



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

PDB ID : 3U88
Title : Crystal structure of human menin in complex with MLL1 and LEDGF
Authors : Huang, J.; Wan, B.; Lei, M.
Deposited on : 2011-10-16
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

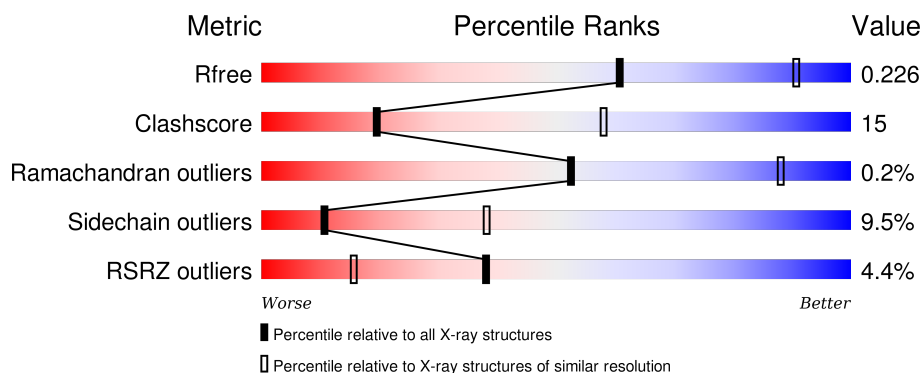
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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) | Similar resolution (#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| R_{free} | 91344 | 1578 (3.00-3.00) |
| Clashscore | 102246 | 1912 (3.00-3.00) |
| Ramachandran outliers | 100387 | 1853 (3.00-3.00) |
| Sidechain outliers | 100360 | 1856 (3.00-3.00) |
| RSRZ outliers | 91569 | 1592 (3.00-3.00) |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 550 | <div> <div>63%</div> <div>20%</div> <div>•</div> <div>13%</div> </div> |
| 1 | B | 550 | <div> <div>62%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> |
| 2 | M | 75 | <div> <div>56%</div> <div>16%</div> <div>•</div> <div>25%</div> </div> |
| 2 | N | 75 | <div> <div>3%</div> <div>48%</div> <div>21%</div> <div>•</div> <div>27%</div> </div> |
| 3 | C | 89 | <div> <div>9%</div> <div>56%</div> <div>28%</div> <div>8%</div> <div>8%</div> </div> |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3 | D | 89 | |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 5 | 0BR | A | 612 | - | - | X | X |
| 5 | 0BR | B | 612 | - | - | - | X |
| 6 | GGB | A | 613 | - | - | X | - |
| 6 | GGB | C | 109 | - | - | X | - |
| 7 | GLV | A | 616 | - | - | - | X |
| 8 | SO4 | M | 154 | - | - | X | - |
| 8 | SO4 | N | 154 | - | - | X | - |

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9881 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Menin.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 1 | A | 477 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3767 | 2414 | 643 | 696 | 14 | | | |
| 1 | B | 485 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3811 | 2444 | 651 | 702 | 14 | | | |

There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| A | 1 | SER | - | EXPRESSION TAG | UNP O00255 |
| A | ? | - | GLY | DELETION | UNP O00255 |
| A | ? | - | TRP | DELETION | UNP O00255 |
| A | ? | - | SER | DELETION | UNP O00255 |
| A | ? | - | PRO | DELETION | UNP O00255 |
| A | ? | - | VAL | DELETION | UNP O00255 |
| B | 1 | SER | - | EXPRESSION TAG | UNP O00255 |
| B | ? | - | GLY | DELETION | UNP O00255 |
| B | ? | - | TRP | DELETION | UNP O00255 |
| B | ? | - | SER | DELETION | UNP O00255 |
| B | ? | - | PRO | DELETION | UNP O00255 |
| B | ? | - | VAL | DELETION | UNP O00255 |

- Molecule 2 is a protein called Histone-lysine N-methyltransferase MLL.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---------|---------|-------|
| 2 | M | 56 | Total | C | N | O | 0 | 0 | 0 |
| | | | 429 | 270 | 93 | 66 | | | |
| 2 | N | 55 | Total | C | N | O | 0 | 0 | 0 |
| | | | 420 | 265 | 92 | 63 | | | |

