wwPDB EM Validation Summary Report

May 13, 2024 – 11:25 pm BST

PDB ID	:	6R83
EMDB ID	:	EMD-4750
Title	:	CryoEM structure and molecular model of squid hemocyanin (Todarodes pacificus , TpH)
Authors	:	Tanaka, Y.; Kato, S.; Stabrin, M.; Raunser, S.; Matsui, T.; Gatsogiannis, C.
Deposited on	:	2019-03-31
Resolution	:	5.10 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

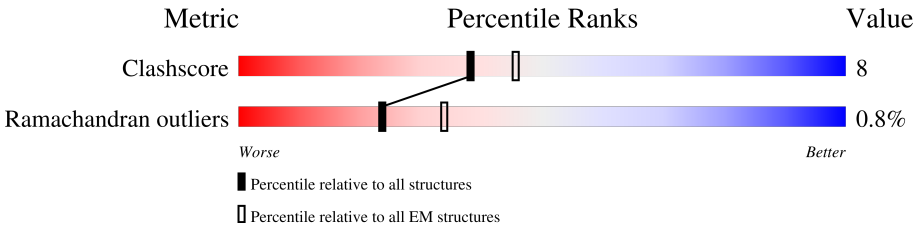
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	10a	3314	98%
1	1a	3314	98%
1	2a	3314	98%
1	3a	3314	98%
1	4a	3314	98%
1	5a	3314	98%
1	6a	3314	98%
1	7a	3314	98%
1	8a	3314	98%
1	9a	3314	98%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 161300 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Hemocyanin subunit 1.

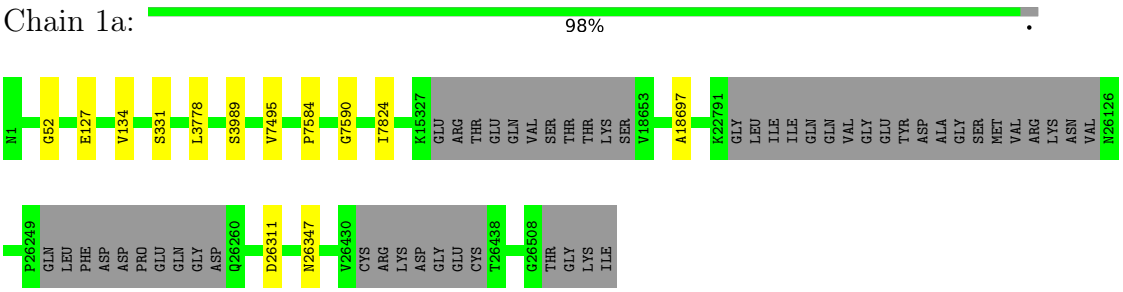
Mol	Chain	Residues	Atoms				AltConf	Trace
1	1a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	2a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	3a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	4a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	5a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	6a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	7a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	8a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	9a	3262	Total 16130	C 9606	N 3262	O 3262	0	0
1	10a	3262	Total 16130	C 9606	N 3262	O 3262	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. 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. 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.

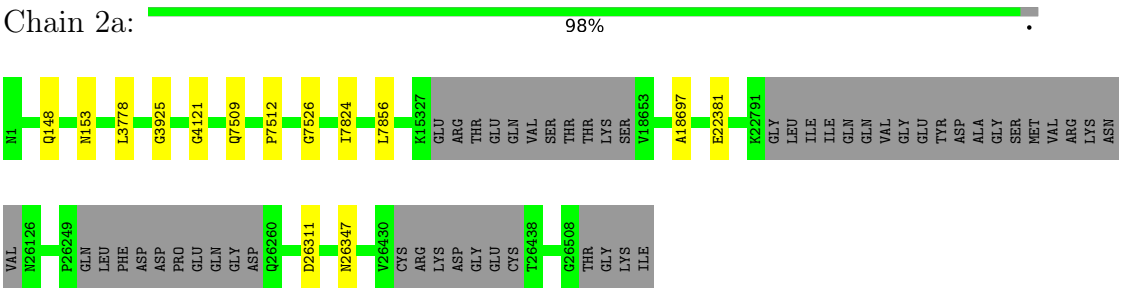
• Molecule 1: Hemocyanin subunit 1

Chain 1a:



