

Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 06:08 PM JST

PDB ID : 8IA9

Title : SpnK Methyltransferase from the Spinosyn Biosynthetic Pathway in Complex

with Mg

Authors: Huang, S.; Zheng, J.

Deposited on : 2023-02-08

Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} \text{MolProbity} & : & 4.02\text{b-}467 \\ \text{Xtriage (Phenix)} & : & 1.13 \end{array}$

EDS : 2.35.1buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

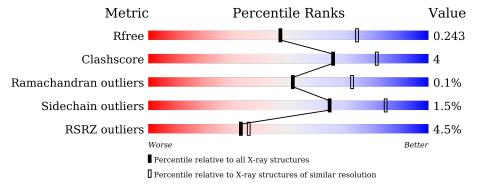
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.50 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}(\mathring{\rm A})) \end{array}$
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	397	85%	10%	5%
1	В	397	5% 86%	9%	5%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6026 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 Demethylmacrocin O-methyltransferase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	378	Total 2929	C 1856	11	O 552	S 5	0	0	0
1	В	379	Total 2940	C 1864	11	O 554	S 5	0	0	0

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

• Molecule 3 is water.

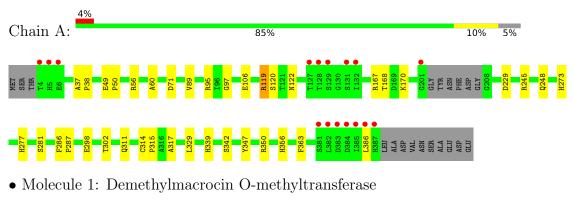
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0
3	В	74	Total O 74 74	0	0

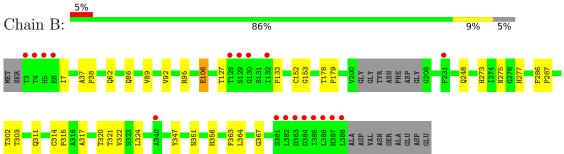


3 Residue-property plots (i)

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: Demethylmacrocin O-methyltransferase







4 Data and refinement statistics (i)

Property	Value	Source	
Space group	P 43 21 2	Depositor	
Cell constants	134.11Å 134.11Å 159.72Å	Donogitor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	47.46 - 2.50	Depositor	
Resolution (A)	47.42 - 2.50	EDS	
% Data completeness	97.9 (47.46-2.50)	Depositor	
(in resolution range)	98.0 (47.42-2.50)	EDS	
R_{merge}	0.13	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.17 (at 2.51Å)	Xtriage	
Refinement program	REFMAC 5.8.0267	Depositor	
D D.	0.208 , 0.243	Depositor	
R, R_{free}	0.212 , 0.243	DCC	
R_{free} test set	2606 reflections (5.20%)	wwPDB-VP	
Wilson B-factor (Å ²)	33.0	Xtriage	
Anisotropy	0.269	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.34, 32.4	EDS	
L-test for twinning ²	$ < L > = 0.45, < L^2> = 0.28$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
F_o, F_c correlation	0.94	EDS	
Total number of atoms	6026	wwPDB-VP	
Average B, all atoms (Å ²)	42.0	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 70.05 % 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 3.3337e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.65	0/2998	0.72	0/4076	
1	В	0.65	0/3009	0.72	0/4092	
All	All	0.65	0/6007	0.72	0/8168	

There are no bond length outliers.

There are no bond angle outliers.