There are 48 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| M | 5 | SER | - | EXPRESSION TAG | UNP Q03164 |
| M | 6 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 7 | TRP | - | EXPRESSION TAG | UNP Q03164 |
| M | 8 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 9 | PHE | - | EXPRESSION TAG | UNP Q03164 |
| M | 10 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| M | 11 | ALA | - | EXPRESSION TAG | UNP Q03164 |
| M | 12 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 13 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| M | 14 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| M | 15 | THR | - | EXPRESSION TAG | UNP Q03164 |
| M | 23 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| M | 24 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 25 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 26 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| M | 27 | LEU | - | EXPRESSION TAG | UNP Q03164 |
| M | 28 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| M | 29 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| M | 30 | ALA | - | EXPRESSION TAG | UNP Q03164 |
| M | 31 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| M | 32 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 33 | GLN | - | EXPRESSION TAG | UNP Q03164 |
| M | 34 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| M | 35 | VAL | - | EXPRESSION TAG | UNP Q03164 |
| N | 5 | SER | - | EXPRESSION TAG | UNP Q03164 |
| N | 6 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 7 | TRP | - | EXPRESSION TAG | UNP Q03164 |
| N | 8 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 9 | PHE | - | EXPRESSION TAG | UNP Q03164 |
| N | 10 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| N | 11 | ALA | - | EXPRESSION TAG | UNP Q03164 |
| N | 12 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 13 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| N | 14 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| N | 15 | THR | - | EXPRESSION TAG | UNP Q03164 |
| N | 23 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| N | 24 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 25 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 26 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| N | 27 | LEU | - | EXPRESSION TAG | UNP Q03164 |
| N | 28 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| N | 29 | GLY | - | EXPRESSION TAG | UNP Q03164 |
| N | 30 | ALA | - | EXPRESSION TAG | UNP Q03164 |

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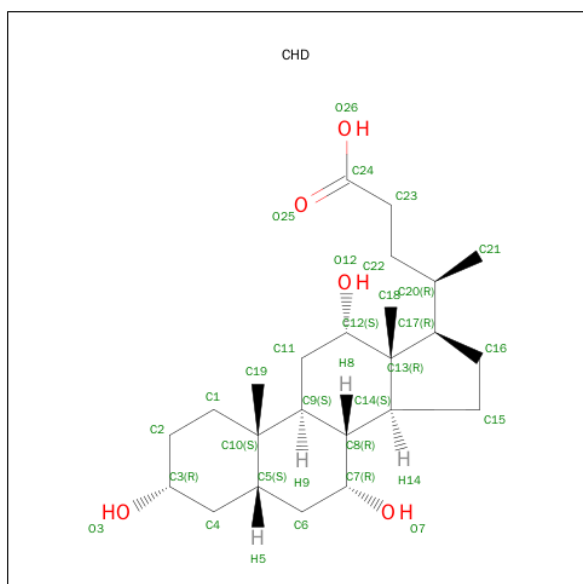
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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| N | 31 | PRO | - | EXPRESSION TAG | UNP Q03164 |
| N | 32 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 33 | GLN | - | EXPRESSION TAG | UNP Q03164 |
| N | 34 | ARG | - | EXPRESSION TAG | UNP Q03164 |
| N | 35 | VAL | - | EXPRESSION TAG | UNP Q03164 |

- Molecule 3 is a protein called Lens epithelium-derived growth factor.

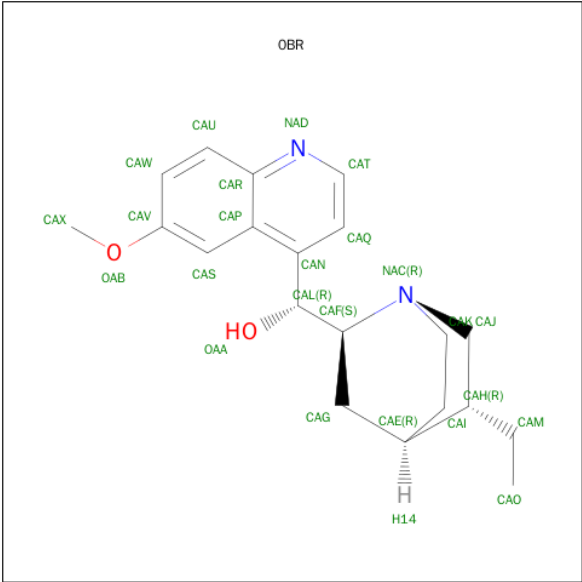
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
| 3 | C | 82 | Total | C | N | O | S | 18 | 0 | 0 |
| | | | 674 | 424 | 121 | 122 | 7 | | | |
| 3 | D | 67 | Total | C | N | O | S | 15 | 0 | 0 |
| | | | 544 | 343 | 97 | 98 | 6 | | | |

