# wwPDB X-ray Structure Validation Summary Report (i)

Jun 1, 2021 – 08:08 PM JST

| | | |
|---|---|---|
| PDB ID | : | 6LE0 |
| Title | : | A nonspecific heme-binding cyclase catalyzes [4 + 2] cycloaddition during neoabyssomicin biosynthesis |
| Authors | : | Ju, J.J. |
| Deposited on | : | 2019-11-23 |
| Resolution | : | 2.51 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

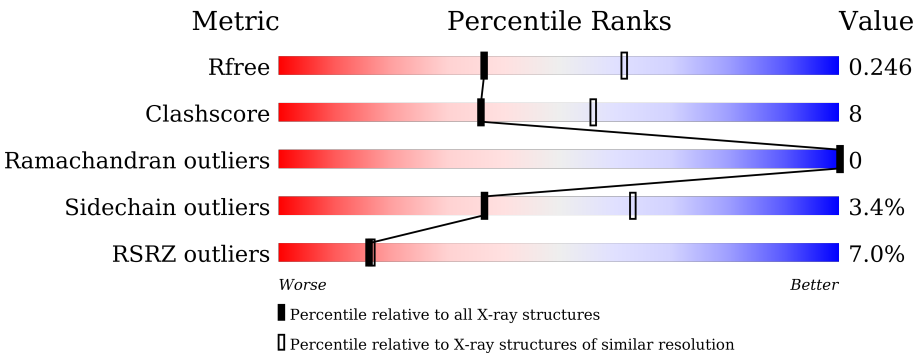
| | | |
|---|---|---|
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.19 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.19 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 4661 (2.50-2.50) |
| Clashscore | 141614 | 5346 (2.50-2.50) |
| Ramachandran outliers | 138981 | 5231 (2.50-2.50) |
| Sidechain outliers | 138945 | 5233 (2.50-2.50) |
| RSRZ outliers | 127900 | 4559 (2.50-2.50) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 219 | 5% 79% 16% • 5% |
| 1 | B | 219 | .% 75% 16% • 8% |
| 1 | C | 219 | 11% 70% 23% 6% |
| 1 | D | 219 | 8% 72% 18% • 9% |

# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6419 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 AbmU.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | Se | | | |
| 1 | A | 209 | 1602 | 1013 | 279 | 305 | 5 | 0 | 0 | 0 |
| 1 | B | 201 | 1540 | 976 | 267 | 292 | 5 | 0 | 0 | 0 |
| 1 | C | 206 | 1572 | 998 | 273 | 296 | 5 | 0 | 0 | 0 |
| 1 | D | 200 | 1531 | 971 | 266 | 289 | 5 | 0 | 0 | 0 |

There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 2 | MSE | - | initiating methionine | UNP A0A2P1BT29 |
| B | 2 | MSE | - | initiating methionine | UNP A0A2P1BT29 |
| C | 2 | MSE | - | initiating methionine | UNP A0A2P1BT29 |
| D | 2 | MSE | - | initiating methionine | UNP A0A2P1BT29 |

- Molecule 2 is water.

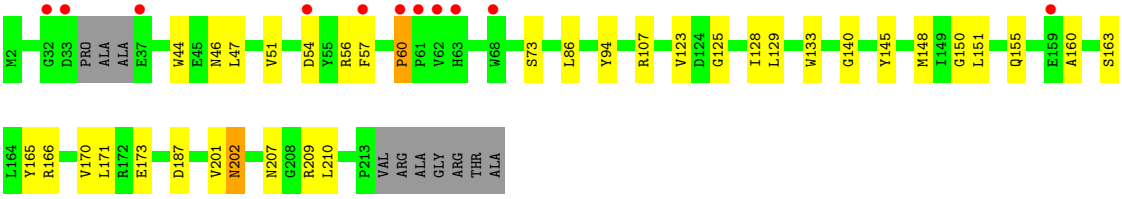
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 2 | A | 81 | 81 | 81 | 0 | 0 |
| 2 | B | 66 | 66 | 66 | 0 | 0 |
| 2 | C | 16 | 16 | 16 | 0 | 0 |
| 2 | D | 11 | 11 | 11 | 0 | 0 |