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	2929	0	2876	23	0
1	В	2940	0	2891	24	0
2	A	1	0	0	0	0
2	В	1	0	0	0	0
3	A	81	0	0	3	0
3	В	74	0	0	1	0
All	All	6026	0	5767	47	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 4.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:167:ARG:HD3	3:A:565:HOH:O	1.69	0.93
1:A:71:ASP:HB3	1:A:89:VAL:CG1	2.24	0.68
1:B:37:ALA:HB3	1:B:38:PRO:HD3	1.75	0.67
1:B:62:GLN:HE21	1:B:89:VAL:HG11	1.61	0.65
1:B:62:GLN:NE2	1:B:89:VAL:HG11	2.11	0.65
1:B:311:GLN:HG3	1:B:317:ALA:CB	2.27	0.64
1:A:37:ALA:HB3	1:A:38:PRO:HD3	1.78	0.64
1:B:106:GLU:HG2	1:B:152:CYS:O	1.98	0.63
1:A:119:ARG:NH2	3:A:503:HOH:O	2.33	0.61
1:A:71:ASP:HB3	1:A:89:VAL:HG13	1.88	0.54
1:B:273:HIS:HD2	3:B:560:HOH:O	1.90	0.54
1:A:350:ARG:HH11	1:A:350:ARG:HG3	1.71	0.54
1:A:314:CYS:HA	1:A:315:PRO:C	2.28	0.54
1:B:314:CYS:HA	1:B:315:PRO:C	2.29	0.53
1:A:386:LEU:O	1:A:386:LEU:HD23	2.10	0.52
1:A:60:ALA:HB3	1:A:95:ARG:HG2	1.92	0.51
1:B:106:GLU:HG3	1:B:153:GLY:HA2	1.93	0.50
1:B:311:GLN:HG3	1:B:317:ALA:HB3	1.94	0.50
1:A:170:LYS:HE3	1:A:298:GLU:OE2	2.12	0.49
1:A:287:PRO:HA	1:A:347:TYR:CE2	2.48	0.49
1:A:248:GLN:HB2	1:A:281:SER:OG	2.13	0.49
1:B:351:ASN:HA	1:B:367:GLY:O	2.12	0.49
1:B:356:HIS:HB2	1:B:363:PHE:HB2	1.96	0.48
1:A:311:GLN:HG3	1:A:317:ALA:CB	2.43	0.48
1:B:127:THR:HG21	1:B:133:PRO:HG3	1.95	0.48
1:A:167:ARG:CD	3:A:565:HOH:O	2.44	0.47
1:B:248:GLN:HG3	1:B:277:HIS:HB3	1.97	0.47
1:A:229:ASP:O	1:A:245:ARG:HA	2.16	0.45
1:B:273:HIS:CB	1:B:302:THR:HG21	2.47	0.44
1:B:178:THR:N	1:B:179:PRO:CD	2.81	0.44
1:B:273:HIS:HB3	1:B:302:THR:HG21	2.00	0.44
1:A:97:GLY:HA3	1:A:120:SER:OG	2.18	0.43
1:B:303:THR:HG21	1:B:322:VAL:HB	2.01	0.43
1:A:329:LEU:C	1:A:329:LEU:HD23	2.40	0.43
1:B:286:PHE:HB3	1:B:287:PRO:HD3	2.00	0.42
1:B:275:ASN:OD1	1:B:320:THR:HA	2.20	0.42
1:A:356:HIS:HB2	1:A:363:PHE:HB2	2.02	0.42
1:B:92:VAL:O	1:B:95:ARG:NH1	2.53	0.42
1:A:49:GLU:HA	1:A:50:PRO:HA	1.86	0.42
1:A:248:GLN:HG3	1:A:277:HIS:HB3	2.02	0.41
1:B:287:PRO:HA	1:B:347:TYR:CE2	2.55	0.41

Continued on next page...



Continued from previous page...

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	$ ext{overlap }(ext{Å})$
1:B:321:THR:O	1:B:324:LEU:HB3	2.21	0.41
1:A:273:HIS:CB	1:A:302:THR:HG21	2.50	0.41
1:B:364:LEU:N	1:B:364:LEU:HD12	2.35	0.41
1:A:49:GLU:HG2	1:A:50:PRO:HA	2.03	0.41
1:A:286:PHE:N	1:A:287:PRO:CD	2.84	0.40
1:B:286:PHE:N	1:B:287:PRO:CD	2.84	0.40

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	Percen	tiles
1	A	374/397~(94%)	362 (97%)	11 (3%)	1 (0%)	41	61
1	В	375/397 (94%)	356 (95%)	19 (5%)	0	100	100
All	All	749/794 (94%)	718 (96%)	30 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ARG

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	309/324~(95%)	303 (98%)	6 (2%)	57 80		
1	В	311/324 (96%)	308 (99%)	3 (1%)	76 90		
All	All	620/648 (96%)	611 (98%)	9 (2%)	65 85		

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	119	ARG
1	A	122	ASN
1	A	168	THR
1	A	339	HIS
1	A	342	SER
1	В	7	ILE
1	В	86	GLN
1	В	106	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	62	GLN
1	В	143	GLN
1	В	273	HIS
1	В	311	GLN