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



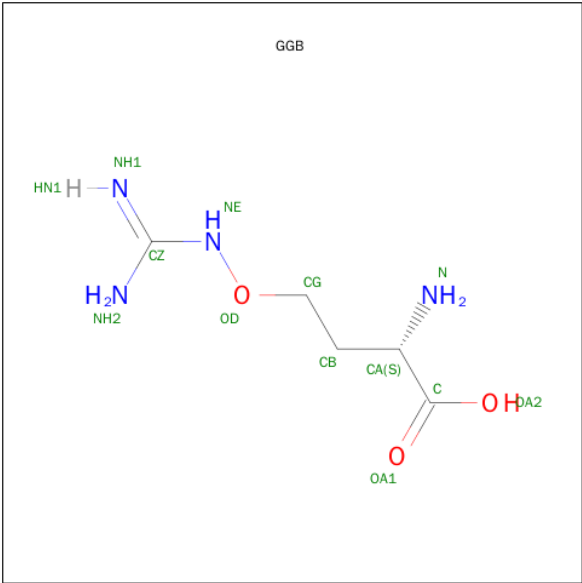
| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---------|---------|
| 4 | A | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |
| 4 | B | 1 | Total | C | O | 0 | 0 |
| | | | 29 | 24 | 5 | | |

- Molecule 5 is (4BETA,8ALPHA,9R)-6'-METHOXY-10,11-DIHYDROCINCHONAN-9-OL (three-letter code: 0BR) (formula: $C_{20}H_{26}N_2O_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---|---|---------|---------|
| 5 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 24 | 20 | 2 | 2 | | |
| 5 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 24 | 20 | 2 | 2 | | |

- Molecule 6 is L-CANAVANINE (three-letter code: GGB) (formula: $C_5H_{12}N_4O_3$).



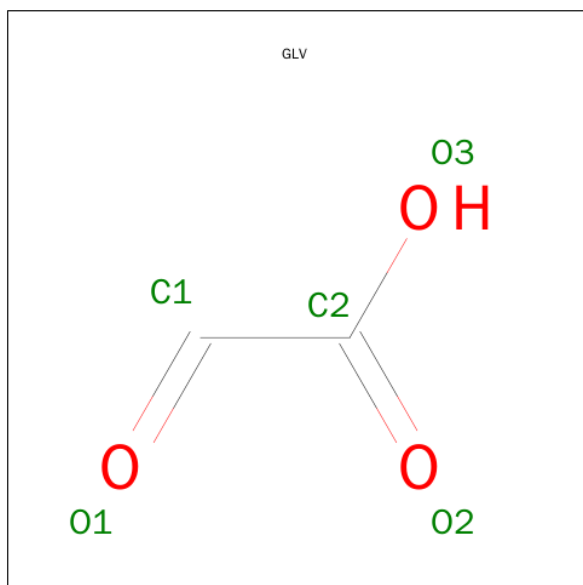
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 6 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 5 | 4 | 3 | | |
| 6 | B | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 5 | 4 | 3 | | |

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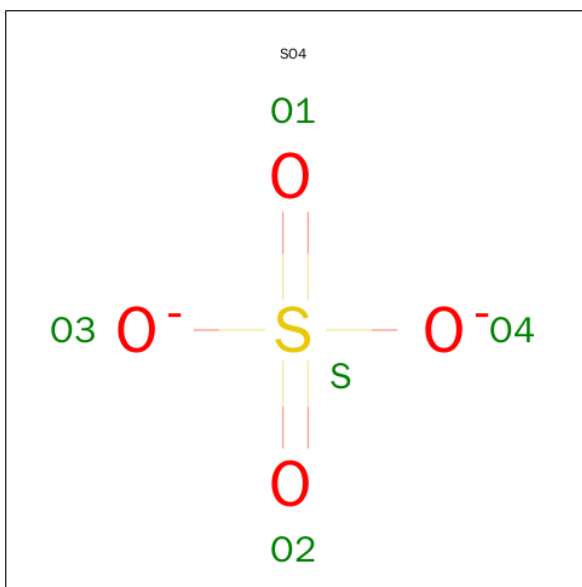
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 6 | A | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 5 | 4 | 3 | | |
| 6 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 5 | 4 | 3 | | |
| 6 | C | 1 | Total | C | N | O | 0 | 0 |
| | | | 12 | 5 | 4 | 3 | | |

- Molecule 7 is GLYOXYLIC ACID (three-letter code: GLV) (formula: $C_2H_2O_3$).



| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 7 | A | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |
| 7 | A | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |
| 7 | A | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |
| 7 | B | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |
| 7 | C | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |
| 7 | D | 1 | Total | C | O | 0 | 0 |
| | | | 5 | 2 | 3 | | |