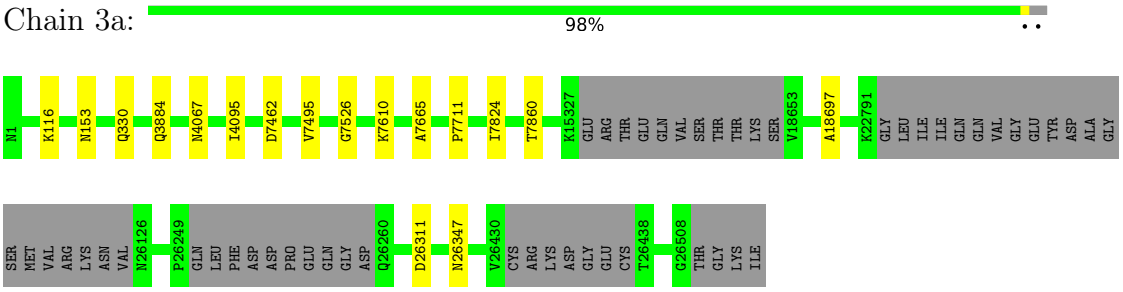
• Molecule 1: Hemocyanin subunit 1

Chain 2a:



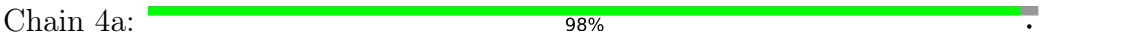
• Molecule 1: Hemocyanin subunit 1

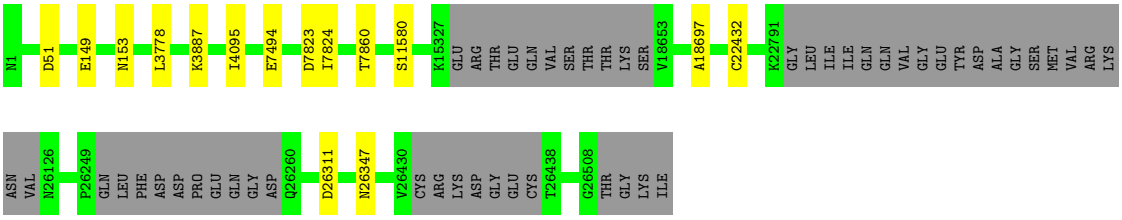
Chain 3a:



• Molecule 1: Hemocyanin subunit 1

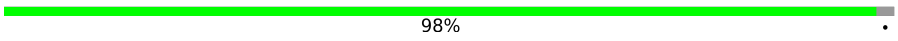
Chain 4a:

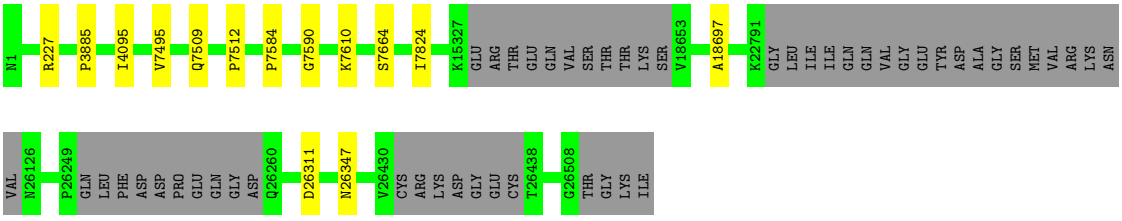




• Molecule 1: Hemocyanin subunit 1

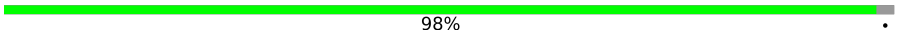
Chain 5a:

