



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:40 AM UTC

PDB ID : 6FGZ / pdb_00006fgz
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

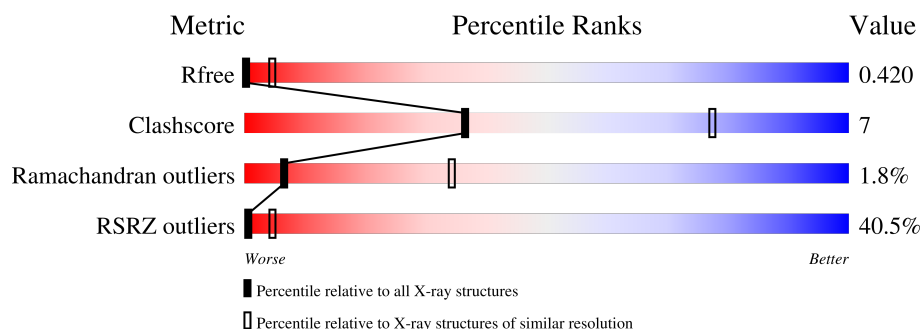
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

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 $\leq 5\%$. 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	774	

2 Entry composition

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.

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

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	188.22Å 188.22Å 163.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.84 – 7.00 40.84 – 7.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.84-7.00) 99.1 (40.84-7.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 7.33Å)	Xtriage
Refinement program	PHENIX dev_1932	Depositor
R, R_{free}	0.344 , 0.411 0.350 , 0.420	Depositor DCC
R_{free} test set	295 reflections (9.92%)	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)	0.21 , 588.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.14	2/2597 (0.1%)	1.70	29/3607 (0.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	PRO	C-N	-29.72	0.93	1.33
1	A	11	LEU	C-N	22.42	1.66	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	PRO	O-C-N	-10.16	108.92	122.64
1	A	17	GLU	N-CA-C	-10.05	100.33	111.28
1	A	724	ARG	N-CA-C	-8.16	102.36	111.82
1	A	455	VAL	N-CA-CB	7.32	115.11	110.50
1	A	744	ARG	N-CA-C	-7.11	103.71	112.38
1	A	727	GLU	N-CA-C	-6.97	103.77	111.36
1	A	18	THR	N-CA-C	-6.78	103.92	111.71
1	A	704	VAL	N-CA-C	6.38	116.55	110.42
1	A	248	THR	CA-C-N	6.04	129.19	120.38
1	A	248	THR	C-N-CA	6.04	129.19	120.38
1	A	22	SER	CA-C-N	5.76	127.04	119.84
1	A	22	SER	C-N-CA	5.76	127.04	119.84
1	A	742	ALA	N-CA-C	-5.66	104.50	111.75
1	A	731	GLU	N-CA-C	-5.66	105.11	111.28
1	A	391	TYR	O-C-N	-5.64	116.08	122.68
1	A	709	ASP	CA-C-N	5.62	127.81	120.28
1	A	709	ASP	C-N-CA	5.62	127.81	120.28
1	A	160	SER	N-CA-C	-5.58	101.78	108.25
1	A	231	GLY	CA-C-N	5.58	128.02	120.44
1	A	231	GLY	C-N-CA	5.58	128.02	120.44
1	A	479	GLU	CA-C-N	5.43	128.95	120.75
1	A	479	GLU	C-N-CA	5.43	128.95	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ALA	CA-C-N	5.39	128.05	120.28
1	A	211	ALA	C-N-CA	5.39	128.05	120.28
1	A	21	ASP	N-CA-C	-5.19	102.66	110.70
1	A	357	ASP	CA-C-N	5.14	127.17	120.28
1	A	357	ASP	C-N-CA	5.14	127.17	120.28
1	A	2	GLU	CA-C-N	5.07	127.78	120.38
1	A	2	GLU	C-N-CA	5.07	127.78	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	27	0
All	All	2606	0	1166	27	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 7.

