# WORLDWIDE PDB

## PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 3, 2017 – 11:36 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 4EZH |
| Title | : | the crystal structure of KDM6B bound with H3K27me3 peptide |
| Authors | : | Cheng, Z.J.; Patel, D.J. |
| Deposited on | : | unknown |
| Resolution | : | 2.52 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.

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

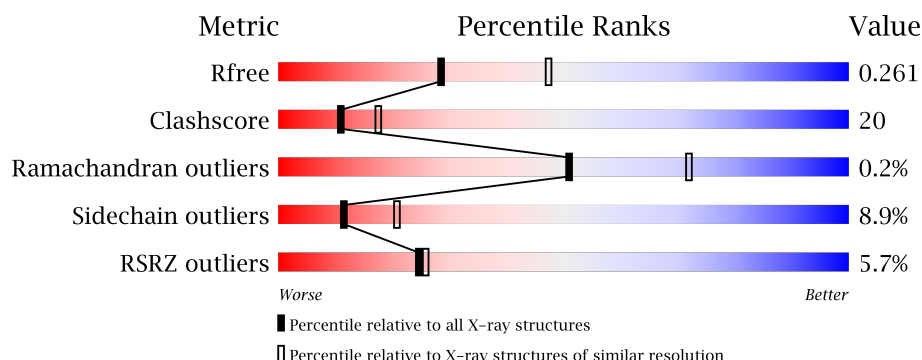| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.7.2 (RC1), CSD as538be (2017) |
| Xtriage (Phenix) | : | 1.9-1692 |
| EDS | : | rb-20029824 |
| Percentile statistics | : | 20161228.v01 (using entries in the PDB archive December 28th 2016) |
| Refmac | : | 5.8.0135 |
| CCP4 | : | 6.5.0 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | rb-20029824 |

# 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 2.52 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 | Percentile Ranks | Value |
|---|---|---|
| Rfree | | 0.261 |
| Clashscore | | 20 |
| Ramachandran outliers | | 0.2% |
| Sidechain outliers | | 8.9% |
| RSRZ outliers | | 5.7% |

Worse          Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

| Metric | Whole archive (#Entries) | Similar resolution (#Entries, resolution range(Å)) |
|---|---|---|
| R$_{free}$ | 100719 | 4636 (2.54-2.50) |
| Clashscore | 112137 | 5382 (2.54-2.50) |
| Ramachandran outliers | 110173 | 5282 (2.54-2.50) |
| Sidechain outliers | 110143 | 5284 (2.54-2.50) |
| RSRZ outliers | 101464 | 4669 (2.54-2.50) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 486 | 6% / 59% 30% 5% 6% |
| 1 | B | 486 | 4% / 58% 31% • 7% |
| 2 | C | 11 | 18% / 55% 36% 9% |
| 2 | D | 11 | 64% 27% 9% |

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 crite-

ria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|------|-----------|----------|---------|------------------|
| 5 | OGA | B | 1703 | - | - | - | X |

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7543 atoms, of which 8 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 Lysine-specific demethylase 6B.

| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---|---|---------|---------|-------|
| 1 | A | 455 | Total<br>3668 | C<br>2331 | H<br>8 | N<br>635 | O<br>675 | S<br>19 | 0 | 0 | 0 |
| 1 | B | 451 | Total<br>3627 | C<br>2313 | | N<br>629 | O<br>666 | S<br>19 | 0 | 0 | 0 |

There are 52 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 1296 | LEU | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1297 | GLU | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1298 | VAL | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1299 | LEU | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1300 | PHE | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1301 | GLN | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1303 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1304 | PRO | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1305 | THR | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1306 | LYS | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1307 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1308 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1309 | ARG | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1310 | LYS | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1311 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1312 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1313 | PRO | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1314 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1315 | THR | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1316 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1317 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1318 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1319 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1320 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| A | 1321 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------|-----------|
| A | 1322 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1296 | LEU | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1297 | GLU | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1298 | VAL | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1299 | LEU | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1300 | PHE | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1302 | GLN | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1303 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1304 | PRO | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1305 | THR | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1306 | LYS | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1307 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1308 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1309 | ARG | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1310 | LYS | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1311 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1312 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1313 | PRO | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1314 | ALA | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1315 | THR | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1316 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1317 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1318 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1319 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1320 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1321 | GLY | - | SEE REMARK 999 | UNP Q5NCY0 |
| B | 1322 | SER | - | SEE REMARK 999 | UNP Q5NCY0 |

