



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:47 PM BST

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 EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

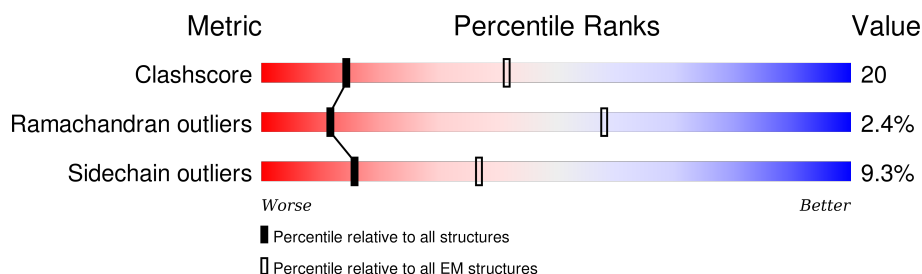
1 Overall quality at a glance ⓘ

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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	54% 36% 8% .
1	C	626	59% 33% 7% .
1	D	626	58% 34% 8% .
1	E	626	58% 34% 6% .
1	F	626	58% 32% 8% .
1	G	626	59% 33% 7% .
1	H	626	60% 32% 7% .
1	I	626	58% 34% 8% .
1	J	626	57% 35% 7% .

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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>

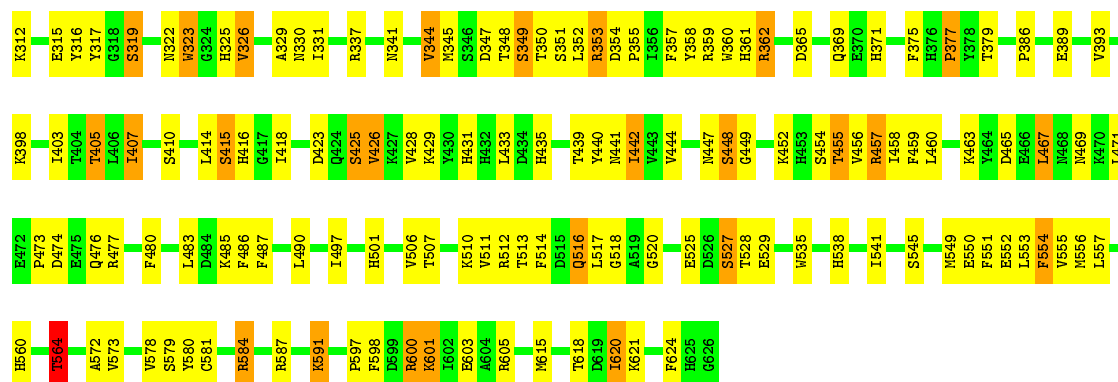
2 Entry composition

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.

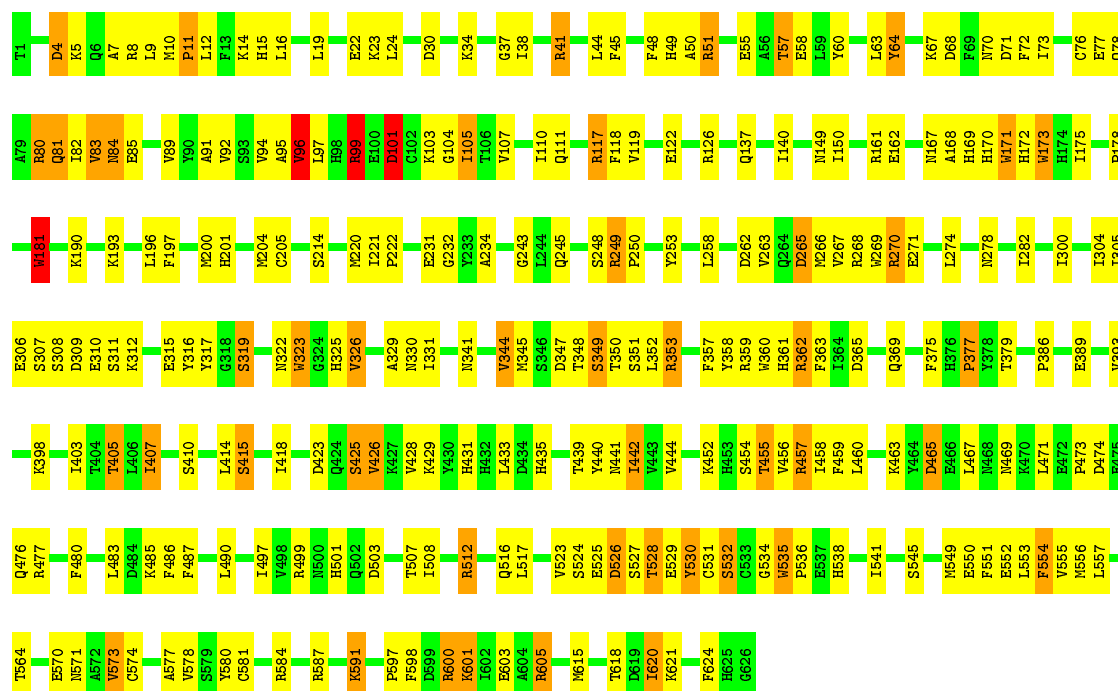
- Molecule 1 is a protein called Hemocyanin AA6 chain.

