



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:23 am GMT

PDB ID : 3IXW
EMDB ID: : EMD-5101
Title : Scorpion Hemocyanin activated state pseudo atomic model built based on cryo-EM density map
Authors : Cong, Y.; Zhang, Q.; Woolford, D.; Schweikardt, T.; Khant, H.; Ludtke, S.; Chiu, W.; Decker, H.
Deposited on : 2009-02-13
Resolution : 8.00 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

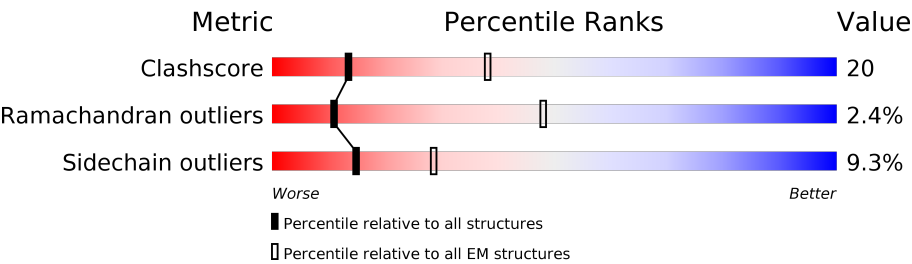
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

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 8.00 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	626	<div><div>54%</div><div>36%</div><div>8%</div><div>.</div></div>
1	C	626	<div><div>59%</div><div>33%</div><div>7%</div><div>.</div></div>
1	D	626	<div><div>58%</div><div>34%</div><div>8%</div><div>.</div></div>
1	E	626	<div><div>58%</div><div>34%</div><div>6%</div><div>.</div></div>
1	F	626	<div><div>58%</div><div>32%</div><div>8%</div><div>.</div></div>
1	G	626	<div><div>59%</div><div>33%</div><div>7%</div><div>.</div></div>
1	H	626	<div><div>60%</div><div>32%</div><div>7%</div><div>.</div></div>
1	I	626	<div><div>58%</div><div>34%</div><div>8%</div><div>.</div></div>
1	J	626	<div><div>57%</div><div>35%</div><div>7%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	K	626	<div><div></div><div>58%34%7%</div></div>
1	L	626	<div><div></div><div>59%33%8%</div></div>
1	M	626	<div><div></div><div>55%36%8%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 74208 atoms, of which 13476 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.

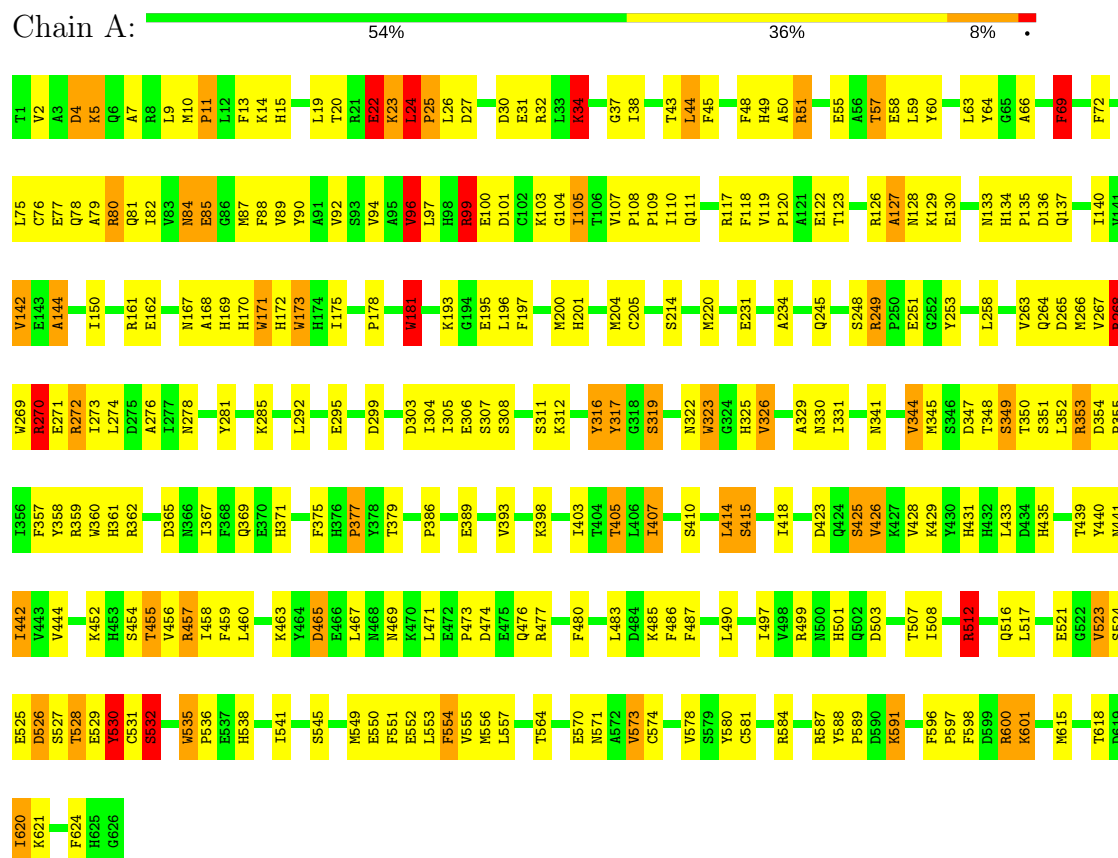
- Molecule 1 is a protein called Hemocyanin AA6 chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	C	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	D	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	E	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	F	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	G	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	H	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	I	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	J	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	K	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	L	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	M	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		