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 (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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	378/397~(95%)	-0.06	16 (4%) 36 39	20, 38, 101, 138	0
1	В	379/397~(95%)	0.05	18 (4%) 31 33	18, 36, 92, 226	0
All	All	757/794 (95%)	-0.00	34 (4%) 33 36	18, 37, 98, 226	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	388	LEU	22.1
1	В	386	LEU	19.9
1	В	385	ILE	18.8
1	В	387	HIS	12.1
1	В	382	LEU	11.6
1	A	386	LEU	7.3
1	A	385	ILE	6.1
1	A	387	HIS	5.8
1	A	131	SER	5.7
1	A	129	SER	5.4
1	В	383	ASP	5.4
1	В	132	ILE	5.3
1	В	4	THR	5.3
1	A	383	ASP	4.8
1	В	3	THR	4.6
1	A	382	LEU	4.4
1	В	5	HIS	4.4
1	A	128	THR	4.4
1	A	201	GLY	4.0
1	A	5	HIS	3.7
1	В	384	ASP	3.5
1	В	129	SER	3.4
1	A	4	THR	3.3
1	A	381	SER	3.2

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	128	THR	3.2
1	В	130	GLY	3.0
1	A	384	ASP	2.7
1	В	381	SER	2.5
1	A	127	THR	2.4
1	В	231	PHE	2.4
1	A	132	ILE	2.4
1	В	340	ALA	2.1
1	В	6	GLU	2.1
1	A	6	GLU	2.0

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.

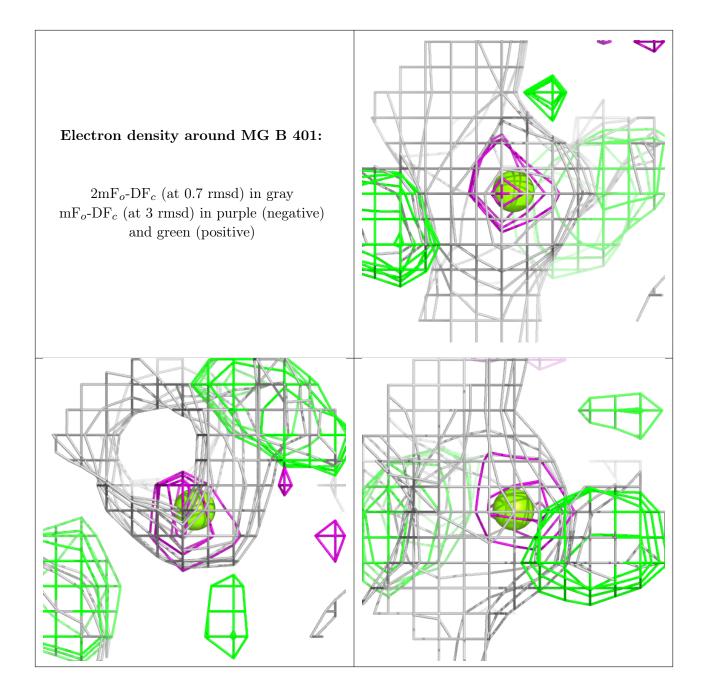
6.4 Ligands (i)

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. 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.

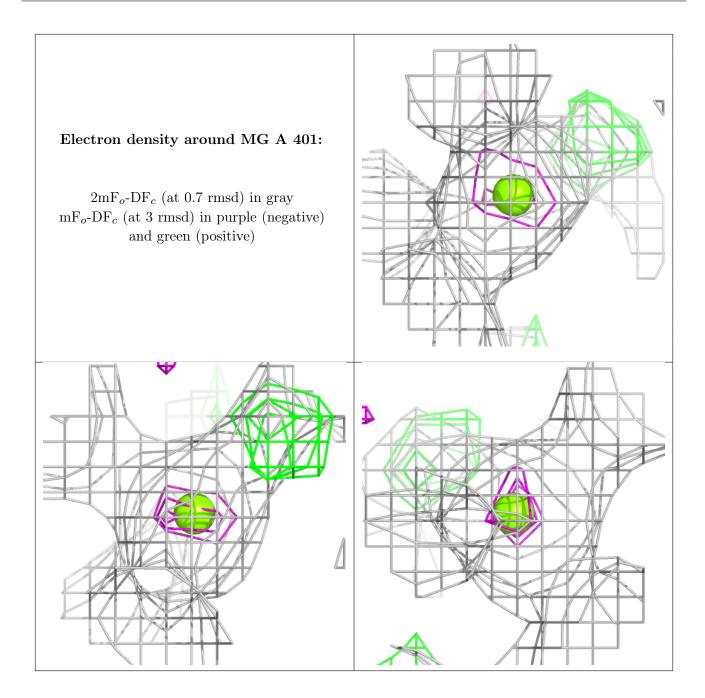
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MG	В	401	1/1	0.62	0.19	30,30,30,30	0
2	MG	A	401	1/1	0.93	0.20	30,30,30,30	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.









6.5 Other polymers (i)

There are no such residues in this entry.