All (27) 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: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:16:ALA:C	1:A:19:GLY:H	2.03	0.66
1:A:740:ALA:O	1:A:743:LYS:CB	2.46	0.64
1:A:722:PRO:C	1:A:724:ARG:H	2.06	0.61
1:A:741:THR:O	1:A:744:ARG:N	2.34	0.60
1:A:743:LYS:C	1:A:745:MET:N	2.58	0.59
1:A:726:SER:O	1:A:730:ASN:CB	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ALA:O	1:A:745:MET:CB	2.52	0.57
1:A:485:GLU:C	1:A:487:LEU:H	2.14	0.56
1:A:485:GLU:O	1:A:487:LEU:N	2.39	0.56
1:A:730:ASN:O	1:A:733:SER:CB	2.56	0.54
1:A:743:LYS:C	1:A:745:MET:H	2.15	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:20:LEU:C	1:A:22:SER:H	2.17	0.52
1:A:485:GLU:C	1:A:487:LEU:N	2.66	0.51
1:A:16:ALA:O	1:A:19:GLY:CA	2.60	0.50
1:A:20:LEU:C	1:A:22:SER:N	2.73	0.46
1:A:722:PRO:C	1:A:724:ARG:N	2.75	0.44
1:A:741:THR:O	1:A:742:ALA:C	2.60	0.43
1:A:741:THR:C	1:A:743:LYS:N	2.74	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	Percentiles	
1	A	508/774 (66%)	479 (94%)	20 (4%)	9 (2%)	6	34

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

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Mol	Chain	Res	Type
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 oligosaccharides 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	C	12:GLN	N	1.65
1	A	23:PRO	C	24:ILE	N	0.93

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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	526/774 (67%)	1.94	213 (40%) 0 4	259, 373, 561, 649	0