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

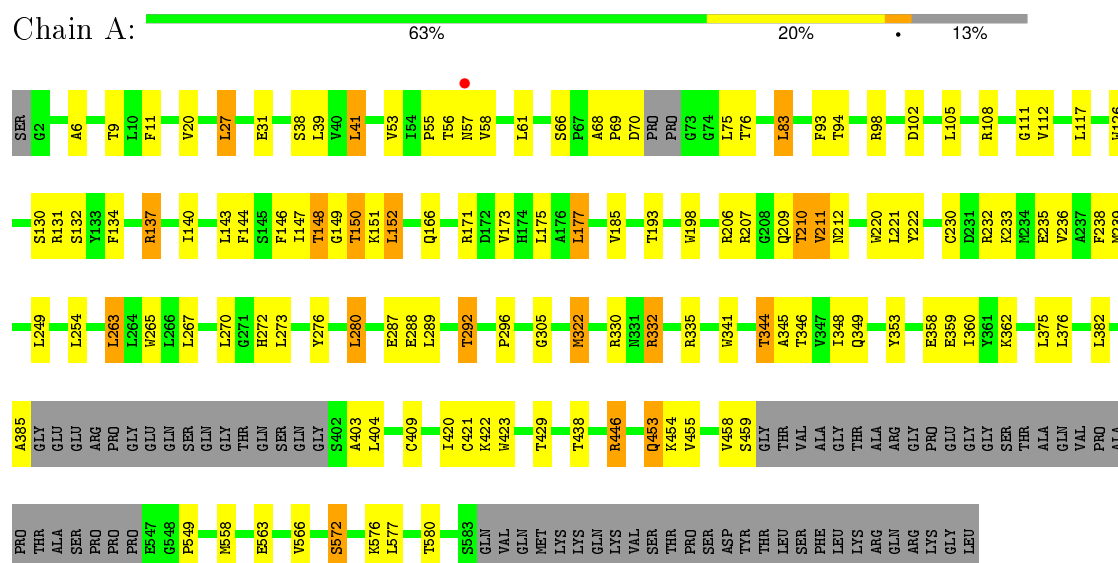


| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---------|---------|
| 8 | N | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | M | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | A | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | B | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | N | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |
| 8 | M | 1 | Total | O | S | 0 | 0 |
| | | | 5 | 4 | 1 | | |

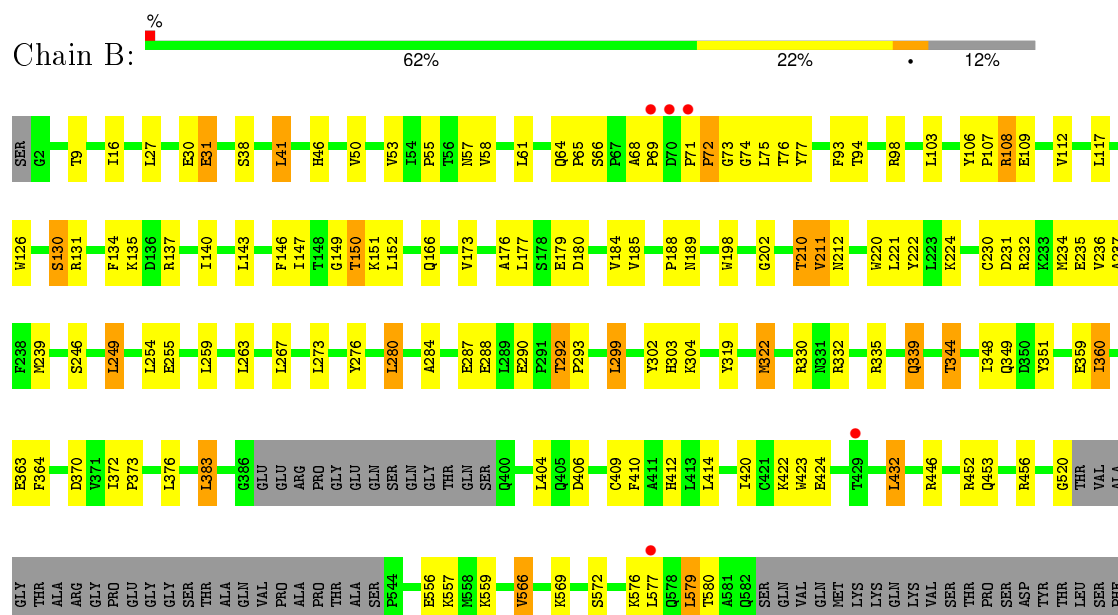
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Menin



• Molecule 1: Menin



LEU
LYS
ARG
GLN
ARG
LYS
GLY
LEU

• Molecule 2: Histone-lysine N-methyltransferase MLL

Chain M:  56% 16% 25%

SER R6 R12 P13 L27 R34 L38 P110 G111 L116 Q117 V118 I122 L126 R127 F129 R130 E135 SER GLY GLY GLY GLY SER SER GLU ASP GLU GLN PHE LEU PHE GLY SER

• Molecule 2: Histone-lysine N-methyltransferase MLL

Chain N:  3% 48% 21% 27%

SER R6 R7 R8 R12 T15 G23 R24 G26 L27 Q33 L38 L39 R107 V108 G109 P110 G111 L116 L126 R127 R128 F129 R130 A131 V132 F133 G134 SER SER GLY GLY GLY GLY GLY GLY GLY GLU ASP GLU GLN PHE LEU PHE GLY SER


