 (90%) | 21 (7%) | 11 (3%) | 3 | 26 |
| 9 | 8 | 418/656 (64%) | 379 (91%) | 28 (7%) | 11 (3%) | 5 | 31 |
| 9 | H | 418/656 (64%) | 379 (91%) | 28 (7%) | 11 (3%) | 5 | 31 |
| 9 | Q | 418/656 (64%) | 379 (91%) | 28 (7%) | 11 (3%) | 5 | 31 |
| 9 | Z | 418/656 (64%) | 379 (91%) | 28 (7%) | 11 (3%) | 5 | 31 |
| 10 | A | 1043/1391 (75%) | 961 (92%) | 58 (6%) | 24 (2%) | 6 | 34 |
| 10 | B | 1043/1391 (75%) | 961 (92%) | 58 (6%) | 24 (2%) | 6 | 34 |
| All | All | 18636/28774 (65%) | 16944 (91%) | 1227 (7%) | 465 (2%) | 9 | 32 |

5 of 465 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | 1 | 55 | ARG |
| 2 | 1 | 73 | VAL |
| 2 | 1 | 159 | GLN |
| 2 | 1 | 404 | THR |
| 2 | 1 | 428 | VAL |

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 |
|-----|-------|------------------|
| 2 | J | 1 |
| 2 | a | 1 |
| 2 | S | 1 |
| 9 | 8 | 1 |
| 9 | H | 1 |
| 9 | Q | 1 |
| 9 | Z | 1 |

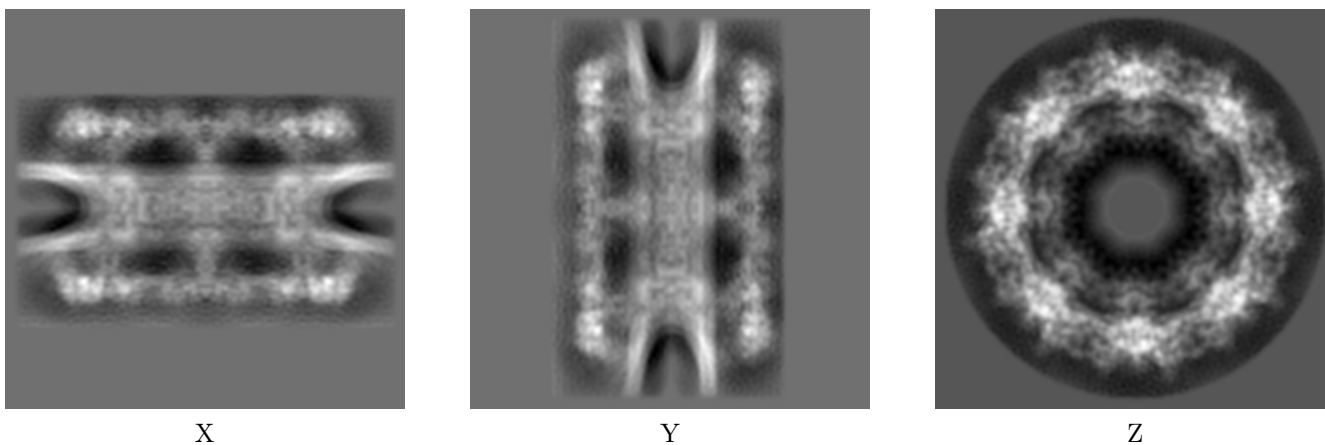
The worst 5 of 7 chain breaks are listed below:

| Model | Chain | Residue-1 | Atom-1 | Residue-2 | Atom-2 | Distance (Å) |
|-------|-------|-----------|--------|-----------|--------|--------------|
| 1 | J | 1013:HIS | C | 1014:ASN | N | 6.20 |
| 1 | a | 1013:HIS | C | 1014:ASN | N | 6.01 |
| 1 | S | 1013:HIS | C | 1014:ASN | N | 4.29 |
| 1 | 8 | 64:TYR | C | 65:SER | N | 1.89 |
| 1 | H | 64:TYR | C | 65:SER | N | 1.89 |