- Molecule 2 is a protein called SYNTHESIZED methylation peptide.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|---|---|---|---------|---------|-------|
| 2 | C | 11 | Total | C | N | O | 0 | 0 | 0 |
| | | | 71 | 43 | 15 | 13 | | | |
| 2 | D | 11 | Total | C | N | O | 0 | 0 | 0 |
| | | | 71 | 43 | 15 | 13 | | | |

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | B | 1 | Total | Ni | 0 | 0 |
| | | | 1 | 1 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 3 | A | 1 | Total Ni<br>1　　1 | | 0 | 0 |

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 4 | B | 1 | Total Zn<br>1　　1 | | 0 | 0 |
| 4 | A | 1 | Total Zn<br>1　　1 | | 0 | 0 |

- Molecule 5 is N-OXALYLGLYCINE (three-letter code: OGA) (formula: $C_4H_5NO_5$).



OGA
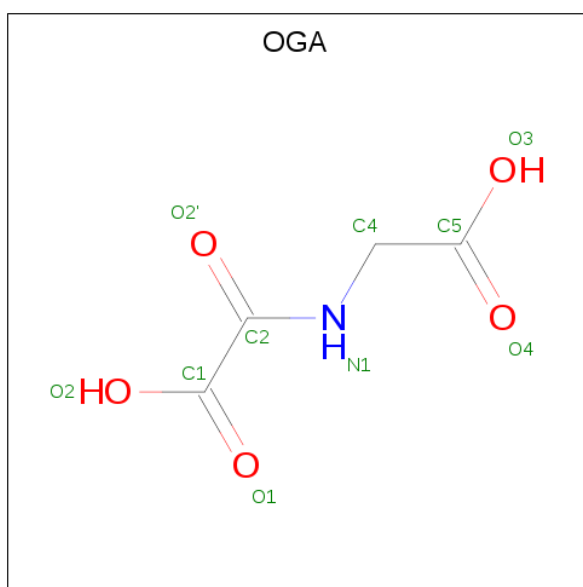
| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
| 5 | A | 1 | Total　C　N　O<br>10　　4　1　5 | | | | 0 | 0 |
| 5 | B | 1 | Total　C　N　O<br>10　　4　1　5 | | | | 0 | 0 |

- Molecule 6 is water.

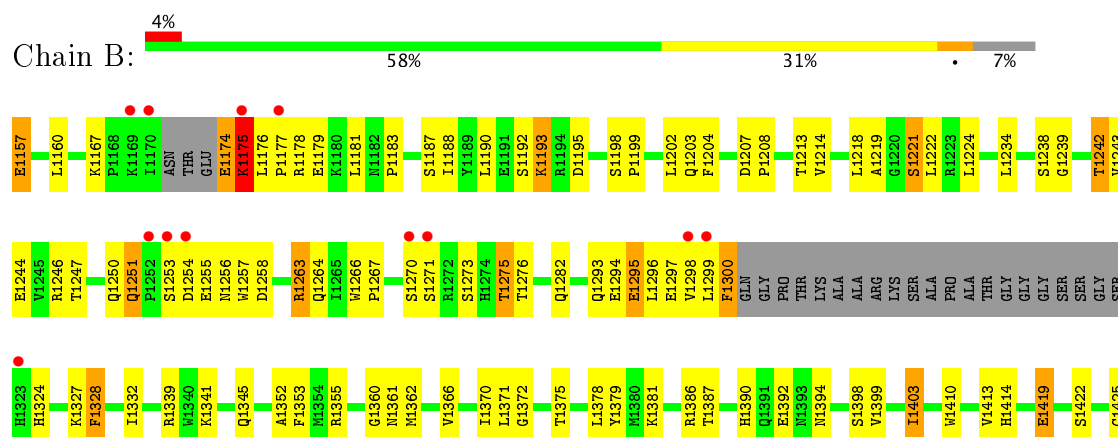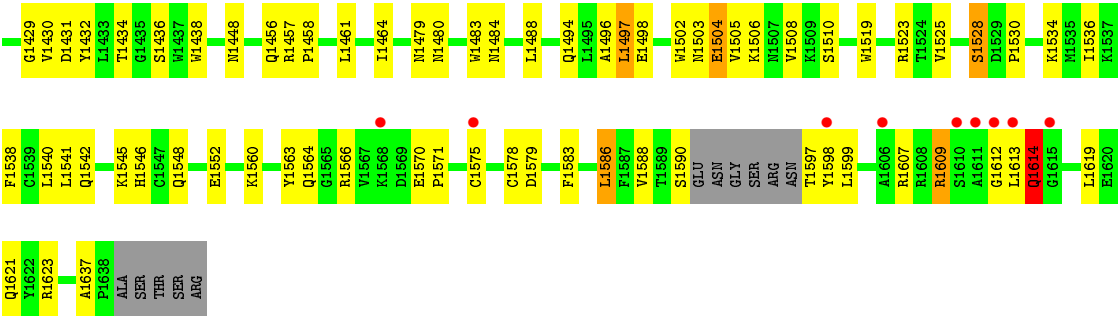| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---------|---------|
| 6 | A | 43 | Total　O<br>43　　43 | | 0 | 0 |
| 6 | B | 39 | Total　O<br>39　　39 | | 0 | 0 |