All (213) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	SER	10.2
1	A	150	SER	9.3
1	A	344	GLU	9.2
1	A	255	THR	7.5
1	A	348	LEU	7.3
1	A	216	ALA	7.3
1	A	349	GLY	6.8
1	A	478	THR	6.7
1	A	270	CYS	6.6
1	A	69	TYR	6.5
1	A	1	MET	6.5
1	A	442	ALA	6.4
1	A	523	VAL	6.3
1	A	17	GLU	6.3
1	A	521	ILE	6.2
1	A	483	ARG	6.1
1	A	476	CYS	6.0
1	A	153	ALA	6.0
1	A	479	GLU	5.9
1	A	526	LYS	5.9
1	A	741	THR	5.9
1	A	475	ASN	5.9
1	A	35	GLN	5.9
1	A	443	PHE	5.8
1	A	724	ARG	5.8
1	A	723	GLU	5.7
1	A	423	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	59	VAL	5.5
1	A	744	ARG	5.4
1	A	269	ILE	5.4
1	A	151	PRO	5.4
1	A	185	ASP	5.3
1	A	55	GLY	5.3
1	A	390	LEU	5.3
1	A	152	LYS	5.2
1	A	165	ASN	5.1
1	A	733	SER	5.1
1	A	345	LEU	5.1
1	A	440	GLU	5.0
1	A	138	GLU	5.0
1	A	22	SER	5.0
1	A	481	LEU	5.0
1	A	709	ASP	4.9
1	A	712	GLN	4.9
1	A	233	ARG	4.9
1	A	215	LEU	4.7
1	A	61	ARG	4.6
1	A	341	TRP	4.6
1	A	726	SER	4.6
1	A	347	THR	4.5
1	A	53	PRO	4.5
1	A	525	HIS	4.5
1	A	391	TYR	4.5
1	A	728	LEU	4.5
1	A	176	LYS	4.4
1	A	249	ASP	4.4
1	A	139	THR	4.3
1	A	446	LEU	4.2
1	A	60	THR	4.2
1	A	54	ARG	4.2
1	A	175	THR	4.2
1	A	40	SER	4.1
1	A	420	GLU	4.0
1	A	141	ARG	4.0
1	A	247	GLY	4.0
1	A	272	GLY	4.0
1	A	283	GLN	4.0
1	A	439	PRO	4.0
1	A	308	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	3.9
1	A	480	LEU	3.9
1	A	518	THR	3.9
1	A	672	ASP	3.9
1	A	461	CYS	3.8
1	A	16	ALA	3.7
1	A	722	PRO	3.7
1	A	718	ASP	3.7
1	A	135	ILE	3.7
1	A	740	ALA	3.7
1	A	309	ASN	3.6
1	A	273	PRO	3.6
1	A	173	GLY	3.6
1	A	409	GLN	3.6
1	A	271	ARG	3.5
1	A	486	ASN	3.5
1	A	302	LEU	3.5
1	A	25	ASP	3.5
1	A	290	ILE	3.5
1	A	154	ILE	3.5
1	A	50	SER	3.4
1	A	493	ALA	3.4
1	A	303	LEU	3.4
1	A	192	ALA	3.4
1	A	245	ASP	3.3
1	A	749	LEU	3.3
1	A	63	PRO	3.3
1	A	118	LEU	3.3
1	A	45	ASN	3.3
1	A	155	ASN	3.3
1	A	730	ASN	3.3
1	A	392	GLY	3.3
1	A	411	MET	3.3
1	A	214	ASP	3.3
1	A	254	LEU	3.3
1	A	304	PRO	3.3
1	A	484	TYR	3.2
1	A	14	LEU	3.2
1	A	737	GLU	3.2
1	A	325	ASP	3.2
1	A	685	ASP	3.2
1	A	129	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	358	LEU	3.2
1	A	407	GLU	3.1
1	A	305	GLN	3.1
1	A	161	PRO	3.1
1	A	745	MET	3.1
1	A	196	SER	3.0
1	A	727	GLU	3.0
1	A	682	SER	3.0
1	A	15	PHE	3.0
1	A	119	HIS	3.0
1	A	23	PRO	2.9
1	A	295	SER	2.9
1	A	281	SER	2.9
1	A	424	THR	2.9
1	A	441	LEU	2.9
1	A	419	ARG	2.9
1	A	716	VAL	2.9
1	A	365	VAL	2.8
1	A	142	VAL	2.8
1	A	751	ARG	2.8
1	A	329	SER	2.8
1	A	520	TYR	2.8
1	A	367	ASN	2.7
1	A	52	PHE	2.7
1	A	13	ASP	2.7
1	A	524	ASN	2.7
1	A	230	GLU	2.7
1	A	217	THR	2.7
1	A	736	ALA	2.7
1	A	372	GLU	2.7
1	A	38	GLY	2.7
1	A	410	SER	2.7
1	A	62	ARG	2.6
1	A	286	ARG	2.6
1	A	752	GLY	2.6
1	A	671	ASP	2.6
1	A	379	GLY	2.6
1	A	438	VAL	2.6
1	A	301	ARG	2.6
1	A	170	ASP	2.6
1	A	713	SER	2.6
1	A	397	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	LEU	2.5
1	A	747	ASP	2.5
1	A	201	PRO	2.5
1	A	428	ASN	2.5
1	A	519	SER	2.5
1	A	328	PRO	2.5
1	A	720	TYR	2.5
1	A	157	ARG	2.5
1	A	27	PRO	2.4
1	A	276	LEU	2.4
1	A	246	LYS	2.4
1	A	232	ARG	2.4
1	A	342	ARG	2.4
1	A	750	GLN	2.4
1	A	729	LEU	2.4
1	A	748	LEU	2.4
1	A	458	ALA	2.4
1	A	220	ALA	2.3
1	A	683	TYR	2.3
1	A	482	GLN	2.3
1	A	485	GLU	2.3
1	A	447	VAL	2.3
1	A	677	GLN	2.3
1	A	248	THR	2.3
1	A	371	SER	2.3
1	A	369	TYR	2.3
1	A	494	CYS	2.3
1	A	256	GLY	2.3
1	A	338	LEU	2.3
1	A	172	PRO	2.3
1	A	346	GLN	2.3
1	A	24	ILE	2.3
1	A	477	GLU	2.2
1	A	188	ARG	2.2
1	A	33	GLY	2.2
1	A	679	LEU	2.2
1	A	36	SER	2.2
1	A	113	ALA	2.2
1	A	193	MET	2.2
1	A	444	GLU	2.2
1	A	171	LEU	2.2
1	A	450	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	227	ALA	2.2
1	A	259	ILE	2.1
1	A	448	LYS	2.1
1	A	473	ALA	2.1
1	A	260	PRO	2.1
1	A	128	PHE	2.1
1	A	265	TYR	2.1
1	A	378	GLU	2.1
1	A	690	ASN	2.1
1	A	298	VAL	2.1
1	A	714	ARG	2.1
1	A	357	ASP	2.1
1	A	297	PRO	2.1
1	A	445	LEU	2.0
1	A	31	VAL	2.0
1	A	697	LYS	2.0
1	A	158	VAL	2.0
1	A	364	ASN	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 oligosaccharides 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.