6 Tomogram visualisation [i](#)

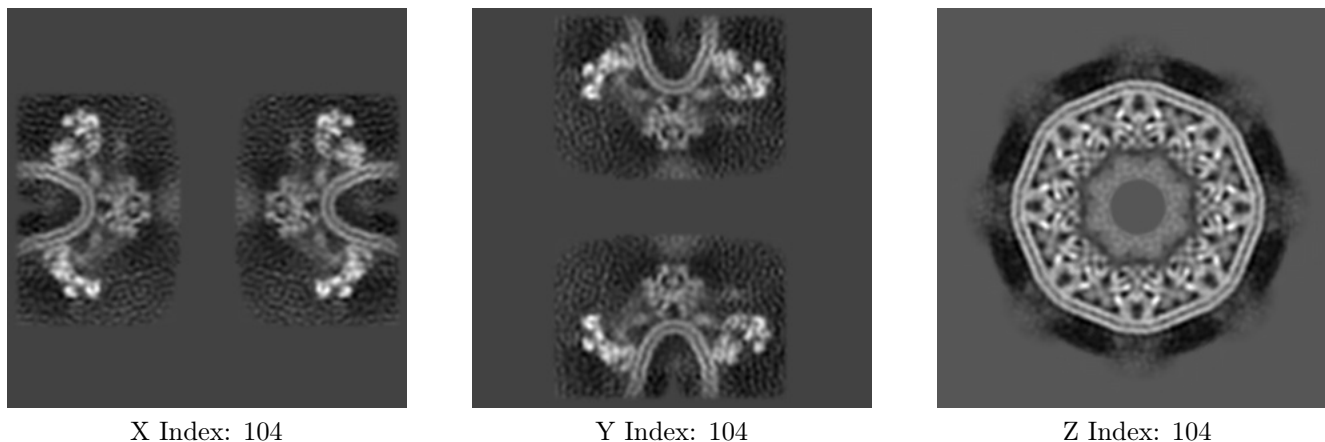
This section contains visualisations of the EMDB entry EMD-3103. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



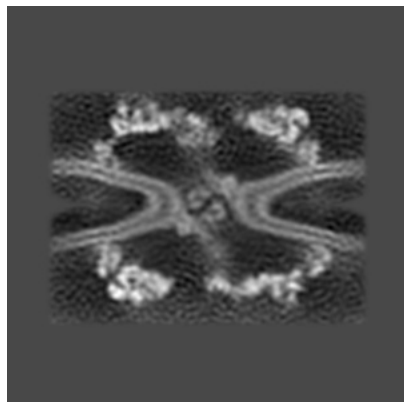
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)

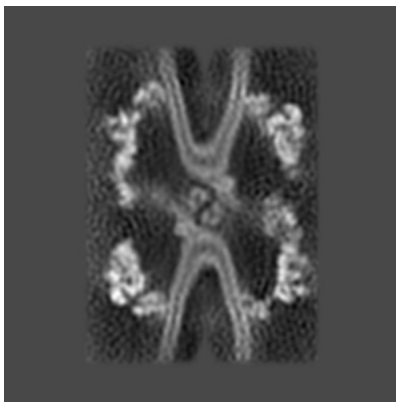


The images above show central slices of the tomogram in three orthogonal directions.