# 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 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.

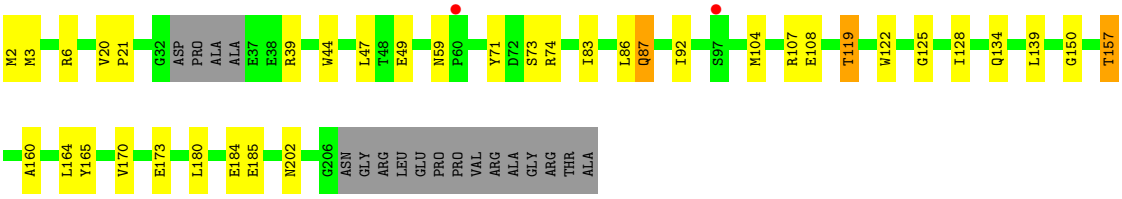
• Molecule 1: AbmU

Chain A:



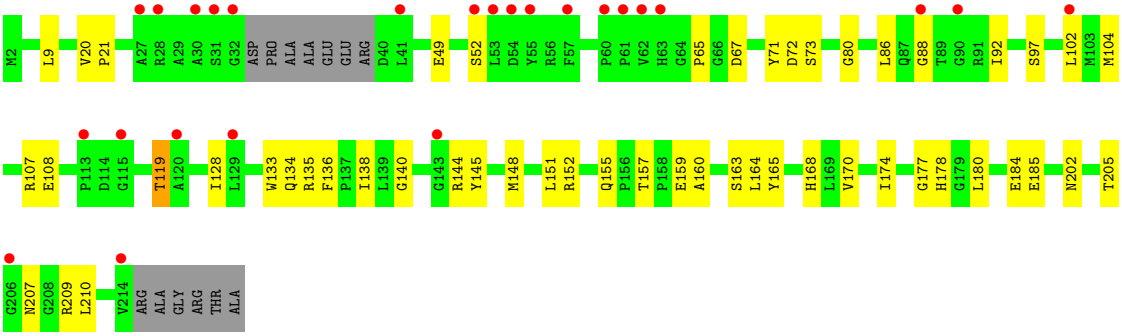

• Molecule 1: AbmU

Chain B:



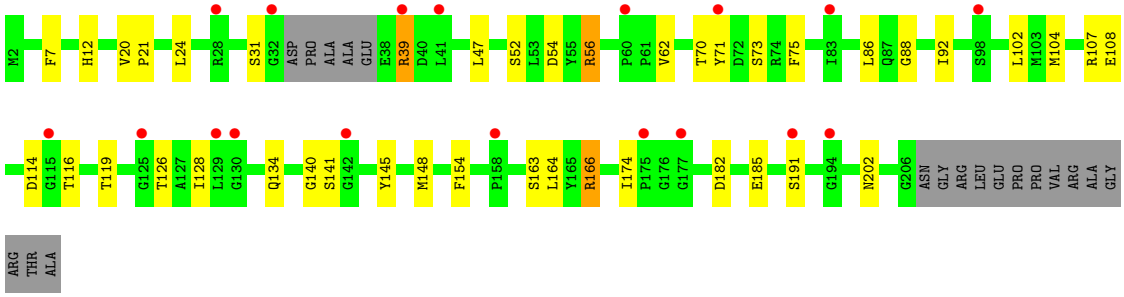

• Molecule 1: AbmU

Chain C:




• Molecule 1: AbmU

Chain D:


M2
F7
H12
V20
P21
L24
R28
S31
G32
ASP
PRO
ALA
ALA
GLU
E33
R39
D40
L41
L47
S52
L53
D54
Y55
R56
P60
P61
V62
T70
Y71
D72
S73
R74
F75
I83
L86
Q87
G88
I92
S98
L102
M103
M104
R107
E108
D114
G115
T116
T119
G125
T126
A127
I128
L129
G130
Q134
G140
S141
G142
Y145
M148
F154
P158
S163
L164
Y165
R166
I174
P175
G176
G177
D182
E185
S191
G194
N202
G206
ASN
GLY
ARG
LEU
GLU
PRO
PRO
VAL
ARG
ALA
GLY
ARG
THR
ALA

# 4 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 66.61Å 65.35Å 101.40Å<br>90.00° 90.19° 90.00° | Depositor |
| Resolution (Å) | 27.88 – 2.51<br>34.37 – 2.51 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 98.3 (27.88-2.51)<br>98.3 (34.37-2.51) | Depositor<br>EDS |
| $R_{merge}$ | 0.08 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.75 (at 2.51Å) | Xtriage |
| Refinement program | PHENIX 1.13_2998 | Depositor |
| R, $R_{free}$ | 0.200 , 0.245<br>0.200 , 0.246 | Depositor<br>DCC |
| $R_{free}$ test set | 1458 reflections (4.94%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 41.7 | Xtriage |
| Anisotropy | 0.385 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 52.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.34$ | Xtriage |
| Estimated twinning fraction | 0.000 for k,h,-l<br>0.006 for -k,-h,-l<br>0.029 for h,-k,-l | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 6419 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 50.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[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)