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		



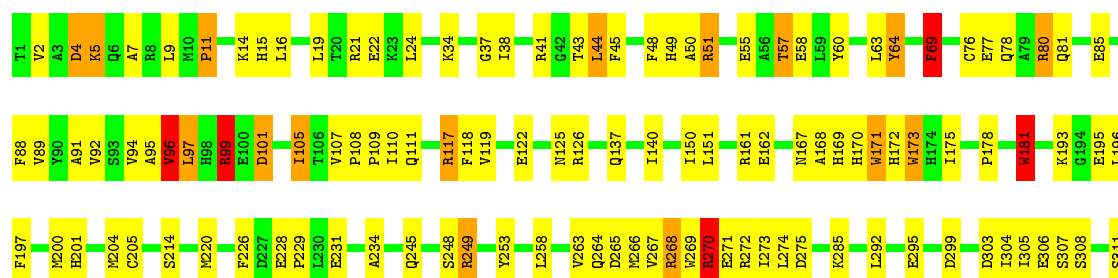
• Molecule 1: Hemocyanin AA6 chain

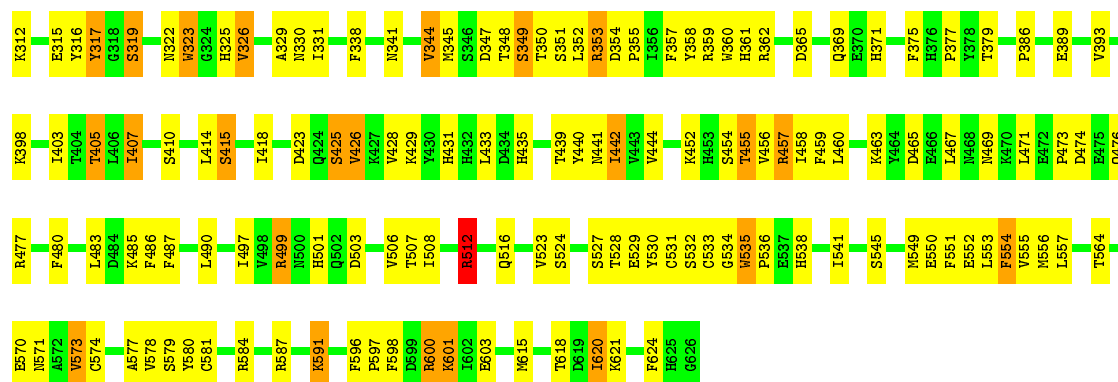
Chain D: 58% 34% 8%



• Molecule 1: Hemocyanin AA6 chain

