



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 07:43 am BST

PDB ID : 1ION  
Title : THE SEPTUM SITE-DETERMINING PROTEIN MIND COMPLEXED  
WITH MG-ADP FROM PYROCOCCUS HORIKOSHII OT3  
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Deposited on : 2001-03-21  
Resolution : 2.30 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](mailto: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 ⓘ 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

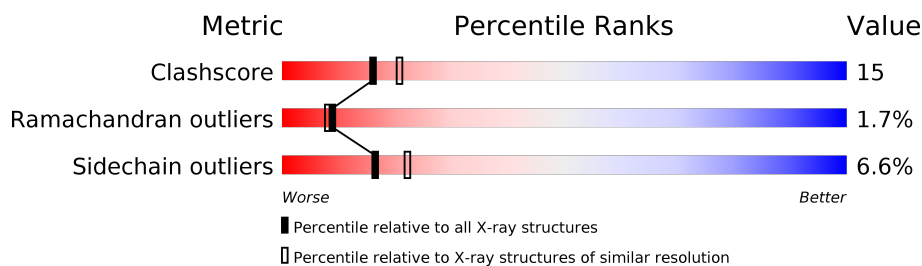
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1887 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 PROBABLE CELL DIVISION INHIBITOR MIND.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	Se	0	0	0
			1824	1165	301	347	2	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	30	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	43	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	75	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	128	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	131	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	152	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	156	MSE	MET	MODIFIED RESIDUE	UNP O58346
A	189	MSE	MET	MODIFIED RESIDUE	UNP O58346

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	35	Total O 35 35	0	0



Note EDS was not executed.

Chain A:

Category	Percentage
Green	75%
Yellow	19%
Orange	6%

Chain A contains 36 items. The items are categorized as follows:

Item	Category
M1	Green
T2	Green
R3	Yellow
G15	Yellow
S24	Yellow
L27	Yellow
M30	Green
G31	Green
R32	Yellow
L46	Orange
L50	Orange
M56	Yellow
L59	Orange
L63	Yellow
L84	Yellow
P85	Yellow
E91	Yellow
K95	Yellow
L101	Orange
P102	Orange
L105	Yellow
L108	Orange
R109	Green
G110	Green
K111	Green
Y112	Green
L116	Yellow
I117	Yellow
R126	Yellow
A127	Yellow
M128	Yellow
M131	Yellow
L132	Green
S133	Yellow
E136	Yellow

Chain A also contains 24 items in the second row:

Item	Category
M156	Yellow
L166	Green
G167	Green
F168	Yellow
R172	Yellow
E177	Yellow
R178	Orange
L193	Orange
I197	Yellow
P198	Yellow
E199	Orange
R204	Yellow
L208	Yellow
K215	Yellow
K221	Yellow
F226	Yellow
E232	Yellow
V233	Green
D234	Yellow
K235	Yellow
L236	Yellow
A237	Yellow
G238	Yellow
I239	Yellow
K240	Yellow
A241	Yellow
K242	Yellow
I243	Yellow

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.59 Å 96.59 Å 96.59 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.30)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.228 , 0.188	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1887	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 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: MG, ADP

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	0.58	3/1840 (0.2%)	0.74	3/2476 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	MSE	SE-CE	-5.61	1.62	1.95
1	A	30	MSE	CG-SE	-5.60	1.76	1.95
1	A	30	MSE	SE-CE	-5.25	1.64	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	242	LYS	N-CA-C	-5.77	95.42	111.00
1	A	84	LEU	N-CA-C	-5.13	97.15	111.00
1	A	199	GLU	N-CA-C	-5.13	97.16	111.00

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	1824	0	1918	55	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	27	0	12	2	0
4	A	35	0	0	2	0
All	All	1887	0	1930	55	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 55 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:A:3:ARG:HD3	1:A:236:LEU:HB3	1.29	1.10
1:A:235:LYS:HA	1:A:235:LYS:NZ	1.77	0.99
1:A:235:LYS:HA	1:A:235:LYS:HZ2	1.33	0.92
1:A:2:THR:HG21	1:A:110:GLY:H	1.36	0.89
1:A:136:GLU:HB3	1:A:166:LEU:HD21	1.56	0.86

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	241/243 (99%)	227 (94%)	10 (4%)	4 (2%)	<b>9</b> <b>8</b>

