



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 10:46 AM UTC

PDB ID : 6YS9 / pdb_00006ys9
Title : T_926 truncate of ChlH from Thermosynechococcus elongatus at 1.64 Å resolution
Authors : Bisson, C.; Hunter, C.N.
Deposited on : 2020-04-21
Resolution : 1.64 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 ⓘ 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

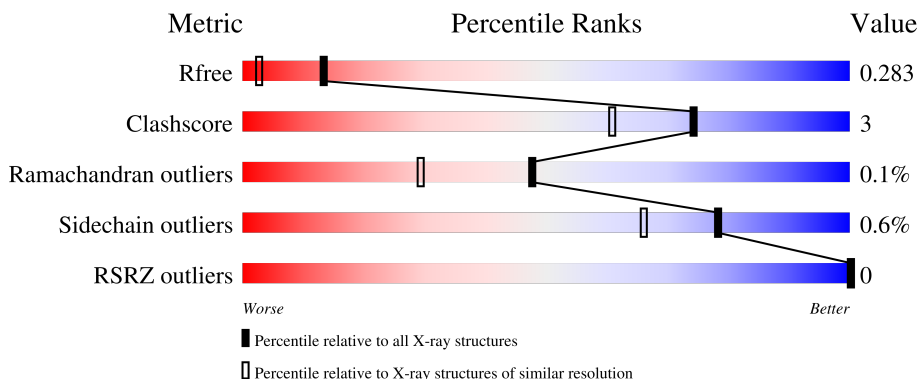
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	410	
1	B	410	
1	C	410	
1	D	410	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12582 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 Magnesium-protoporphyrin methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			3012	1891	525	586	10			
1	B	380	Total	C	N	O	S	0	0	0
			3005	1887	524	584	10			
1	C	378	Total	C	N	O	S	0	1	0
			2999	1884	522	583	10			
1	D	380	Total	C	N	O	S	0	1	0
			3008	1889	525	584	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8DM52
A	403	LEU	-	expression tag	UNP Q8DM52
A	404	GLU	-	expression tag	UNP Q8DM52
A	405	HIS	-	expression tag	UNP Q8DM52
A	406	HIS	-	expression tag	UNP Q8DM52
A	407	HIS	-	expression tag	UNP Q8DM52
A	408	HIS	-	expression tag	UNP Q8DM52
A	409	HIS	-	expression tag	UNP Q8DM52
A	410	HIS	-	expression tag	UNP Q8DM52
B	1	MET	-	initiating methionine	UNP Q8DM52
B	403	LEU	-	expression tag	UNP Q8DM52
B	404	GLU	-	expression tag	UNP Q8DM52
B	405	HIS	-	expression tag	UNP Q8DM52
B	406	HIS	-	expression tag	UNP Q8DM52
B	407	HIS	-	expression tag	UNP Q8DM52
B	408	HIS	-	expression tag	UNP Q8DM52
B	409	HIS	-	expression tag	UNP Q8DM52
B	410	HIS	-	expression tag	UNP Q8DM52
C	1	MET	-	initiating methionine	UNP Q8DM52
C	403	LEU	-	expression tag	UNP Q8DM52
C	404	GLU	-	expression tag	UNP Q8DM52

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Chain	Residue	Modelled	Actual	Comment	Reference
C	405	HIS	-	expression tag	UNP Q8DM52
C	406	HIS	-	expression tag	UNP Q8DM52
C	407	HIS	-	expression tag	UNP Q8DM52
C	408	HIS	-	expression tag	UNP Q8DM52
C	409	HIS	-	expression tag	UNP Q8DM52
C	410	HIS	-	expression tag	UNP Q8DM52
D	1	MET	-	initiating methionine	UNP Q8DM52
D	403	LEU	-	expression tag	UNP Q8DM52
D	404	GLU	-	expression tag	UNP Q8DM52
D	405	HIS	-	expression tag	UNP Q8DM52
D	406	HIS	-	expression tag	UNP Q8DM52
D	407	HIS	-	expression tag	UNP Q8DM52
D	408	HIS	-	expression tag	UNP Q8DM52
D	409	HIS	-	expression tag	UNP Q8DM52
D	410	HIS	-	expression tag	UNP Q8DM52