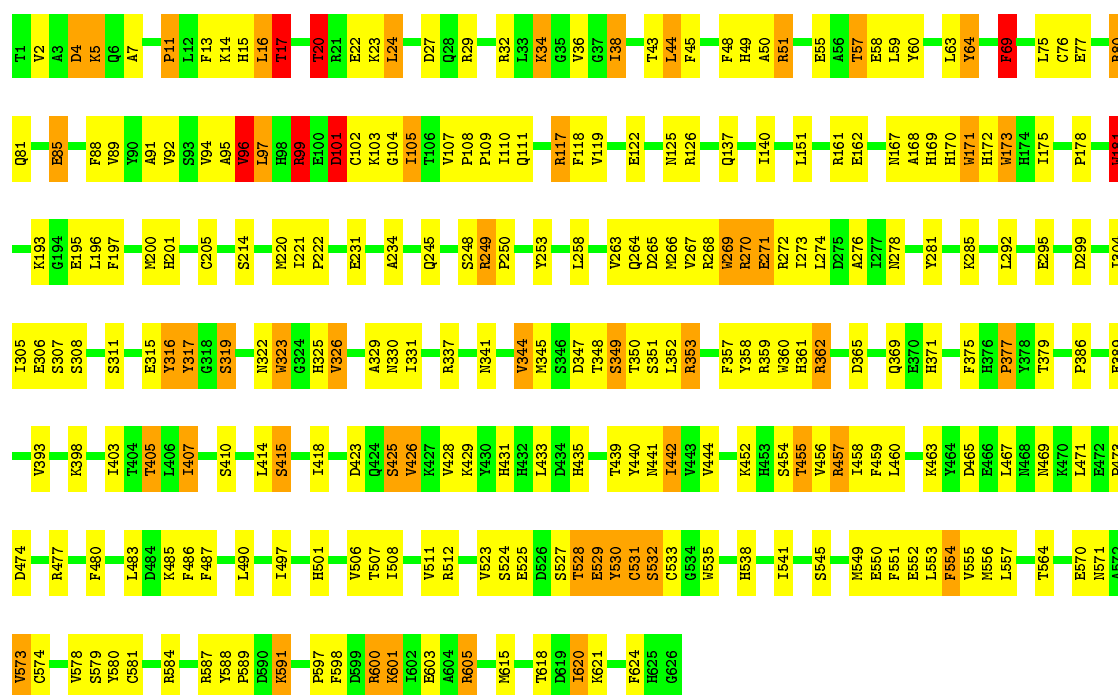
Chain E: 58% 34% 6%





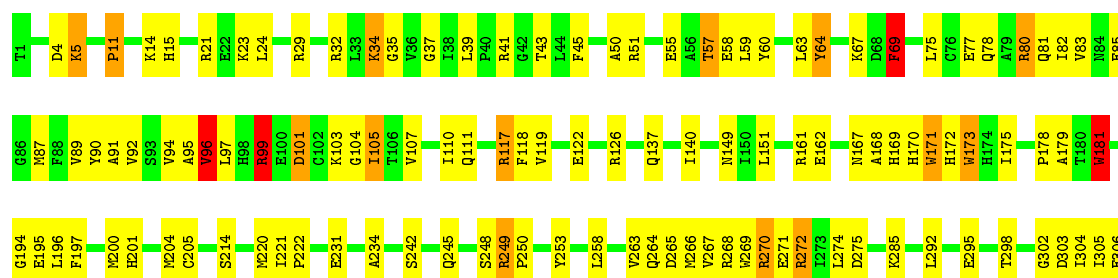
• Molecule 1: Hemocyanin AA6 chain

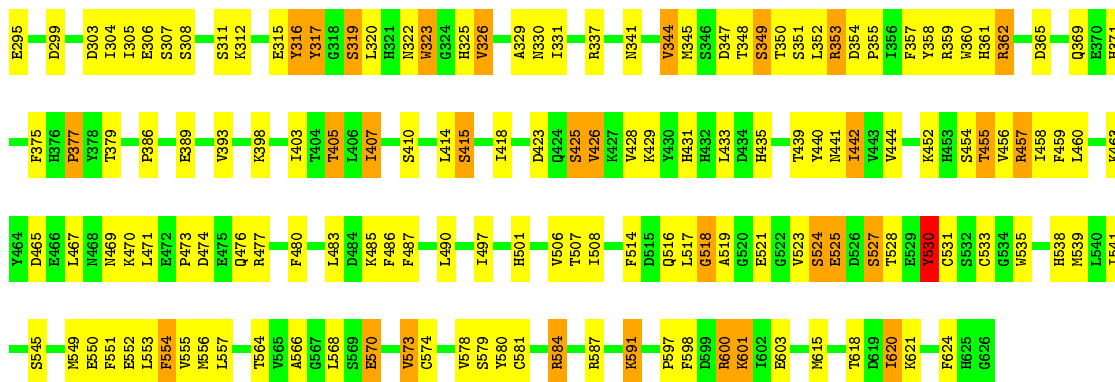
Chain F: 58% 32% 8% .