• Molecule 3: Lens epithelium-derived growth factor

Chain C:  9% 56% 28% 8% 8%

SER R348 R351 R352 Q353 R354 I355 R356 I359 R360 R361 S362 L363 K364 I365 D366 R367 L368 V370 N371 R372 C373 L377 Q384 V385 T386 R392 H393 M396 L400 K401 K402 I403 R404 R405 R406 K407 V408 V411 I412 K415 L419 V429 GLY GLU GLY ASP SER

VAL

• Molecule 3: Lens epithelium-derived growth factor

Chain D:  43% 55% 19% 25%

SER MET ASP SER ARG LEU Q353 R354 I355 H356 A357 R358 I359 R360 R361 S362 L363 LYS ILE ASP ASN LEU ASP V370 N371 R372 C373 I374 A375 A376 L377 D378 E379 L380 A381 S382 L383 Q384 V385 Q388 Q389 A390 Q391 R392 H393 T394 E395 M396 I397 T398 T399 L400 K401 K402 K403 R404 ARG PHE LYS

VAL SER Q410 V411 I412 M413 E414 K415 L419 V420 G430 GLU GLY ASP SER VAL

4 Data and refinement statistics

| Property | Value | Source |
|---|---|------------------|
| Space group | P 61 2 2 | Depositor |
| Cell constants a, b, c, α , β , γ | 187.99 Å 187.99 Å 238.42 Å 90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 48.65 – 3.00 48.65 – 3.00 | Depositor EDS |
| % Data completeness (in resolution range) | 99.8 (48.65-3.00) 99.8 (48.65-3.00) | Depositor EDS |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 3.98 (at 3.01 Å) | Xtriage |
| Refinement program | PHENIX (PHENIX.REFINE: 1.7_650) | Depositor |
| R, R_{free} | 0.202 , 0.233 0.199 , 0.226 | Depositor DCC |
| R_{free} test set | 5048 reflections (11.20%) | DCC |
| Wilson B-factor (Å ²) | 75.4 | Xtriage |
| Anisotropy | 0.031 | Xtriage |
| Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²) | 0.34 , 52.6 | EDS |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$ | Xtriage |
| Outliers | 0 of 50114 reflections | Xtriage |
| F_o, F_c correlation | 0.94 | EDS |
| Total number of atoms | 9881 | wwPDB-VP |
| Average B, all atoms (Å ²) | 77.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: 0BR, CHD, SO4, GLV, GGB

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 | 0.38 | 0/3852 | 0.51 | 1/5228 (0.0%) |
| 1 | B | 0.36 | 0/3902 | 0.51 | 0/5301 |
| 2 | M | 0.36 | 0/439 | 0.60 | 0/591 |
| 2 | N | 0.39 | 0/430 | 0.64 | 1/579 (0.2%) |
| 3 | C | 0.26 | 0/679 | 0.42 | 0/905 |
| 3 | D | 0.24 | 0/546 | 0.43 | 0/725 |
| All | All | 0.36 | 0/9848 | 0.51 | 2/13329 (0.0%) |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | N | 111 | GLY | N-CA-C | -5.29 | 99.88 | 113.10 |
| 1 | A | 385 | ALA | N-CA-CB | -5.17 | 102.86 | 110.10 |

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 3767 | 0 | 3736 | 104 | 0 |
| 1 | B | 3811 | 0 | 3780 | 108 | 0 |
| 2 | M | 429 | 0 | 443 | 12 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | N | 420 | 0 | 437 | 16 | 0 |
| 3 | C | 674 | 0 | 715 | 26 | 0 |
| 3 | D | 544 | 0 | 576 | 17 | 0 |
| 4 | A | 29 | 0 | 39 | 1 | 0 |
| 4 | B | 29 | 0 | 39 | 0 | 0 |
| 5 | A | 24 | 0 | 26 | 20 | 0 |
| 5 | B | 24 | 0 | 26 | 7 | 0 |
| 6 | A | 24 | 0 | 21 | 9 | 0 |
| 6 | B | 12 | 0 | 11 | 2 | 0 |
| 6 | C | 24 | 0 | 22 | 13 | 0 |
| 7 | A | 15 | 0 | 3 | 1 | 0 |
| 7 | B | 5 | 0 | 1 | 0 | 0 |
| 7 | C | 5 | 0 | 1 | 0 | 0 |
| 7 | D | 5 | 0 | 1 | 0 | 0 |
| 8 | A | 10 | 0 | 0 | 0 | 0 |
| 8 | B | 10 | 0 | 0 | 0 | 0 |
| 8 | M | 10 | 0 | 0 | 3 | 0 |
| 8 | N | 10 | 0 | 0 | 2 | 0 |
| All | All | 9881 | 0 | 9877 | 295 | 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 15.