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	D	1	Total K 1 1	0	0

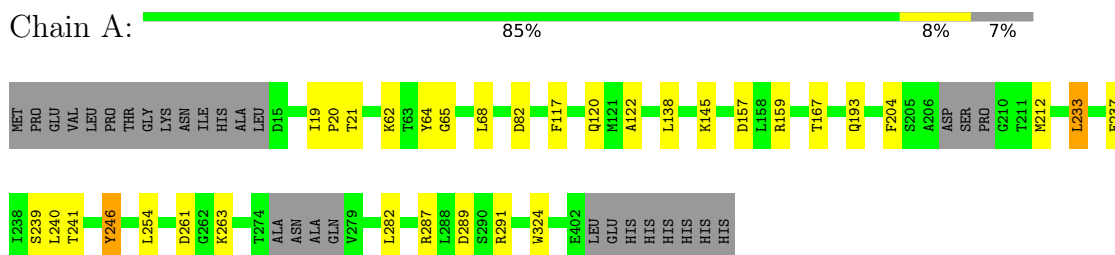
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	179	Total O 179 179	0	0
3	C	102	Total O 102 102	0	0
3	D	166	Total O 166 166	0	0

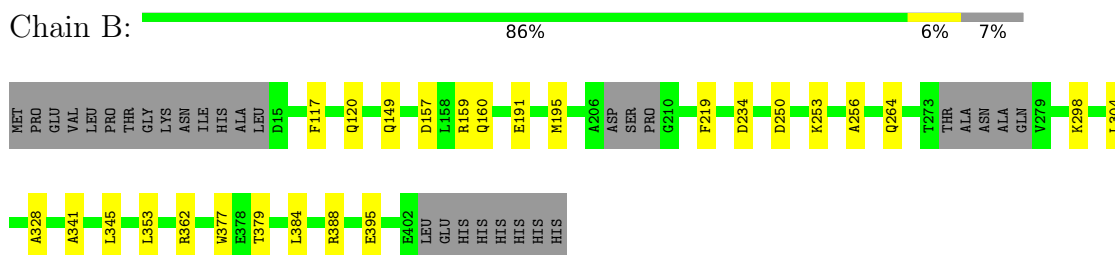
3 Residue-property plots [i](#)

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.

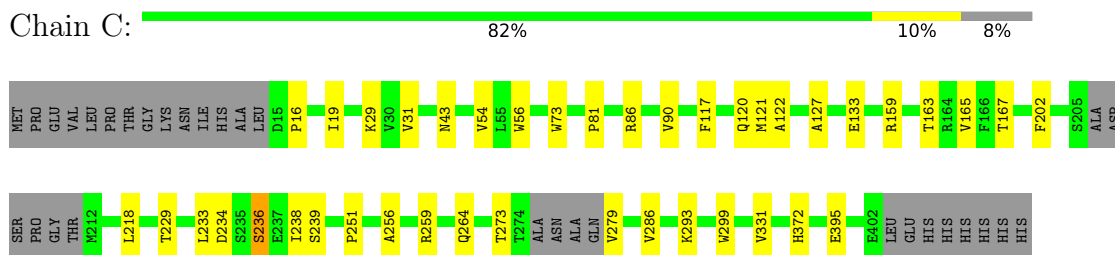
- Molecule 1: Magnesium-protoporphyrin methyltransferase



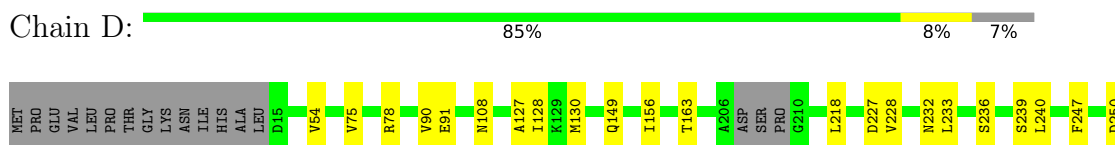
- Molecule 1: Magnesium-protoporphyrin methyltransferase