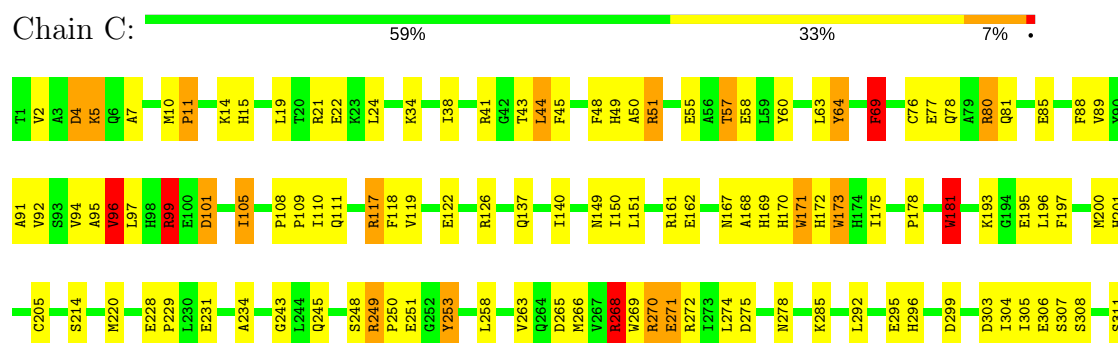
3 Residue-property plots

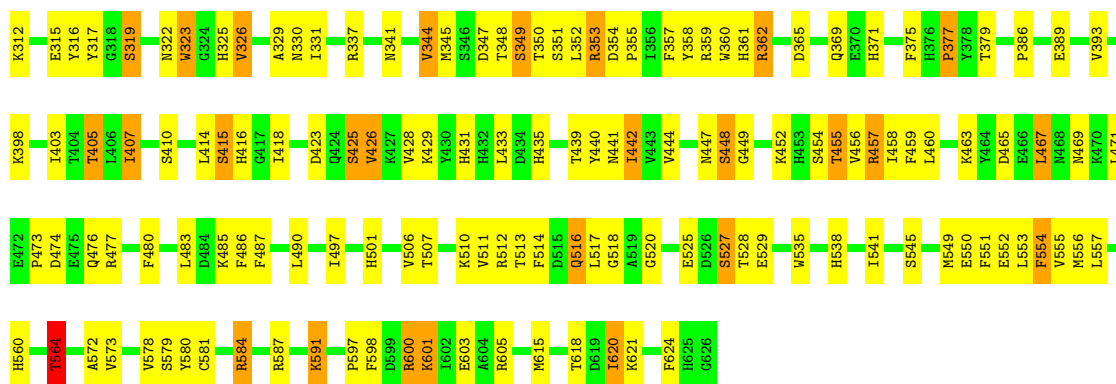
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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 AA6 chain