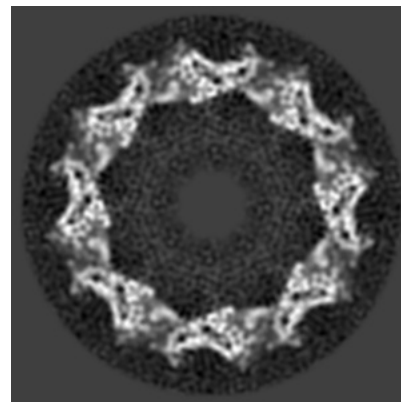
6.3 Largest variance slices [i](#)



X Index: 160



Y Index: 48



Z Index: 62

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

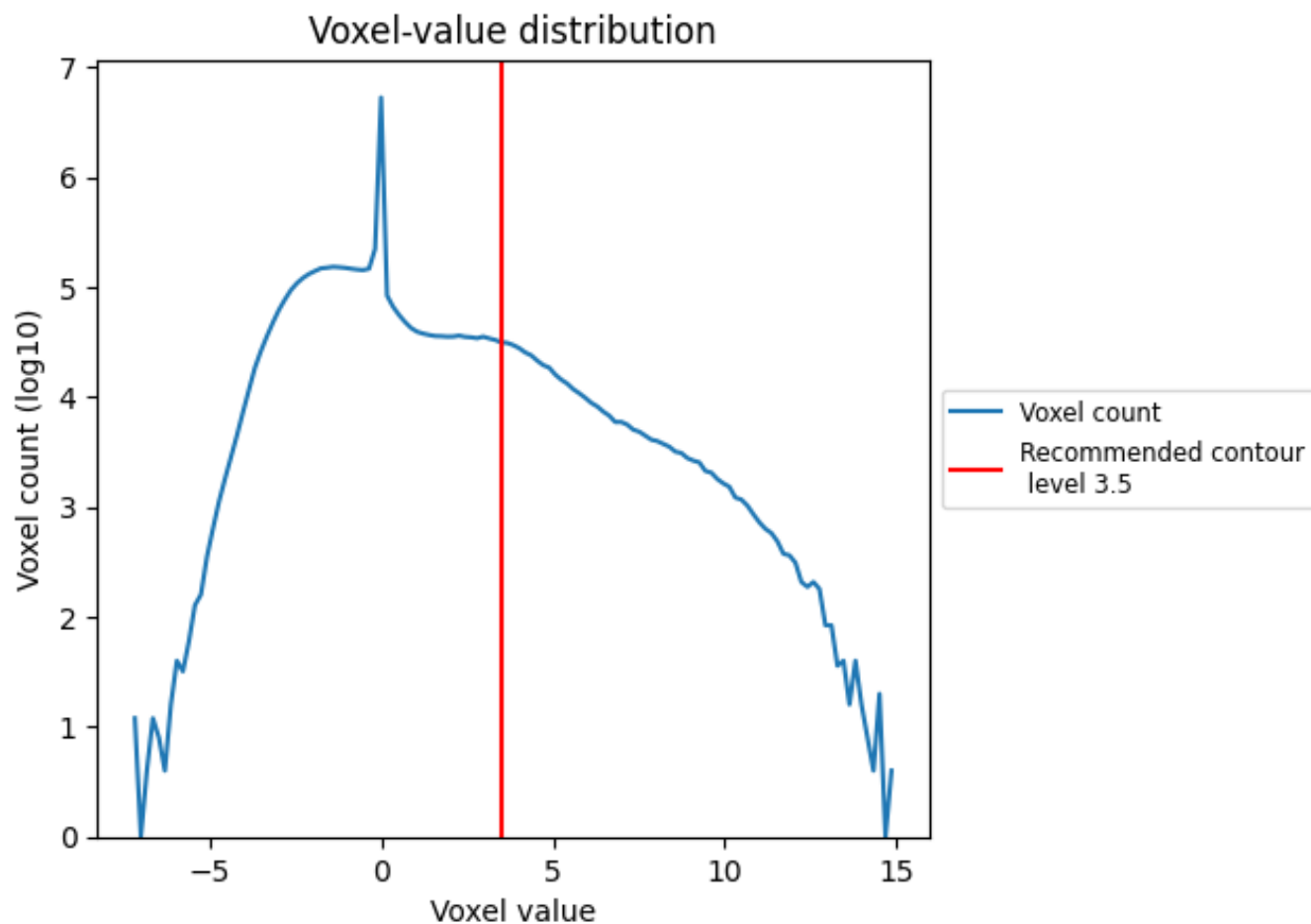
6.4 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