- Molecule 1: Magnesium-protoporphyrin methyltransferase



- Molecule 1: Magnesium-protoporphyrin methyltransferase



L254	K266	T273	THR	ALA	ASN	ALA	Q278	V286	M303	G310	T327	A328	R350	E370	L390	V401	GLU	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.48Å 140.33Å 78.01Å 90.00° 108.66° 90.00°	Depositor
Resolution (Å)	64.38 – 1.64 64.38 – 1.64	Depositor EDS
% Data completeness (in resolution range)	86.2 (64.38-1.64) 90.7 (64.38-1.64)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.201 , 0.247 (Not available) , 0.283	Depositor DCC
R_{free} test set	8572 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 20.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.050 for l,-k,h	Xtriage
Reported twinning fraction	0.893 for H, K, L 0.107 for -L, -K, -H	Depositor
Outliers	0 of 172694 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12582	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 27.52 % 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 2.1657e-03.*

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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	1.05	0/3064	1.47	3/4156 (0.1%)
1	B	1.09	1/3057 (0.0%)	1.42	2/4146 (0.0%)
1	C	1.09	1/3054 (0.0%)	1.46	7/4142 (0.2%)
1	D	1.09	0/3063	1.38	4/4154 (0.1%)
All	All	1.08	2/12238 (0.0%)	1.43	16/16598 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	229	THR	C-O	5.67	1.30	1.23
1	B	219	PHE	C-O	5.22	1.30	1.24

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	HIS	CA-C-N	7.02	127.89	120.03
1	C	372	HIS	C-N-CA	7.02	127.89	120.03
1	C	122	ALA	CA-C-N	6.19	128.48	120.44
1	C	122	ALA	C-N-CA	6.19	128.48	120.44
1	C	31	VAL	CA-C-O	-5.77	115.05	121.17

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	3012	0	2970	21	0
1	B	3005	0	2963	16	0
1	C	2999	0	2960	18	0
1	D	3008	0	2970	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	107	0	0	2	0
3	B	179	0	0	5	0
3	C	102	0	0	1	0
3	D	166	0	0	4	0
All	All	12582	0	11863	74	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 3.

The worst 5 of 74 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:D:149:GLN:OE1	3:D:601:HOH:O	1.87	0.93
1:A:167:THR:HG22	1:A:212:MET:HE2	1.71	0.72
1:D:130:MET:HE1	3:D:730:HOH:O	1.92	0.69
1:A:291:ARG:NH2	3:A:601:HOH:O	2.33	0.61
1:A:19:ILE:HG23	1:A:65:GLY:HA3	1.85	0.58

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	375/410 (92%)	362 (96%)	12 (3%)	1 (0%)	36	20
1	B	374/410 (91%)	364 (97%)	10 (3%)	0	100	100
1	C	373/410 (91%)	359 (96%)	14 (4%)	0	100	100
1	D	375/410 (92%)	362 (96%)	13 (4%)	0	100	100
All	All	1497/1640 (91%)	1447 (97%)	49 (3%)	1 (0%)	48	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP

5.3.2 Protein sidechains ⓘ

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	324/349 (93%)	323 (100%)	1 (0%)	86	79
1	B	323/349 (93%)	322 (100%)	1 (0%)	86	79
1	C	324/349 (93%)	319 (98%)	5 (2%)	57	32
1	D	324/349 (93%)	323 (100%)	1 (0%)	86	79
All	All	1295/1396 (93%)	1287 (99%)	8 (1%)	78	66

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	239	SER
1	C	395	GLU
1	C	239	SER
1	C	238	ILE
1	C	251	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	383	ASN
1	D	88	ASN
1	D	372	HIS
1	D	340	ASN
1	A	232	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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, 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	381/410 (92%)	-0.82	0 100 100	11, 25, 60, 104	0
1	B	380/410 (92%)	-1.10	0 100 100	8, 19, 45, 76	0
1	C	378/410 (92%)	-0.83	0 100 100	12, 24, 60, 85	1 (0%)
1	D	380/410 (92%)	-1.07	0 100 100	9, 20, 47, 80	1 (0%)
All	All	1519/1640 (92%)	-0.96	0 100 100	8, 22, 55, 104	2 (0%)

There are no RSRZ outliers to report.

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](#)

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, 95th 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	B-factors(Å ²)	Q<0.9
2	K	A	501	1/1	0.99	0.04	35,35,35,35	0
2	K	B	501	1/1	1.00	0.03	25,25,25,25	0
2	K	C	501	1/1	1.00	0.04	27,27,27,27	0
2	K	D	501	1/1	1.00	0.04	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.