# 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
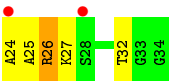
• Molecule 1: Lysine-specific demethylase 6B



• Molecule 1: Lysine-specific demethylase 6B

G1429 V1430 D1431 Y1432 L1433 T1434 G1435 S1436 W1437 W1438 N1448 Q1456 R1457 P1458 L1461 I1464 N1479 N1480 W1483 N1484 L1488 Q1494 L1495 A1496 L1497 E1498 W1502 N1503 E1504 V1505 K1506 M1507 V1508 K1509 S1510 W1519 R1523 T1524 V1525 S1528 D1529 P1530 K1534 M1535 I1536 K1537

F1538 C1539 L1540 L1541 Q1542 K1545 H1546 C1547 Q1548 E1552 K1560 Y1563 Q1564 G1565 R1566 V1567 K1568 D1569 E1570 P1571 C1575 C1578 D1579 F1583 L1586 F1587 V1588 T1589 S1590 GLU ASN GLY SER ARG ASN T1597 Y1598 L1599 A1606 R1607 R1608 R1609 S1610 A1611 G1612 L1613 Q1614 G1615 L1619 E1620

Q1621 Y1622 R1623 A1637 P1638 ALA SER THR SER ARG

• Molecule 2: SYNTHESIZED methylation peptide

Chain C:

18%

55% 36% 9%

A24 A25 R26 K27 S28 T32 G33 G34

• Molecule 2: SYNTHESIZED methylation peptide

Chain D:

64% 27% 9%

A24 A25 R26 K27 T32 G33 G34

# 4   Data and refinement statistics (i)

| Property | Value | Source |
|----------|-------|--------|
| Space group | P 21 21 21 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 83.68Å    102.41Å    143.20Å<br>90.00°     90.00°      90.00° | Depositor |
| Resolution (Å) | 40.00   –    2.52<br>40.16   –    2.52 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.7 (40.00-2.52)<br>87.6 (40.16-2.52) | Depositor<br>EDS |
| $R_{merge}$ | 0.11 | Depositor |
| $R_{sym}$ | 0.07 | Depositor |
| $< I/\sigma(I) >$ [1] | 2.99 (at 2.51Å) | Xtriage |
| Refinement program | PHENIX (phenix.refine: 1.7.1_743) | Depositor |
| R, $R_{free}$ | 0.213    ,    0.254<br>0.215    ,    0.261 | Depositor<br>DCC |
| $R_{free}$ test set | 1872 reflections (5.07%) | DCC |
| Wilson B-factor (Å$^2$) | 46.0 | Xtriage |
| Anisotropy | 0.724 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.30 , 43.4 | EDS |
| L-test for twinning[2] | $< |L| > = 0.54, < L^2 > = 0.38$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o,F_c$ correlation | 0.95 | EDS |
| Total number of atoms | 7543 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 58.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.27 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.6257e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: NI, ZN, M3L, OGA