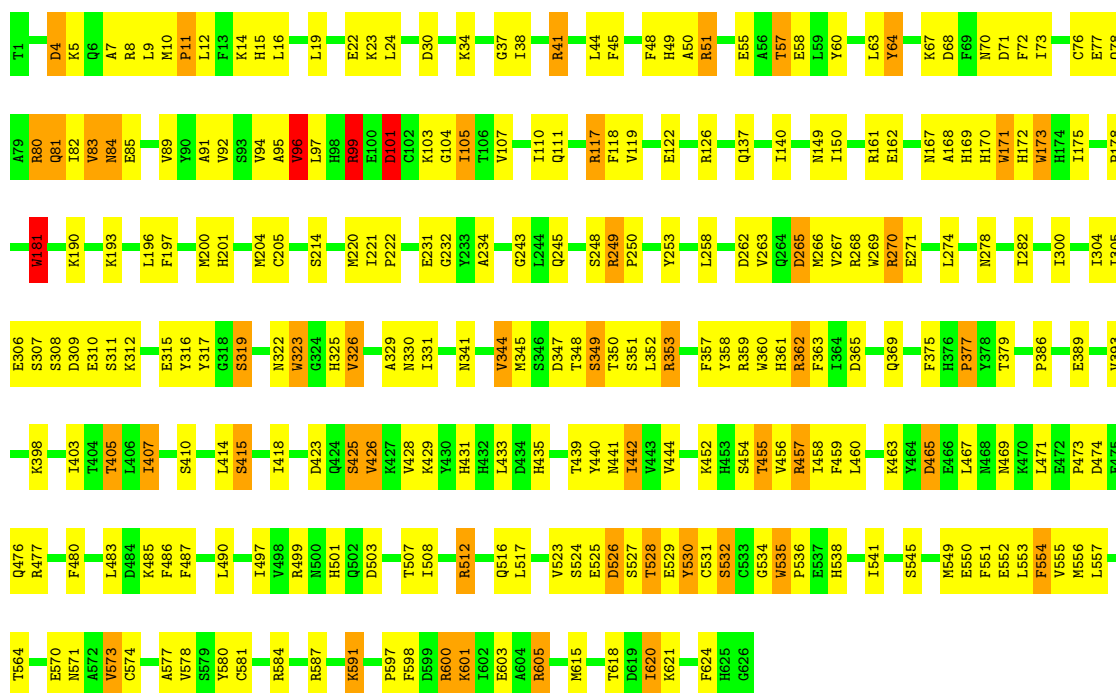
• Molecule 1: Hemocyanin AA6 chain





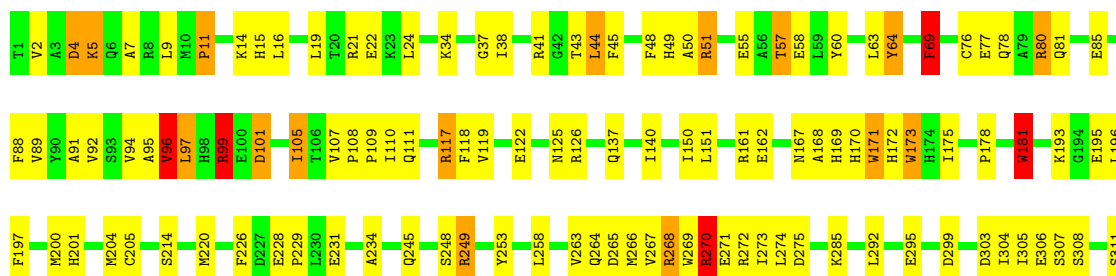
• Molecule 1: Hemocyanin AA6 chain

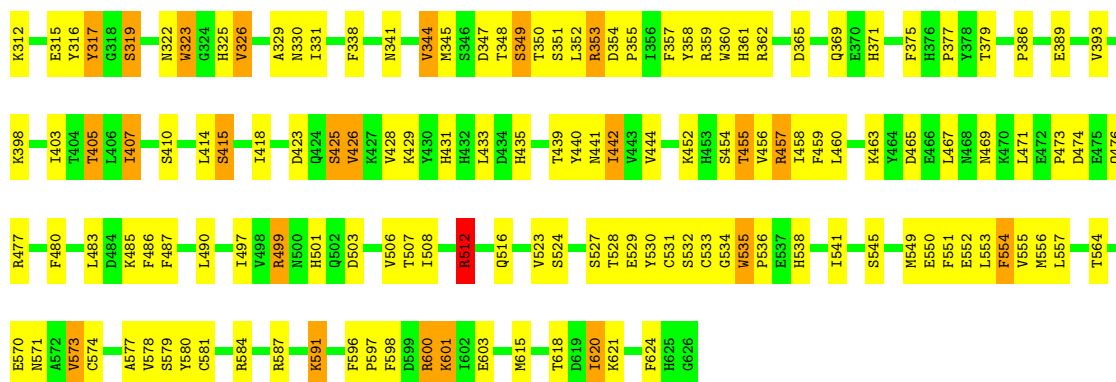
Chain D: 58% 34% 8% .



