

Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 02:59 am BST

PDB ID : 6FGZ

Title : Cyanidioschyzon merolae Dnm1 (CmDnm1)

Authors: Bohuszewicz, O.; Low, H.H.

Deposited on : 2018-01-11

Resolution : 7.00 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 following versions of software and data (see references (1)) were used in the production of this report:

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

nenix) : 1.13 EDS : 2.11

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

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) oteins) : Engh & Huber (2001

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

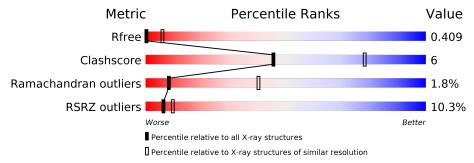
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.00 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
RSRZ outliers	127900	1004 (9.50-3.80)

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 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				
			7%				
1	A	774		64%		32%	



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2606 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 Dynamin.

Mo	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
1	A	526	Total 2606	C 1554	N 526	O 526	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

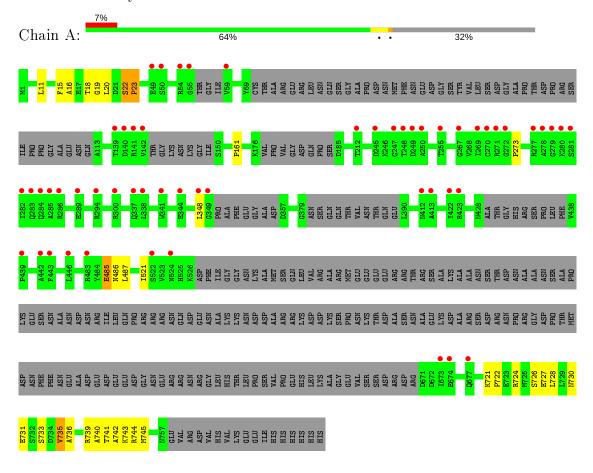
Chain	Residue	Modelled	Actual	Comment	Reference
A	769	HIS	_	expression tag	UNP Q84Y91
A	770	HIS	-	expression tag	UNP Q84Y91
A	771	HIS	_	expression tag	UNP Q84Y91
A	772	HIS	-	expression tag	UNP Q84Y91
A	773	HIS	_	expression tag	UNP Q84Y91
A	774	HIS	-	expression tag	UNP Q84Y91



3 Residue-property plots (i)

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: Dynamin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants	188.22Å 188.22Å 163.63Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.84 - 7.00	Depositor
Resolution (A)	40.84 - 7.00	EDS
% Data completeness	99.8 (40.84-7.00)	Depositor
(in resolution range)	99.8 (40.84-7.00)	EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$4.44 \; ({ m at} \; 7.33 { m \AA})$	Xtriage
Refinement program	PHENIX dev_1932	Depositor
R, R_{free}	0.344 , 0.411	Depositor
10, 10 free	0.347 , 0.409	DCC
R_{free} test set	295 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	477.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 584.3	EDS
L-test for twinning ²	$ < L > = 0.47, < L^2> = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	2606	wwPDB-VP
Average B, all atoms $(Å^2)$	389.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.

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)

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	Boı	nd lengths	Bo	nd angles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Α	0.69	$2/2597 \ (0.1\%)$	0.95	$2/3607 \ (0.1\%)$

All (2) bond length outliers are listed below:

M	[ol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$Ideal(\AA)$
	1	Α	23	PRO	C-N	-17.75	0.93	1.34
-	1	A	11	LEU	C-N	13.87	1.66	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	23	PRO	O-C-N	-8.61	108.92	122.70
1	A	23	PRO	CA-C-N	6.58	131.67	117.20

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	2606	0	1166	24	0
All	All	2606	0	1166	24	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 6.

All (24) close contacts within the same asymmetric unit are listed below, sorted by their clash



magnitude.