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 | 0.63 | 4/3755 (0.1%) | 0.64 | 1/5110 (0.0%) |
| 1 | B | 0.63 | 0/3721 | 0.63 | 1/5062 (0.0%) |
| 2 | C | 1.47 | 0/59 | 1.18 | 0/79 |
| 2 | D | 0.38 | 0/59 | 0.68 | 0/79 |
| All | All | 0.64 | 4/7594 (0.1%) | 0.64 | 2/10330 (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 sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | B | 0 | 1 |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 1 | A | 1411 | PHE | CE1-CZ | -5.76 | 1.26 | 1.37 |
| 1 | A | 1411 | PHE | CG-CD1 | -5.67 | 1.30 | 1.38 |
| 1 | A | 1411 | PHE | CE2-CZ | -5.65 | 1.26 | 1.37 |
| 1 | A | 1411 | PHE | CG-CD2 | -5.40 | 1.30 | 1.38 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 1 | A | 1614 | GLN | CA-CB-CG | 5.37 | 125.21 | 113.40 |
| 1 | B | 1614 | GLN | CA-CB-CG | 5.03 | 124.47 | 113.40 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|------|------|---------|
| 1 | B | 1174 | GLU | Peptide |

## 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 | 3660 | 8 | 3580 | 144 | 1 |
| 1 | B | 3627 | 0 | 3551 | 151 | 0 |
| 2 | C | 71 | 0 | 75 | 6 | 0 |
| 2 | D | 71 | 0 | 75 | 12 | 0 |
| 3 | A | 1 | 0 | 0 | 0 | 0 |
| 3 | B | 1 | 0 | 0 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | B | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 10 | 0 | 3 | 0 | 0 |
| 5 | B | 10 | 0 | 3 | 0 | 0 |
| 6 | A | 43 | 0 | 0 | 4 | 0 |
| 6 | B | 39 | 0 | 0 | 2 | 0 |
| All | All | 7535 | 8 | 7287 | 297 | 1 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 297 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) |
|--------|--------|--------------------------|-------------------|
| 1:B:1251:GLN:NE2 | 1:B:1256:ASN:HA | 1.32 | 1.43 |
| 1:B:1403:ILE:HG23 | 1:B:1479:ASN:O | 1.48 | 1.13 |
| 1:B:1157:GLU:HA | 1:B:1157:GLU:OE1 | 1.48 | 1.09 |
| 1:A:1160:LEU:HD11 | 1:A:1497:LEU:HB3 | 1.35 | 1.08 |
| 1:B:1597:THR:HG22 | 1:B:1598:TYR:H | 1.16 | 1.07 |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1169:LYS:O | 1:A:1339:ARG:NH2[3_544] | 2.04 | 0.16 |

## 5.3  Torsion angles (i)

### 5.3.1  Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 449/486 (92%) | 425 (95%) | 23 (5%) | 1 (0%) | 51 | 72 |
| 1 | B | 443/486 (91%) | 424 (96%) | 18 (4%) | 1 (0%) | 51 | 72 |
| 2 | C | 8/11 (73%) | 7 (88%) | 1 (12%) | 0 | 100 | 100 |
| 2 | D | 8/11 (73%) | 6 (75%) | 2 (25%) | 0 | 100 | 100 |
| All | All | 908/994 (91%) | 862 (95%) | 44 (5%) | 2 (0%) | 51 | 72 |

All (2) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 1175 | LYS |
| 1 | A | 1227 | GLY |

### 5.3.2  Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 404/424 (95%) | 371 (92%) | 33 (8%) | 13 | 24 |
| 1 | B | 400/424 (94%) | 364 (91%) | 36 (9%) | 11 | 20 |
| 2 | C | 4/4 (100%) | 2 (50%) | 2 (50%) | 0 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------|-----------|----------|-----|-----|
| 2 | D | 4/4 (100%) | 3 (75%) | 1 (25%) | 1 | 1 |
| All | All | 812/856 (95%) | 740 (91%) | 72 (9%) | 11 | 21 |

5 of 72 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | A | 1614 | GLN |
| 1 | B | 1221 | SER |
| 1 | B | 1586 | LEU |
| 1 | B | 1157 | GLU |
| 1 | B | 1187 | SER |

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | B | 1251 | GLN |
| 1 | B | 1264 | GLN |
| 1 | B | 1473 | GLN |
| 1 | A | 1621 | GLN |
| 1 | B | 1393 | 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)

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

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|---------|--------|------|---------|
| | | | | | Counts | RMSZ | #$|Z| > 2$ | Counts | RMSZ | #$|Z| > 2$ |
| 2 | M3L | C | 27 | 2 | 11,11,12 | 1.66 | 3 (27%) | 11,14,16 | 0.60 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|--------|--------|------|--------|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 2 | M3L | D | 27 | 2 | 11,11,12 | 0.83 | 0 | 11,14,16 | 0.90 | 1 (9%) |