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 | 0.59 | 1/1644 (0.1%) | 0.79 | 0/2237 |
| 1 | B | 0.54 | 0/1580 | 0.74 | 0/2149 |
| 1 | C | 0.45 | 0/1614 | 0.72 | 0/2198 |
| 1 | D | 0.44 | 0/1571 | 0.72 | 2/2137 (0.1%) |
| All | All | 0.51 | 1/6409 (0.0%) | 0.74 | 2/8721 (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 (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 1 | A | 123 | VAL | CB-CG2 | -5.04 | 1.42 | 1.52 |

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | D | 166 | ARG | CG-CD-NE | -8.37 | 94.23 | 111.80 |
| 1 | D | 166 | ARG | NE-CZ-NH2 | -5.69 | 117.45 | 120.30 |

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | B | 59 | ASN | 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 | 1602 | 0 | 1524 | 21 | 0 |
| 1 | B | 1540 | 0 | 1467 | 21 | 0 |
| 1 | C | 1572 | 0 | 1504 | 36 | 0 |
| 1 | D | 1531 | 0 | 1461 | 29 | 0 |
| 2 | A | 81 | 0 | 0 | 0 | 0 |
| 2 | B | 66 | 0 | 0 | 2 | 0 |
| 2 | C | 16 | 0 | 0 | 2 | 0 |
| 2 | D | 11 | 0 | 0 | 0 | 0 |
| All | All | 6419 | 0 | 5956 | 97 | 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 8.

The worst 5 of 97 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:C:86:LEU:HD21 | 1:C:108:GLU:HB3 | 1.55 | 0.87 |
| 1:D:128:ILE:HD11 | 1:D:134:GLN:HG2 | 1.65 | 0.77 |
| 1:D:108:GLU:HB2 | 1:D:119:THR:HG22 | 1.69 | 0.75 |
| 1:D:182:ASP:HB3 | 1:D:185:GLU:HG2 | 1.70 | 0.73 |
| 1:C:128:ILE:HD11 | 1:C:134:GLN:HG3 | 1.70 | 0.72 |

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 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 | 205/219 (94%) | 200 (98%) | 5 (2%) | 0 | 100 | 100 |
| 1 | B | 197/219 (90%) | 194 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | C | 202/219 (92%) | 199 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | D | 196/219 (90%) | 193 (98%) | 3 (2%) | 0 | 100 | 100 |
| All | All | 800/876 (91%) | 786 (98%) | 14 (2%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 165/165 (100%) | 162 (98%) | 3 (2%) | 59 | 81 |
| 1 | B | 158/165 (96%) | 151 (96%) | 7 (4%) | 28 | 52 |
| 1 | C | 162/165 (98%) | 158 (98%) | 4 (2%) | 47 | 73 |
| 1 | D | 157/165 (95%) | 149 (95%) | 8 (5%) | 24 | 45 |
| All | All | 642/660 (97%) | 620 (97%) | 22 (3%) | 37 | 63 |

5 of 22 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | D | 31 | SER |
| 1 | D | 56 | ARG |
| 1 | D | 52 | SER |
| 1 | D | 62 | VAL |
| 1 | B | 139 | LEU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | B | 87 | GLN |
| 1 | D | 59 | 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 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)

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(Å$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 204/219 (93%) | 0.20 | 11 (5%) 25 27 | 17, 31, 65, 97 | 0 |
| 1 | B | 196/219 (89%) | 0.05 | 2 (1%) 82 84 | 18, 35, 61, 89 | 0 |
| 1 | C | 201/219 (91%) | 0.95 | 25 (12%) 4 3 | 34, 65, 92, 110 | 0 |
| 1 | D | 195/219 (89%) | 0.81 | 18 (9%) 9 9 | 33, 63, 92, 118 | 0 |
| All | All | 796/876 (90%) | 0.50 | 56 (7%) 16 16 | 17, 47, 88, 118 | 0 |

The worst 5 of 56 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | D | 129 | LEU | 8.5 |
| 1 | C | 55 | TYR | 6.0 |
| 1 | D | 142 | GLY | 5.6 |
| 1 | C | 54 | ASP | 4.6 |
| 1 | C | 61 | PRO | 4.5 |

## 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 monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.