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	GLY
1	A	234	ASP
1	A	237	ALA
1	A	239	ILE



### 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	198/189 (105%)	185 (93%)	13 (7%)	16	22

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	59	LEU
1	A	177	GLU
1	A	50	LEU
1	A	108	LEU

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

Mol	Chain	Res	Type
1	A	124	GLN
1	A	142	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

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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$
3	ADP	A	301	2	24,29,29	1.64	6 (25%)	29,45,45	1.57	3 (10%)

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
3	ADP	A	301	2	-	2/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	ADP	C8-N7	-4.20	1.27	1.34
3	A	301	ADP	C2'-C3'	3.00	1.61	1.53
3	A	301	ADP	O4'-C1'	-2.42	1.37	1.41
3	A	301	ADP	C2-N3	2.24	1.35	1.32
3	A	301	ADP	C2'-C1'	2.24	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	ADP	O4'-C1'-C2'	5.33	114.72	106.93
3	A	301	ADP	C3'-C2'-C1'	-2.77	96.80	100.98
3	A	301	ADP	O4'-C4'-C5'	-2.73	100.41	109.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

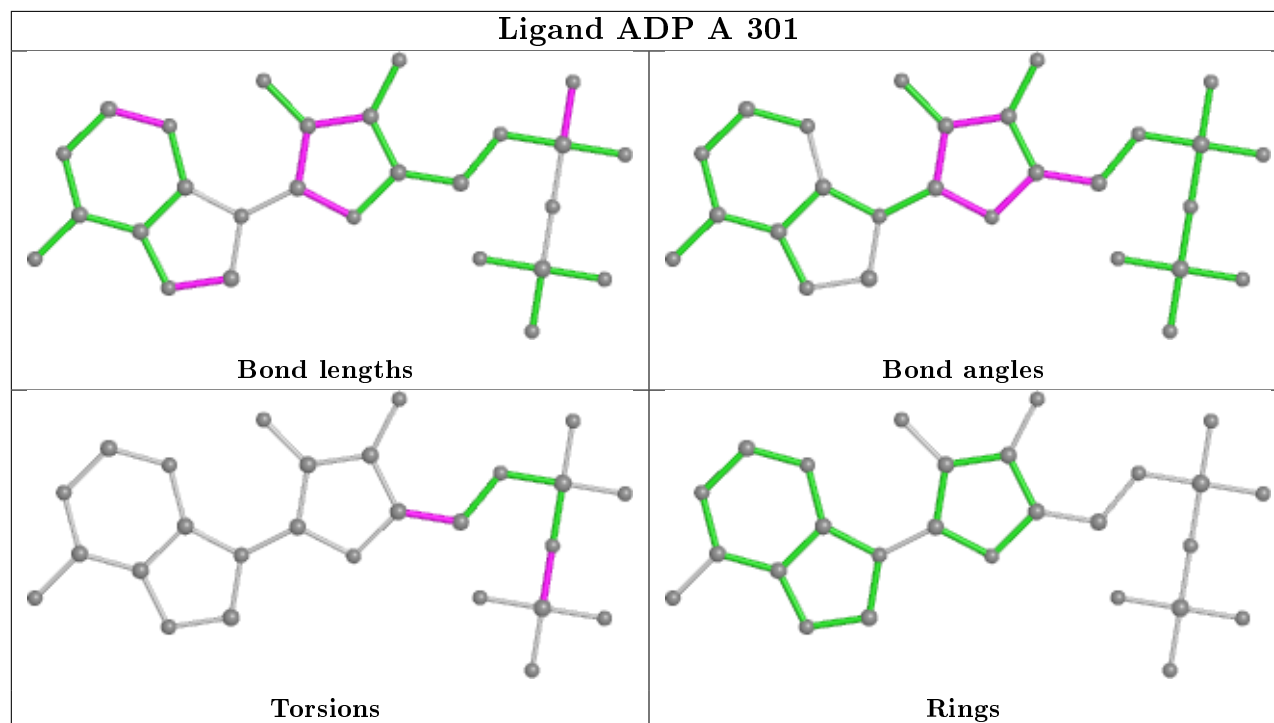
Mol	Chain	Res	Type	Atoms
3	A	301	ADP	PA-O3A-PB-O2B
3	A	301	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.