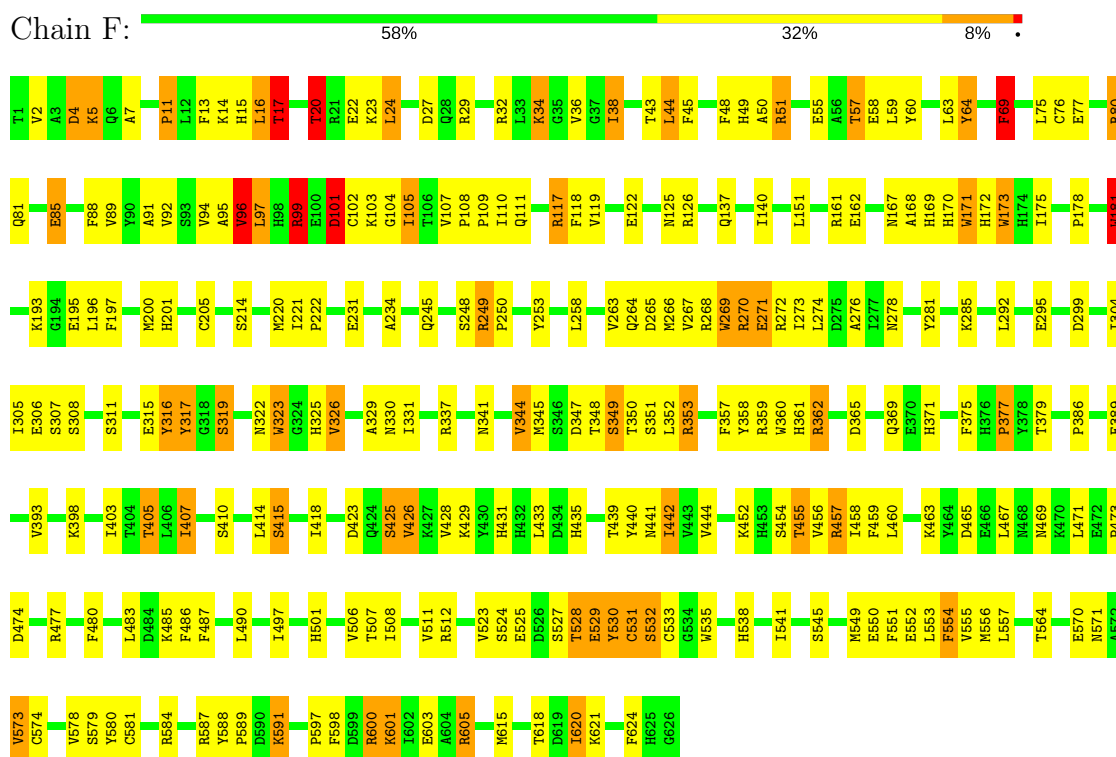
• Molecule 1: Hemocyanin AA6 chain

Chain E: 58% 34% 6% .