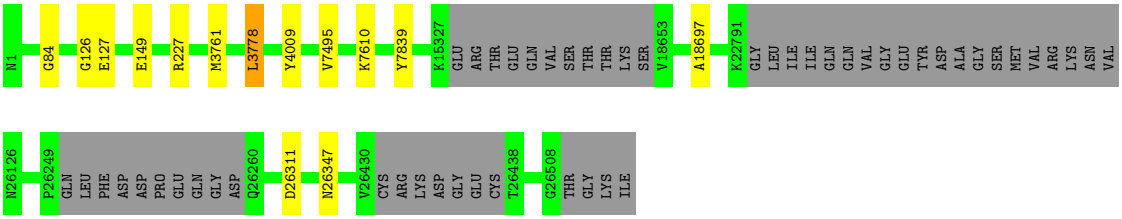




• Molecule 1: Hemocyanin subunit 1

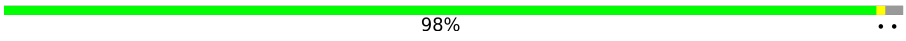
Chain 6a:

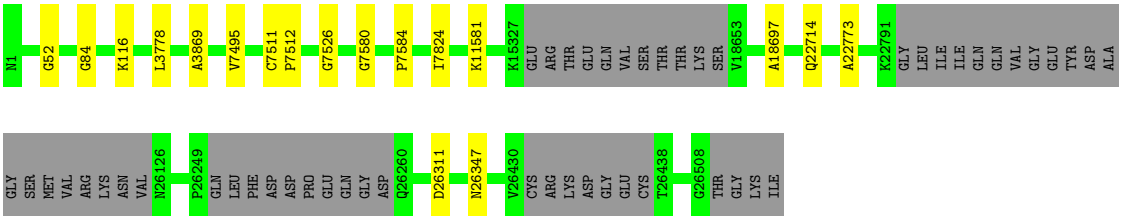




• Molecule 1: Hemocyanin subunit 1

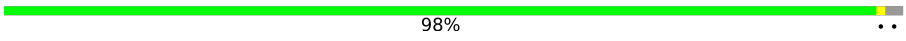
Chain 7a:

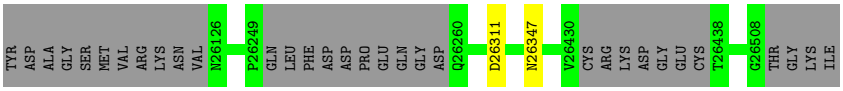




• Molecule 1: Hemocyanin subunit 1

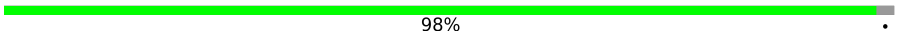
Chain 8a:

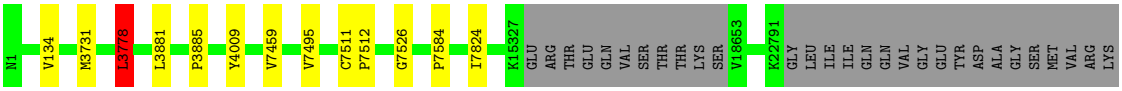


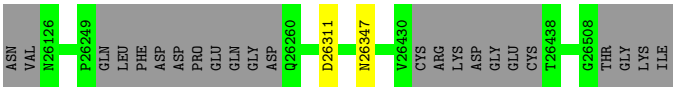


• Molecule 1: Hemocyanin subunit 1

Chain 9a:

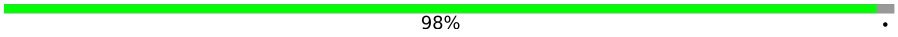


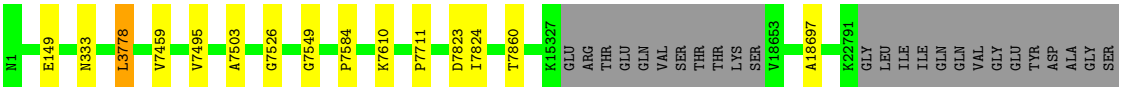


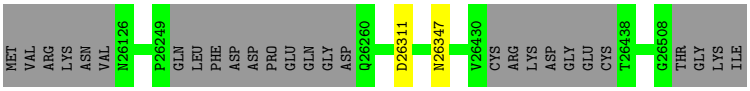


• Molecule 1: Hemocyanin subunit 1

Chain 10a:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	196315	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor