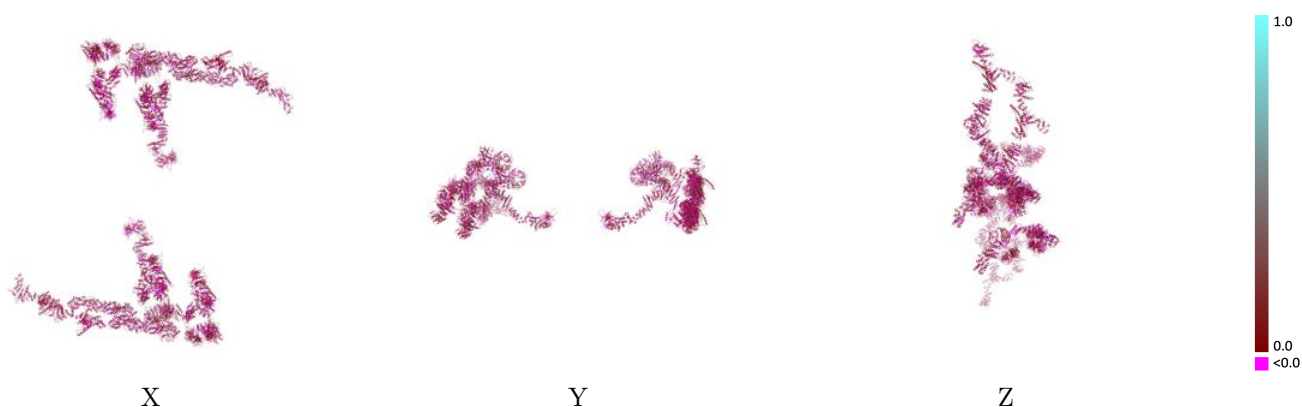
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3103 and PDB model 5A9Q. Per-residue inclusion information can be found in section 3 on page 8.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