The worst 5 of 295 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) |
|------------------|-----------------|--------------------------|-------------------|
| 6:C:108:GGB:HCG1 | 6:C:109:GGB:OA1 | 1.44 | 1.15 |
| 5:A:612:0BR:H26 | 5:A:612:0BR:H16 | 1.30 | 1.11 |
| 5:A:612:0BR:OAA | 5:A:612:0BR:H20 | 1.55 | 1.05 |
| 6:C:109:GGB:OD | 6:C:109:GGB:N | 1.86 | 1.02 |
| 1:A:38:SER:HA | 1:A:239:MET:HE3 | 1.42 | 1.01 |

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1 | A | 469/550 (85%) | 446 (95%) | 23 (5%) | 0 | 100 | 100 |
| 1 | B | 479/550 (87%) | 449 (94%) | 29 (6%) | 1 (0%) | 52 | 88 |
| 2 | M | 54/75 (72%) | 48 (89%) | 5 (9%) | 1 (2%) | 10 | 43 |
| 2 | N | 53/75 (71%) | 50 (94%) | 3 (6%) | 0 | 100 | 100 |
| 3 | C | 80/89 (90%) | 72 (90%) | 8 (10%) | 0 | 100 | 100 |
| 3 | D | 61/89 (68%) | 57 (93%) | 4 (7%) | 0 | 100 | 100 |
| All | All | 1196/1428 (84%) | 1122 (94%) | 72 (6%) | 2 (0%) | 52 | 88 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 72 | PRO |
| 2 | M | 111 | GLY |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|-----------------|-----------|----------|-------------|----|
| 1 | A | 401/461 (87%) | 369 (92%) | 32 (8%) | 15 | 47 |
| 1 | B | 405/461 (88%) | 364 (90%) | 41 (10%) | 9 | 34 |
| 2 | M | 39/50 (78%) | 34 (87%) | 5 (13%) | 5 | 23 |
| 2 | N | 38/50 (76%) | 31 (82%) | 7 (18%) | 2 | 10 |
| 3 | C | 78/83 (94%) | 68 (87%) | 10 (13%) | 5 | 23 |
| 3 | D | 62/83 (75%) | 60 (97%) | 2 (3%) | 46 | 82 |
| All | All | 1023/1188 (86%) | 926 (90%) | 97 (10%) | 11 | 38 |

5 of 97 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 150 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 280 | LEU |
| 2 | N | 8 | ARG |
| 1 | B | 184 | VAL |
| 1 | B | 246 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 272 | HIS |
| 1 | B | 303 | HIS |
| 3 | C | 384 | GLN |
| 3 | C | 393 | HIS |
| 3 | D | 421 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