A , 1	A	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:A:726:SER:O	1:A:730:ASN:N	2.18	0.74
1:A:348:LEU:CB	1:A:739:ARG:CB	2.65	0.74
1:A:724:ARG:O	1:A:728:LEU:N	2.17	0.71
1:A:15:PHE:O	1:A:18:THR:CB	2.40	0.70
1:A:15:PHE:O	1:A:19:GLY:N	2.26	0.67
1:A:16:ALA:O	1:A:19:GLY:N	2.28	0.66
1:A:740:ALA:O	1:A:743:LYS:CB	2.46	0.64
1:A:16:ALA:C	1:A:19:GLY:H	2.03	0.61
1:A:741:THR:O	1:A:744:ARG:N	2.34	0.60
1:A:722:PRO:C	1:A:724:ARG:H	2.06	0.58
1:A:726:SER:O	1:A:730:ASN:CB	2.52	0.57
1:A:742:ALA:O	1:A:745:MET:CB	2.52	0.57
1:A:485:GLU:O	1:A:487:LEU:N	2.39	0.56
1:A:743:LYS:C	1:A:745:MET:N	2.58	0.55
1:A:730:ASN:O	1:A:733:SER:CB	2.56	0.54
1:A:735:VAL:O	1:A:736:ALA:HB3	2.08	0.53
1:A:727:GLU:O	1:A:731:GLU:N	2.39	0.52
1:A:16:ALA:O	1:A:19:GLY:HA2	2.10	0.52
1:A:485:GLU:C	1:A:487:LEU:H	2.14	0.52
1:A:16:ALA:O	1:A:19:GLY:CA	2.60	0.50
1:A:743:LYS:C	1:A:745:MET:H	2.15	0.48
1:A:485:GLU:C	1:A:487:LEU:N	2.66	0.48
1:A:20:LEU:C	1:A:22:SER:H	2.17	0.47
1:A:20:LEU:C	1:A:22:SER:N	2.73	0.42

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	508/774 (66%)	479 (94%)	20 (4%)	9 (2%)	8 40



All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	SER
1	A	23	PRO
1	A	735	VAL
1	A	485	GLU
1	A	486	ASN
1	A	721	LYS
1	A	161	PRO
1	A	521	ILE
1	A	273	PRO

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

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)

The following chains have linkage breaks:



Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	11:LEU	С	12:GLN	N	1.65
1	A	23:PRO	С	24:ILE	N	0.93



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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$	$OWAB(\AA^2)$	Q < 0.9
1	A	526/774 (67%)	0.43	54 (10%) 6 10	259, 373, 561, 649	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	271	ARG	5.6
1	A	248	THR	5.4
1	A	341	TRP	4.7
1	A	247	GLY	4.5
1	A	349	GLY	4.5
1	A	55	GLY	4.3
1	A	442	ALA	4.1
1	A	269	ILE	4.0
1	A	285	ALA	3.9
1	A	142	VAL	3.8
1	A	270	CYS	3.7
1	A	282	ILE	3.6
1	A	281	SER	3.4
1	A	522	SER	3.3
1	A	674	GLU	3.2
1	A	423	ARG	3.0
1	A	272	GLY	3.0
1	A	422	ILE	2.9
1	A	54	ARG	2.9
1	A	483	ARG	2.8
1	A	255	THR	2.8
1	A	413	ALA	2.7
1	A	139	THR	2.7
1	A	249	ASP	2.7
1	A	439	PRO	2.7
1	A	446	LEU	2.7
1	A	59	VAL	2.6

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	250	ALA	2.5
1	A	283	GLN	2.5
1	A	279	GLY	2.5
1	A	289	GLU	2.5
1	A	412	ASN	2.4
1	A	286	ARG	2.4
1	A	338	LEU	2.4
1	A	267	GLY	2.4
1	A	348	LEU	2.4
1	A	245	ASP	2.4
1	A	140	ASP	2.4
1	A	277	ARG	2.3
1	A	673	ILE	2.3
1	A	300	ARG	2.2
1	A	443	PHE	2.2
1	A	344	GLU	2.2
1	A	212	THR	2.2
1	A	284	GLN	2.2
1	A	294	ARG	2.2
1	A	49	GLU	2.1
1	A	280	LYS	2.1
1	A	677	GLN	2.1
1	A	141	ARG	2.1
1	A	524	ASN	2.1
1	A	337	GLN	2.1
1	A	50	SER	2.1
1	A	278	ALA	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 carbohydrates 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.