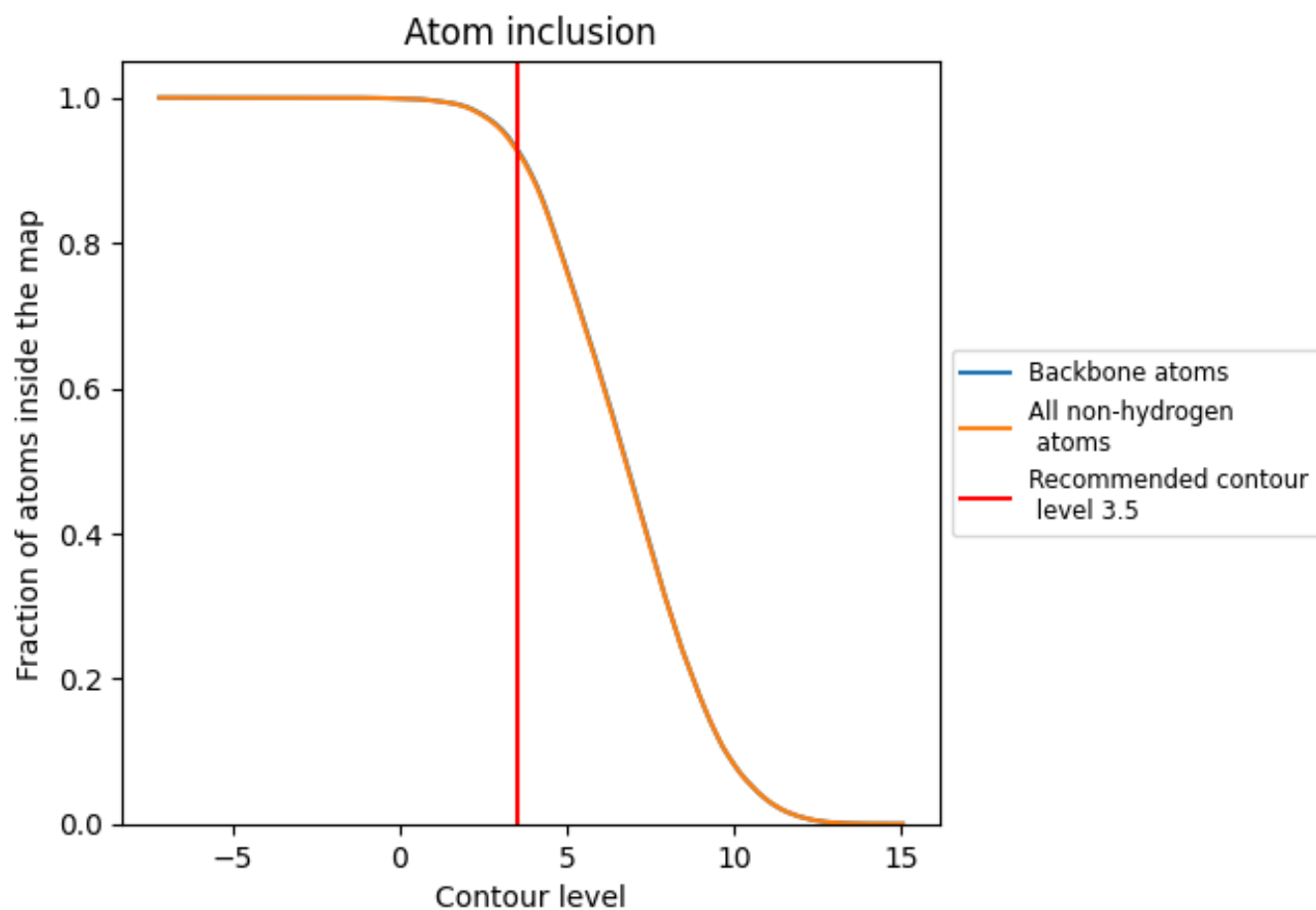


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































































8.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary









The table lists the average atom inclusion at the recommended contour level (3.5) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--|--|
| All |  0.9272 |  0.0490 |
| 0 |  0.9757 |  0.0520 |
| 1 |  0.8031 |  0.0300 |
| 2 |  0.8372 |  0.0400 |
| 3 |  0.8634 |  0.0470 |
| 4 |  0.9594 |  0.0600 |
| 5 |  0.9749 |  0.0640 |
| 6 |  0.9786 |  0.0360 |
| 7 |  0.9743 |  0.0530 |
| 8 |  0.9833 |  0.0540 |
| 9 |  0.9059 |  0.0440 |
| A |  0.8033 |  0.0510 |
| B |  0.8729 |  0.0490 |
| C |  0.8193 |  0.0540 |
| D |  0.9521 |  0.0540 |
| E |  0.9836 |  0.0500 |
| F |  0.9636 |  0.0500 |
| G |  0.9843 |  0.0520 |
| H |  0.9772 |  0.0380 |
| I |  0.9846 |  0.0430 |
| J |  0.9466 |  0.0400 |
| K |  0.9860 |  0.0310 |
| L |  0.9738 |  0.0600 |
| M |  0.9841 |  0.0660 |
| N |  0.9826 |  0.0540 |
| O |  0.9807 |  0.0300 |
| P |  0.9655 |  0.0570 |
| Q |  0.9916 |  0.0490 |
| R |  0.9930 |  0.0530 |
| S |  0.9498 |  0.0410 |
| T |  0.9719 |  0.0500 |
| U |  0.7691 |  0.0610 |
| V |  0.9265 |  0.0520 |
| W |  0.9932 |  0.0550 |
| X |  0.9230 |  0.0440 |



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| Chain | Atom inclusion | Q-score |
|-------|--|--|
| Y |  0.9554 |  0.0430 |
| Z |  0.9758 |  0.0580 |
| a |  0.9454 |  0.0440 |
| b |  0.9266 |  0.0410 |