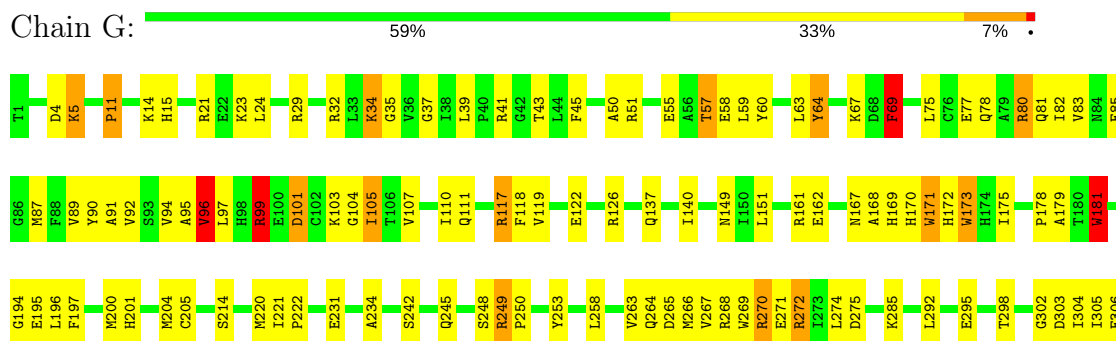


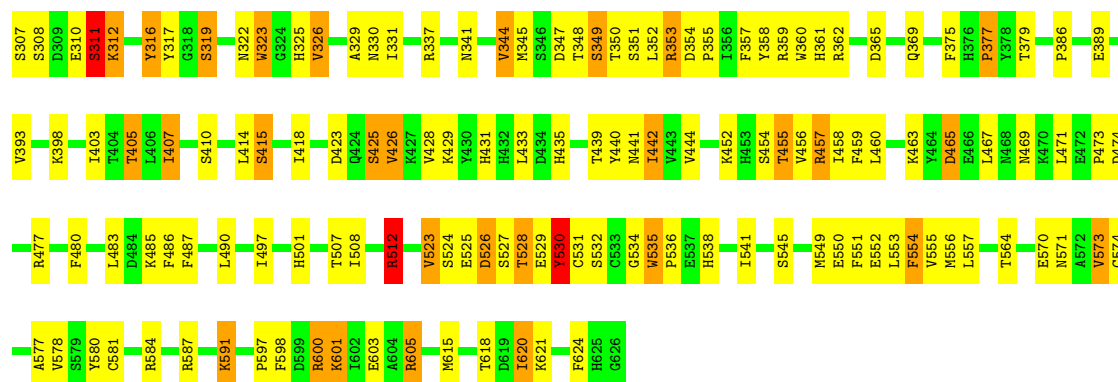


• Molecule 1: Hemocyanin AA6 chain

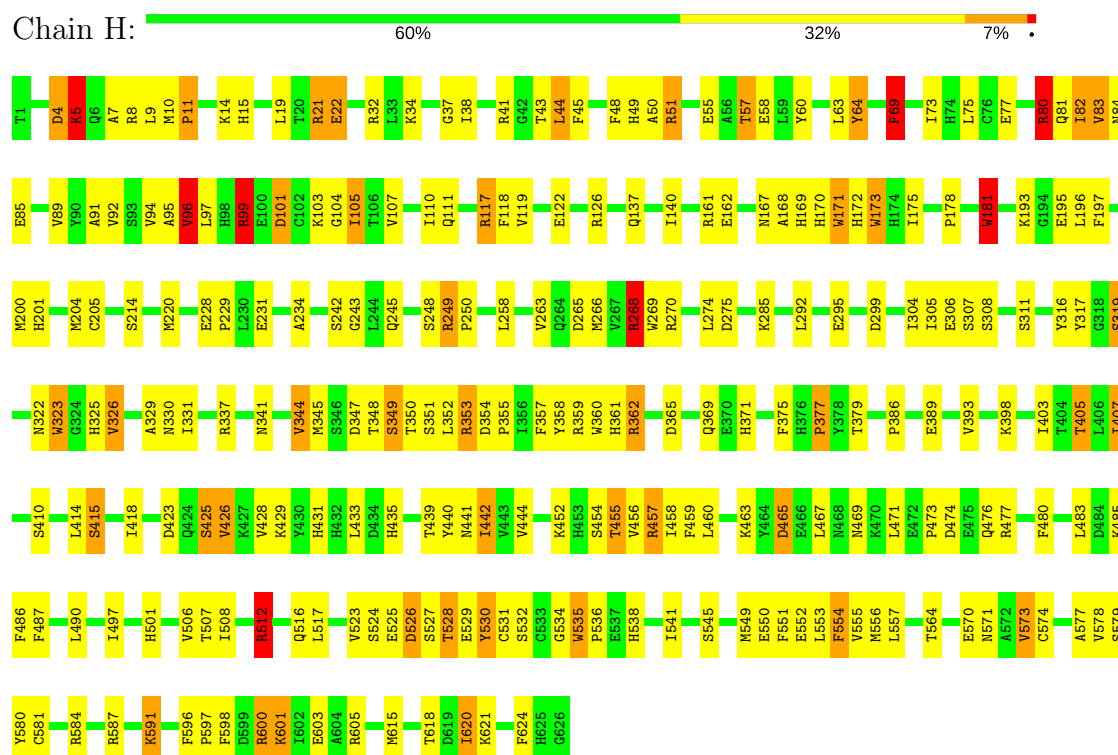


• Molecule 1: Hemocyanin AA6 chain