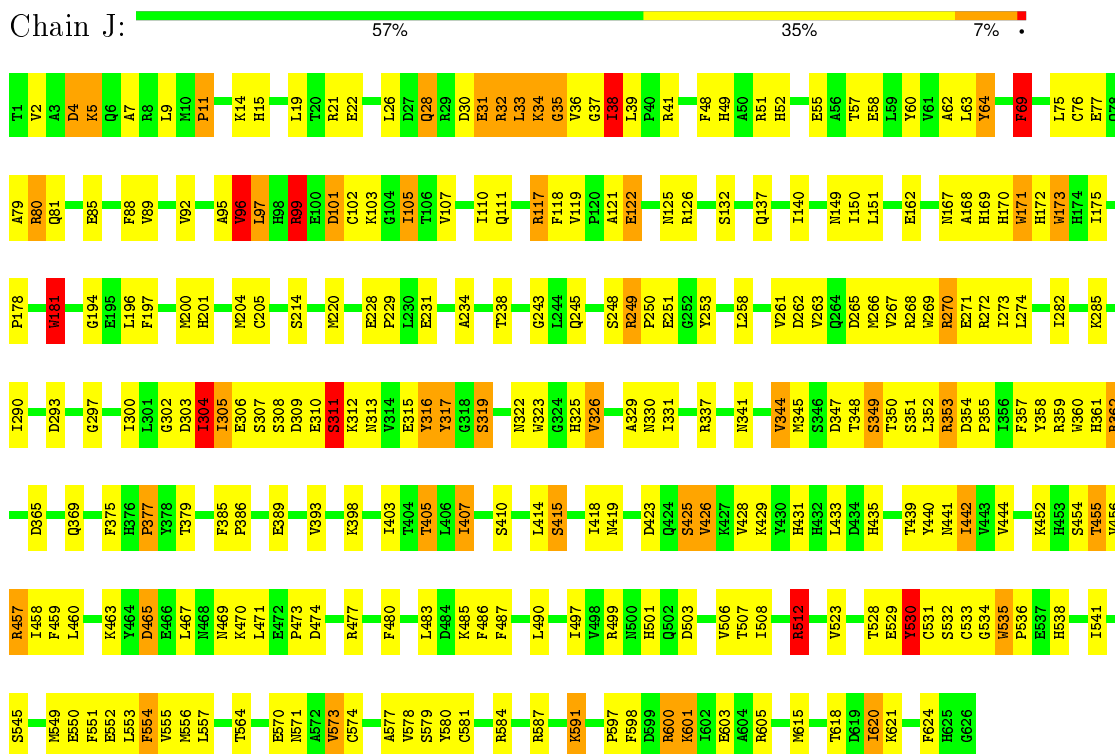
• Molecule 1: Hemocyanin AA6 chain

Chain G: 59% 33% 7% .