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	10a	0.27	0/6115	0.57	2/8514 (0.0%)
1	1a	0.25	0/6115	0.56	0/8514
1	2a	0.24	0/6115	0.53	1/8514 (0.0%)
1	3a	0.25	0/6115	0.53	1/8514 (0.0%)
1	4a	0.25	0/6115	0.53	2/8514 (0.0%)
1	5a	0.26	0/6115	0.54	0/8514
1	6a	0.25	0/6115	0.54	0/8514
1	7a	0.28	0/6115	0.55	1/8514 (0.0%)
1	8a	0.27	0/6115	0.54	0/8514
1	9a	0.27	0/6115	0.56	2/8514 (0.0%)
All	All	0.26	0/61150	0.55	9/85140 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	10a	0	5
1	1a	0	5
1	2a	0	5
1	3a	0	3
1	4a	0	7
1	5a	0	3
1	6a	0	4
1	7a	0	7
1	8a	0	3
1	9a	0	5
All	All	0	47

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	10a	7526	GLY	N-CA-C	5.93	127.94	113.10
1	2a	7526	GLY	N-CA-C	5.60	127.10	113.10
1	9a	7526	GLY	N-CA-C	5.51	126.89	113.10
1	10a	7823	ASP	C-N-CA	5.37	135.12	121.70
1	7a	7526	GLY	N-CA-C	5.34	126.45	113.10

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1a	127	GLU	Peptide
1	1a	18697	ALA	Peptide
1	1a	26311	ASP	Mainchain
1	1a	26347	ASN	Peptide
1	1a	3778	LEU	Peptide

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	10a	16130	0	2800	0	0
1	1a	16130	0	2801	0	0
1	2a	16130	0	2800	0	0
1	3a	16130	0	2800	0	0
1	4a	16130	0	2800	0	0
1	5a	16130	0	2800	0	0
1	6a	16130	0	2800	0	0
1	7a	16130	0	2801	0	0
1	8a	16130	0	2801	0	0
1	9a	16130	0	2800	0	0
All	All	161300	0	28003	0	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 8.

There are no clashes within the asymmetric unit.

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 PDB entries followed by that with respect to all EM entries.

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	10a	1237/3314 (37%)	1157 (94%)	69 (6%)	11 (1%)	17	56
1	1a	1237/3314 (37%)	1167 (94%)	62 (5%)	8 (1%)	25	65
1	2a	1237/3314 (37%)	1176 (95%)	53 (4%)	8 (1%)	25	65
1	3a	1237/3314 (37%)	1167 (94%)	57 (5%)	13 (1%)	14	52
1	4a	1237/3314 (37%)	1185 (96%)	46 (4%)	6 (0%)	29	68
1	5a	1237/3314 (37%)	1164 (94%)	62 (5%)	11 (1%)	17	56
1	6a	1237/3314 (37%)	1169 (94%)	57 (5%)	11 (1%)	17	56
1	7a	1237/3314 (37%)	1143 (92%)	84 (7%)	10 (1%)	19	60
1	8a	1237/3314 (37%)	1162 (94%)	59 (5%)	16 (1%)	12	48
1	9a	1237/3314 (37%)	1151 (93%)	76 (6%)	10 (1%)	19	60
All	All	12370/33140 (37%)	11641 (94%)	625 (5%)	104 (1%)	24	60

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1a	134	VAL
1	1a	331	SER
1	1a	3989	SER
1	2a	148	GLN
1	3a	7495	VAL

5.3.2 Protein sidechains

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

5.3.3 RNA

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)

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	3a	1
1	4a	1
1	7a	1
1	10a	1
1	8a	1
1	2a	1
1	1a	1
1	6a	1
1	5a	1
1	9a	1

The worst 5 of 10 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3a	11598:ASP	C	14913:VAL	N	29.53
1	4a	11598:ASP	C	14913:VAL	N	27.35
1	7a	11598:ASP	C	14913:VAL	N	27.29
1	10a	11598:ASP	C	14913:VAL	N	25.41
1	8a	11598:ASP	C	14913:VAL	N	24.86

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4750. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.