23 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | CHD | A | 611 | - | 29,32,32 | 1.97 | 10 (34%) | 48,51,51 | 2.03 | 17 (35%) |
| 5 | 0BR | A | 612 | - | 27,27,27 | 0.99 | 2 (7%) | 39,39,39 | 1.42 | 8 (20%) |
| 6 | GGB | A | 613 | - | 4,11,11 | 4.84 | 1 (25%) | 1,13,13 | 0.55 | 0 |
| 6 | GGB | A | 614 | - | 4,11,11 | 5.29 | 1 (25%) | 1,13,13 | 0.48 | 0 |
| 7 | GLV | A | 615 | - | 1,4,4 | 0.85 | 0 | 0,4,4 | 0.00 | - |
| 7 | GLV | A | 616 | - | 1,4,4 | 0.56 | 0 | 0,4,4 | 0.00 | - |
| 7 | GLV | A | 617 | - | 1,4,4 | 0.39 | 0 | 0,4,4 | 0.00 | - |
| 8 | SO4 | A | 618 | - | 4,4,4 | 0.10 | 0 | 6,6,6 | 0.19 | 0 |
| 8 | SO4 | A | 619 | - | 4,4,4 | 0.11 | 0 | 6,6,6 | 0.21 | 0 |
| 4 | CHD | B | 611 | - | 29,32,32 | 1.98 | 12 (41%) | 48,51,51 | 1.83 | 11 (22%) |
| 5 | 0BR | B | 612 | - | 27,27,27 | 0.99 | 2 (7%) | 39,39,39 | 1.42 | 8 (20%) |
| 6 | GGB | B | 615 | - | 4,11,11 | 4.87 | 1 (25%) | 1,13,13 | 0.10 | 0 |
| 7 | GLV | B | 616 | - | 1,4,4 | 0.65 | 0 | 0,4,4 | 0.00 | - |
| 8 | SO4 | B | 617 | - | 4,4,4 | 0.11 | 0 | 6,6,6 | 0.14 | 0 |
| 8 | SO4 | B | 618 | - | 4,4,4 | 0.19 | 0 | 6,6,6 | 0.22 | 0 |
| 6 | GGB | C | 108 | - | 4,11,11 | 5.14 | 1 (25%) | 1,13,13 | 0.06 | 0 |
| 6 | GGB | C | 109 | - | 4,11,11 | 5.10 | 1 (25%) | 1,13,13 | 0.08 | 0 |
| 7 | GLV | C | 113 | - | 1,4,4 | 0.44 | 0 | 0,4,4 | 0.00 | - |
| 7 | GLV | D | 114 | - | 1,4,4 | 0.41 | 0 | 0,4,4 | 0.00 | - |
| 8 | SO4 | M | 154 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.08 | 0 |
| 8 | SO4 | M | 2 | - | 4,4,4 | 0.14 | 0 | 6,6,6 | 0.13 | 0 |
| 8 | SO4 | N | 1 | - | 4,4,4 | 0.08 | 0 | 6,6,6 | 0.09 | 0 |
| 8 | SO4 | N | 154 | - | 4,4,4 | 0.23 | 0 | 6,6,6 | 0.08 | 0 |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | CHD | A | 611 | - | - | 0/7/74/74 | 0/4/4/4 |
| 5 | 0BR | A | 612 | - | - | 0/12/33/33 | 0/2/4/4 |
| 6 | GGB | A | 613 | - | - | 0/5/11/11 | 0/0/0/0 |
| 6 | GGB | A | 614 | - | - | 0/5/11/11 | 0/0/0/0 |
| 7 | GLV | A | 615 | - | - | 0/0/2/2 | 0/0/0/0 |
| 7 | GLV | A | 616 | - | - | 0/0/2/2 | 0/0/0/0 |
| 7 | GLV | A | 617 | - | - | 0/0/2/2 | 0/0/0/0 |
| 8 | SO4 | A | 618 | - | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SO4 | A | 619 | - | - | 0/0/0/0 | 0/0/0/0 |
| 4 | CHD | B | 611 | - | - | 0/7/74/74 | 0/4/4/4 |
| 5 | 0BR | B | 612 | - | - | 0/12/33/33 | 0/2/4/4 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 6 | GGB | B | 615 | - | - | 0/5/11/11 | 0/0/0/0 |
| 7 | GLV | B | 616 | - | - | 0/0/2/2 | 0/0/0/0 |
| 8 | SO4 | B | 617 | - | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SO4 | B | 618 | - | - | 0/0/0/0 | 0/0/0/0 |
| 6 | GGB | C | 108 | - | - | 0/5/11/11 | 0/0/0/0 |
| 6 | GGB | C | 109 | - | - | 1/5/11/11 | 0/0/0/0 |
| 7 | GLV | C | 113 | - | - | 0/0/2/2 | 0/0/0/0 |
| 7 | GLV | D | 114 | - | - | 0/0/2/2 | 0/0/0/0 |
| 8 | SO4 | M | 154 | - | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SO4 | M | 2 | - | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SO4 | N | 1 | - | - | 0/0/0/0 | 0/0/0/0 |
| 8 | SO4 | N | 154 | - | - | 0/0/0/0 | 0/0/0/0 |

The worst 5 of 31 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|--------|-------------|----------|
| 6 | A | 614 | GGB | OD-NE | -10.49 | 1.33 | 1.45 |
| 6 | C | 108 | GGB | OD-NE | -10.20 | 1.33 | 1.45 |
| 6 | C | 109 | GGB | OD-NE | -10.12 | 1.33 | 1.45 |
| 6 | B | 615 | GGB | OD-NE | -9.65 | 1.34 | 1.45 |
| 6 | A | 613 | GGB | OD-NE | -9.60 | 1.34 | 1.45 |

The worst 5 of 44 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | B | 611 | CHD | C18-C13-C17 | -5.58 | 102.41 | 111.22 |
| 4 | A | 611 | CHD | C18-C13-C17 | -4.75 | 103.72 | 111.22 |
| 4 | A | 611 | CHD | C19-C10-C9 | -3.64 | 105.72 | 111.18 |
| 5 | B | 612 | 0BR | CAX-OAB-CAV | -3.44 | 109.47 | 117.51 |
| 5 | A | 612 | 0BR | CAX-OAB-CAV | -3.42 | 109.52 | 117.51 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 6 | C | 109 | GGB | CG-OD-NE-CZ |

There are no ring outliers.