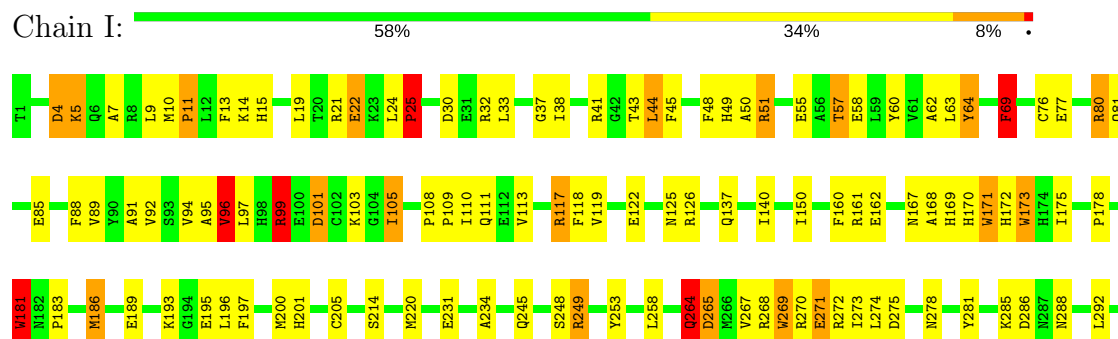


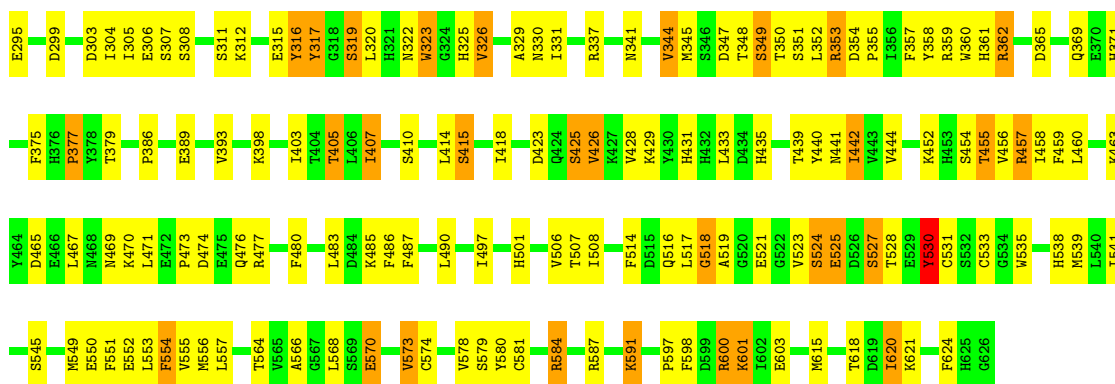


• Molecule 1: Hemocyanin AA6 chain



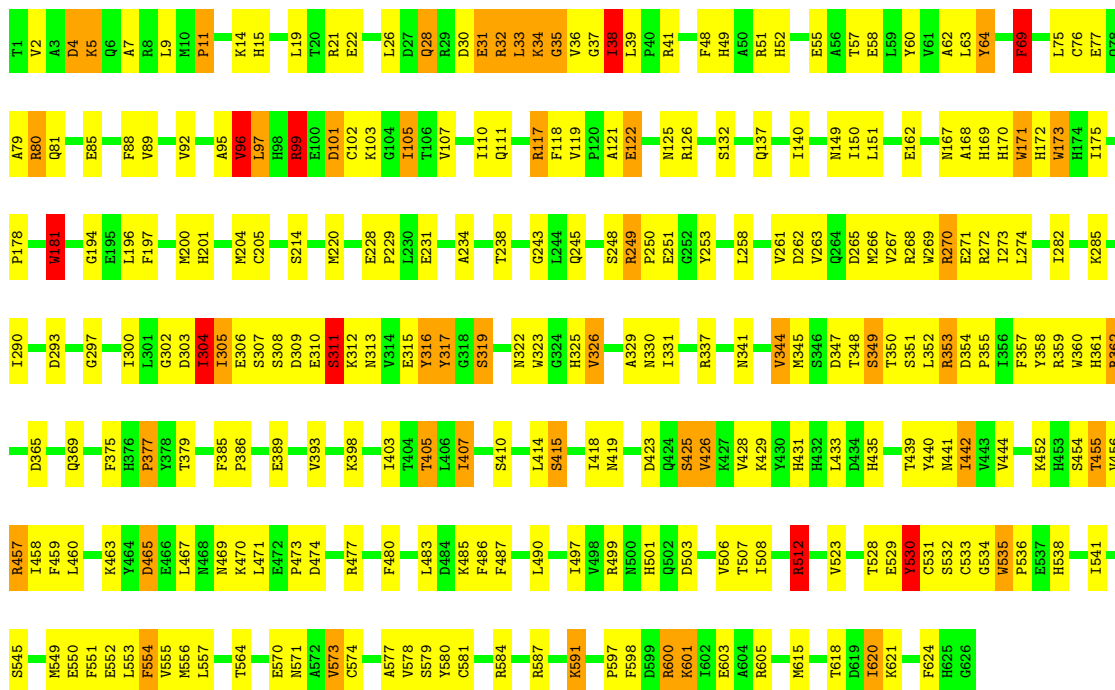
• Molecule 1: Hemocyanin AA6 chain