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 |
|-----|------|-------|-----|------|---------|----------|-------|
| 2 | M3L | C | 27 | 2 | - | 0/8/10/12 | 0/0/0/0 |
| 2 | M3L | D | 27 | 2 | - | 0/8/10/12 | 0/0/0/0 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 2 | C | 27 | M3L | CM2-NZ | -3.09 | 1.41 | 1.50 |
| 2 | C | 27 | M3L | CB-CA | -2.64 | 1.50 | 1.53 |
| 2 | C | 27 | M3L | CE-NZ | -2.42 | 1.43 | 1.51 |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------|-----|-------------|----------|
| 2 | D | 27 | M3L | O-C-CA | -2.71 | 117.54 | 125.02 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 2 | C | 27 | M3L | 3 | 0 |
| 2 | D | 27 | M3L | 6 | 0 |

## 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------|------|-----------|--------|------|-----------|
| | | | | | Counts | RMSZ | $\#|Z| > 2$ | Counts | RMSZ | $\#|Z| > 2$ |
| 5 | OGA | A | 1703 | 3 | 3,9,9 | 0.42 | 0 | 3,11,11 | 0.45 | 0 |
| 5 | OGA | B | 1703 | 3 | 3,9,9 | 0.62 | 0 | 3,11,11 | 2.56 | 1 (33%) |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|----------|-------|
| 5 | OGA | A | 1703 | 3 | - | 0/3/9/9 | 0/0/0/0 |
| 5 | OGA | B | 1703 | 3 | - | 0/3/9/9 | 0/0/0/0 |

There are no bond length outliers.

All (1) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5 | B | 1703 | OGA | C1-C2-N1 | -4.33 | 111.95 | 115.80 |

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  ⓘ

There are no such residues in this entry.

## 5.8  Polymer linkage issues  ⓘ

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, $95^{th}$ percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

| Mol | Chain | Analysed | <RSRZ> | #RSRZ>2 | | | OWAB($\text{Å}^2$) | Q<0.9 |
|-----|-------|----------|--------|---------|------|------|-------------------|-------|
| 1 | A | 455/486 (93%) | 0.31 | 30 (6%) | 19 | 20 | 24, 53, 94, 122 | 0 |
| 1 | B | 451/486 (92%) | 0.24 | 21 (4%) | 32 | 34 | 36, 54, 92, 119 | 0 |
| 2 | C | 10/11 (90%) | 0.75 | 2 (20%) | 1 | 1 | 58, 81, 109, 109 | 0 |
| 2 | D | 10/11 (90%) | 1.01 | 0 | 100 | 100 | 53, 76, 115, 118 | 0 |
| All | All | 926/994 (93%) | 0.29 | 53 (5%) | 24 | 26 | 24, 54, 95, 122 | 0 |

The worst 5 of 53 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1 | B | 1298 | VAL | 7.1 |
| 1 | B | 1299 | LEU | 6.8 |
| 1 | A | 1299 | LEU | 6.8 |
| 1 | A | 1174 | GLU | 5.6 |
| 1 | B | 1253 | SER | 4.8 |

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

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors($\text{Å}^2$) | Q<0.9 |
|-----|------|-------|-----|-------|------|-----|------|------------------------|-------|
| 2 | M3L | D | 27 | 12/13 | 0.83 | 0.30 | - | 48,66,75,78 | 0 |
| 2 | M3L | C | 27 | 12/13 | 0.89 | 0.27 | - | 44,62,69,72 | 0 |

## 6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.4 Ligands (i)

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

| Mol | Type | Chain | Res | Atoms | RSCC | RSR | LLDF | B-factors($Å^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|---|
| 5 | OGA | B | 1703 | 10/10 | 0.88 | 0.25 | 3.20 | 20,20,20,20 | 0 |
| 5 | OGA | A | 1703 | 10/10 | 0.90 | 0.21 | 0.57 | 20,20,20,20 | 0 |
| 4 | ZN | B | 1702 | 1/1 | 0.96 | 0.14 | -0.78 | 57,57,57,57 | 0 |
| 4 | ZN | A | 1702 | 1/1 | 0.97 | 0.09 | -2.70 | 56,56,56,56 | 0 |
| 3 | NI | A | 1701 | 1/1 | 0.95 | 0.20 | - | 34,34,34,34 | 0 |
| 3 | NI | B | 1701 | 1/1 | 0.94 | 0.20 | - | 40,40,40,40 | 0 |

## 6.5 Other polymers (i)

There are no such residues in this entry.