11 monomers are involved in 55 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 4 | A | 611 | CHD | 1 | 0 |
| 5 | A | 612 | 0BR | 20 | 0 |
| 6 | A | 613 | GGB | 6 | 0 |
| 6 | A | 614 | GGB | 3 | 0 |
| 7 | A | 615 | GLV | 1 | 0 |
| 5 | B | 612 | 0BR | 7 | 0 |
| 6 | B | 615 | GGB | 2 | 0 |
| 6 | C | 108 | GGB | 4 | 0 |
| 6 | C | 109 | GGB | 12 | 0 |
| 8 | M | 154 | SO4 | 3 | 0 |
| 8 | N | 154 | SO4 | 2 | 0 |

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | OWAB(Å ²) | Q<0.9 |
|-----|-------|-----------------|--------|---------------|-----------------------|---------|
| 1 | A | 477/550 (86%) | -0.28 | 1 (0%) 95 87 | 44, 62, 94, 139 | 0 |
| 1 | B | 485/550 (88%) | -0.33 | 5 (1%) 84 60 | 49, 67, 102, 145 | 0 |
| 2 | M | 56/75 (74%) | -0.08 | 0 100 100 | 51, 80, 109, 123 | 0 |
| 2 | N | 55/75 (73%) | -0.03 | 2 (3%) 46 20 | 53, 87, 123, 136 | 0 |
| 3 | C | 82/89 (92%) | 0.76 | 8 (9%) 10 4 | 85, 129, 154, 156 | 6 (7%) |
| 3 | D | 67/89 (75%) | 2.38 | 38 (56%) 0 0 | 99, 144, 165, 171 | 5 (7%) |
| All | All | 1222/1428 (85%) | -0.07 | 54 (4%) 38 16 | 44, 69, 143, 171 | 11 (0%) |

The worst 5 of 54 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 3 | D | 361 | ASN | 6.4 |
| 3 | D | 370 | VAL | 5.8 |
| 3 | D | 363 | LEU | 5.7 |
| 3 | D | 396 | MET | 5.2 |
| 3 | D | 373 | CYS | 5.1 |

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors(Å ²) | Q<0.9 |
|-----|------|-------|-----|-------|------|------|-------|----------------------------|-------|
| 5 | 0BR | A | 612 | 24/24 | 0.91 | 0.31 | 4.17 | 54,61,67,70 | 7 |
| 7 | GLV | A | 616 | 5/5 | 0.82 | 0.34 | 3.78 | 61,74,76,88 | 2 |
| 5 | 0BR | B | 612 | 24/24 | 0.91 | 0.28 | 3.77 | 53,61,67,72 | 0 |
| 7 | GLV | B | 616 | 5/5 | 0.85 | 0.28 | 1.81 | 64,65,76,78 | 1 |
| 7 | GLV | A | 615 | 5/5 | 0.90 | 0.26 | 1.58 | 57,64,71,76 | 1 |
| 4 | CHD | A | 611 | 29/29 | 0.94 | 0.28 | 1.17 | 55,64,72,74 | 5 |
| 4 | CHD | B | 611 | 29/29 | 0.95 | 0.26 | 1.06 | 52,62,75,77 | 6 |
| 6 | GGB | A | 614 | 12/12 | 0.88 | 0.24 | 0.58 | 78,93,108,108 | 5 |
| 8 | SO4 | B | 617 | 5/5 | 0.88 | 0.18 | -0.05 | 114,115,124,136 | 0 |
| 7 | GLV | D | 114 | 5/5 | 0.80 | 0.32 | -0.36 | 109,110,110,111 | 0 |
| 7 | GLV | A | 617 | 5/5 | 0.94 | 0.17 | -0.64 | 72,73,85,88 | 1 |
| 6 | GGB | C | 109 | 12/12 | 0.69 | 0.40 | -0.75 | 115,126,131,132 | 0 |
| 8 | SO4 | N | 154 | 5/5 | 0.87 | 0.17 | -0.87 | 119,120,135,137 | 0 |
| 7 | GLV | C | 113 | 5/5 | 0.87 | 0.16 | -1.06 | 88,94,100,101 | 0 |
| 8 | SO4 | N | 1 | 5/5 | 0.95 | 0.11 | -1.73 | 89,95,105,115 | 0 |
| 8 | SO4 | M | 2 | 5/5 | 0.96 | 0.14 | -1.86 | 87,88,103,105 | 0 |
| 8 | SO4 | M | 154 | 5/5 | 0.93 | 0.12 | -1.90 | 107,122,128,136 | 0 |
| 8 | SO4 | A | 618 | 5/5 | 0.94 | 0.14 | -3.17 | 84,100,102,114 | 0 |
| 6 | GGB | A | 613 | 12/12 | 0.87 | 0.29 | - | 67,87,98,100 | 4 |
| 6 | GGB | B | 615 | 12/12 | 0.86 | 0.32 | - | 76,84,106,107 | 6 |
| 8 | SO4 | B | 618 | 5/5 | 0.93 | 0.11 | - | 93,95,98,114 | 0 |
| 6 | GGB | C | 108 | 12/12 | 0.87 | 0.33 | - | 113,120,132,133 | 0 |
| 8 | SO4 | A | 619 | 5/5 | 0.94 | 0.13 | - | 80,88,103,113 | 0 |

6.5 Other polymers ⓘ

There are no such residues in this entry.