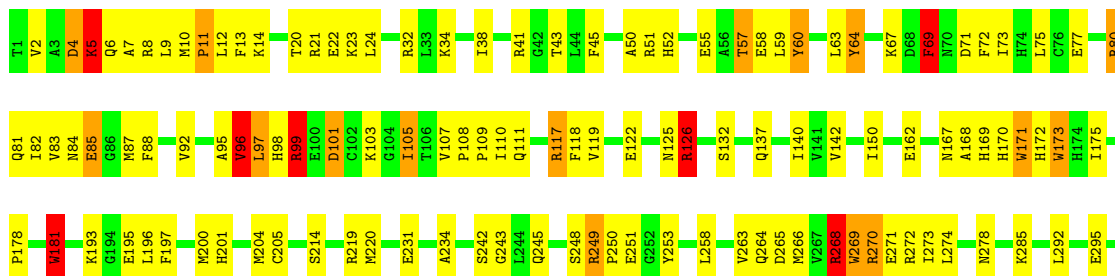
• Molecule 1: Hemocyanin AA6 chain

Chain J: 57% 35% 7% .

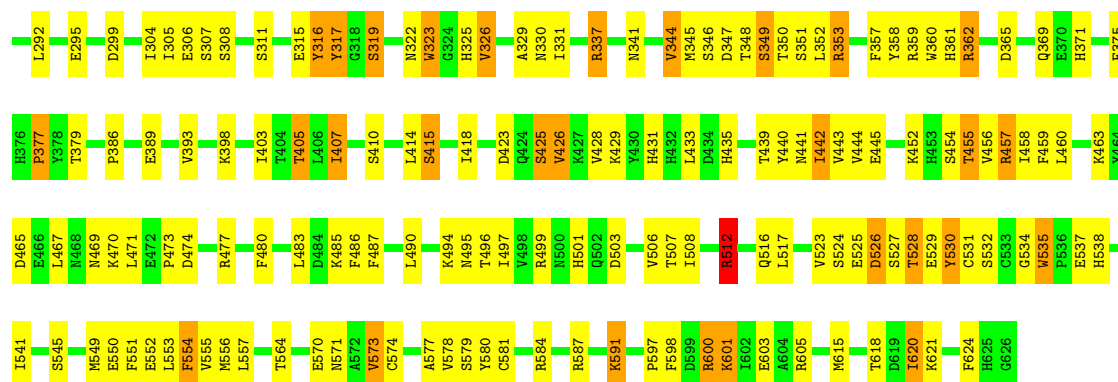


• Molecule 1: Hemocyanin AA6 chain

Chain K: 58% 34% 7% .







4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of particles used	13400	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEM3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.55	11/5191 (0.2%)	1.55	54/7033 (0.8%)
1	C	1.54	8/5190 (0.2%)	1.48	38/7030 (0.5%)
1	D	0.73	1/5191 (0.0%)	1.39	46/7033 (0.7%)
1	E	1.55	9/5191 (0.2%)	1.49	44/7033 (0.6%)
1	F	1.54	8/5191 (0.2%)	1.50	46/7033 (0.7%)
1	G	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
1	H	1.53	9/5191 (0.2%)	1.51	49/7033 (0.7%)
1	I	1.54	8/5190 (0.2%)	1.51	46/7030 (0.7%)
1	J	1.53	8/5191 (0.2%)	1.38	40/7033 (0.6%)
1	K	1.51	8/5191 (0.2%)	1.39	42/7033 (0.6%)
1	L	1.53	9/5191 (0.2%)	1.49	43/7033 (0.6%)
1	M	1.52	8/5191 (0.2%)	1.40	47/7033 (0.7%)
All	All	1.48	95/62290 (0.2%)	1.46	542/84390 (0.6%)

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	A	0	20
1	C	0	15
1	D	0	13
1	E	0	15
1	F	0	16
1	G	0	16
1	H	0	16
1	I	0	15
1	J	0	14
1	K	0	18
1	L	0	18
1	M	0	19
All	All	0	195

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	5	LYS	CE-NZ	50.53	2.75	1.49
1	G	5	LYS	CE-NZ	50.45	2.75	1.49
1	H	5	LYS	CE-NZ	50.33	2.74	1.49
1	L	5	LYS	CE-NZ	50.29	2.74	1.49
1	I	5	LYS	CE-NZ	50.17	2.74	1.49

The worst 5 of 542 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	44	LEU	O-C-N	-41.48	56.33	122.70
1	A	44	LEU	O-C-N	-41.46	56.37	122.70
1	F	44	LEU	O-C-N	-41.45	56.38	122.70
1	C	44	LEU	O-C-N	-41.43	56.41	122.70
1	I	44	LEU	O-C-N	-41.43	56.41	122.70

There are no chirality outliers.

5 of 195 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	GLU	Peptide
1	A	23	LYS	Peptide
1	A	24	LEU	Peptide
1	A	43	THR	Peptide
1	A	69	PHE	Sidechain

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	5061	1123	4864	260	0
1	C	5061	1123	4863	199	0
1	D	5061	1123	4865	181	0
1	E	5061	1123	4864	190	0
1	F	5061	1123	4864	193	0
1	G	5061	1123	4865	214	0
1	H	5061	1123	4864	205	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	5061	1123	4863	207	0
1	J	5061	1123	4865	242	0
1	K	5061	1123	4865	225	0
1	L	5061	1123	4864	210	0
1	M	5061	1123	4865	230	0
All	All	60732	13476	58371	2404	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 20.

The worst 5 of 2404 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:24:LEU:CB	1:A:24:LEU:CG	1.76	1.56
1:K:69:PHE:CZ	1:K:69:PHE:CE1	1.94	1.55
1:G:69:PHE:CD2	1:G:69:PHE:CE2	1.96	1.54
1:G:69:PHE:CE1	1:G:69:PHE:CD1	1.96	1.54
1:H:69:PHE:CD2	1:H:69:PHE:CE2	1.96	1.53

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	A	624/626 (100%)	527 (84%)	77 (12%)	20 (3%)	5	36
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	9	47
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	6	40
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	8	44
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	5	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	6	40
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	5	38
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	7	43
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	6	40
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	10	49
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	9	47
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	6	40
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	11	42

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	351	SER
1	A	530	TYR
1	C	34	LYS
1	C	351	SER

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

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	556/556 (100%)	496 (89%)	60 (11%)	7	31
1	C	556/556 (100%)	508 (91%)	48 (9%)	12	42
1	D	556/556 (100%)	503 (90%)	53 (10%)	10	36
1	E	556/556 (100%)	506 (91%)	50 (9%)	11	38
1	F	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	G	556/556 (100%)	508 (91%)	48 (9%)	12	42
1	H	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	I	556/556 (100%)	504 (91%)	52 (9%)	10	36
1	J	556/556 (100%)	503 (90%)	53 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	556/556 (100%)	505 (91%)	51 (9%)	11	37
1	L	556/556 (100%)	504 (91%)	52 (9%)	10	36
1	M	556/556 (100%)	504 (91%)	52 (9%)	10	36
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	15	37

5 of 621 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	349	SER
1	H	512	ARG
1	M	85	GLU
1	G	439	THR
1	H	85	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	278	ASN
1	I	125	ASN
1	L	431	HIS
1	G	431	HIS
1	H	224	HIS

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](#)

There are no chain breaks in this entry.