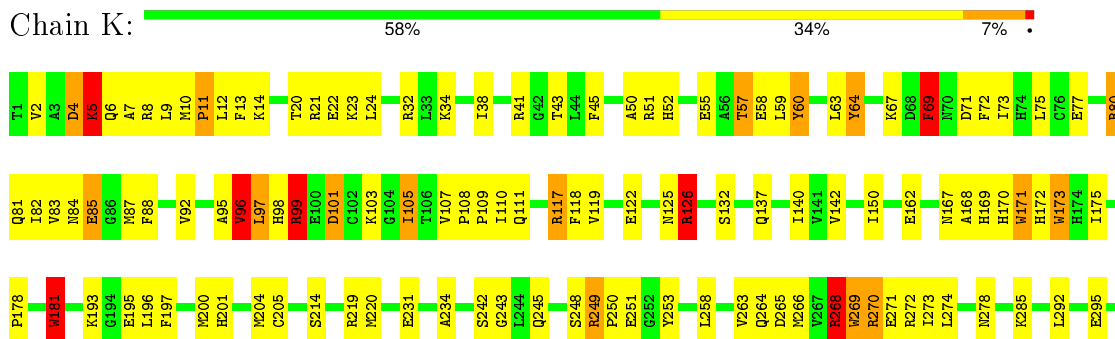


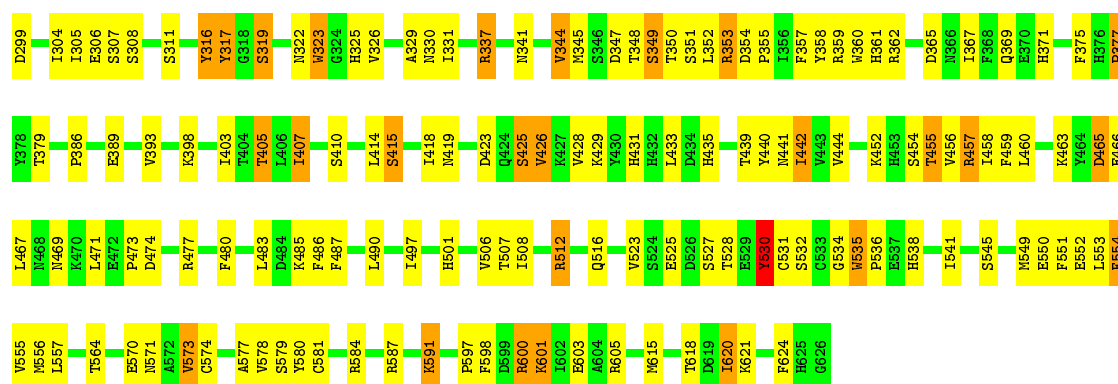


• Molecule 1: Hemocyanin AA6 chain



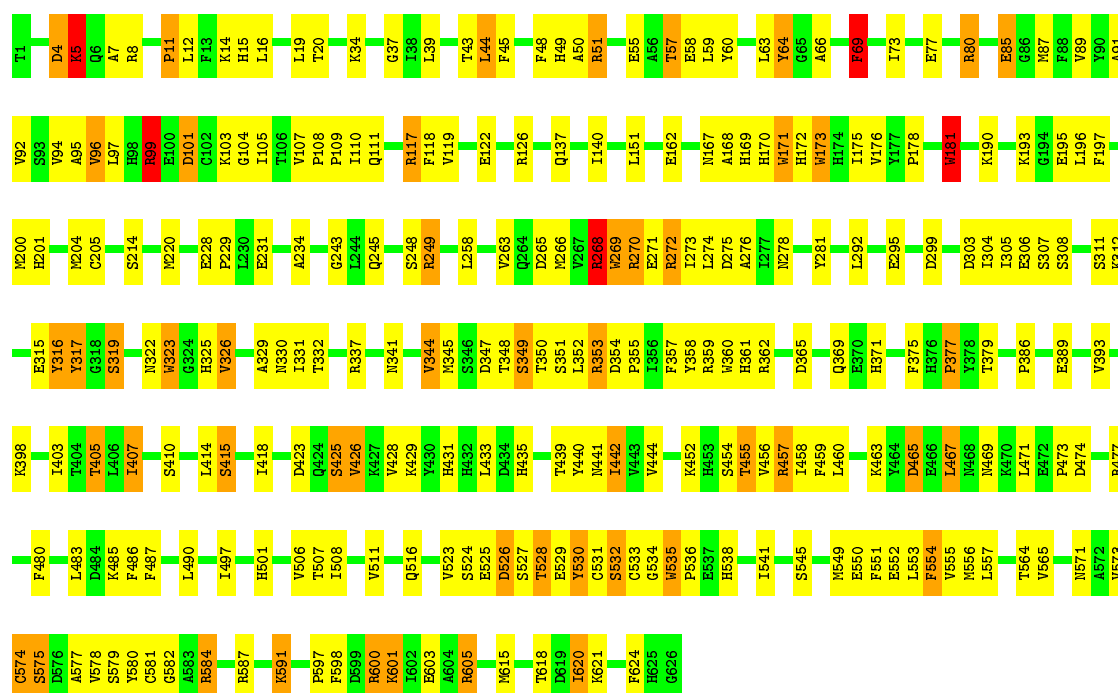
• Molecule 1: Hemocyanin AA6 chain





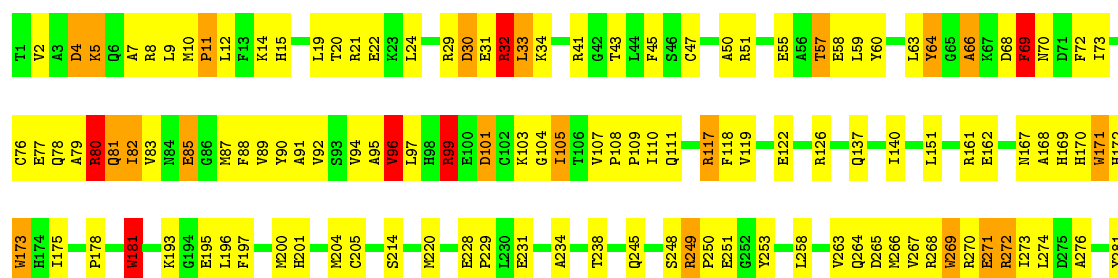
• Molecule 1: Hemocyanin AA6 chain

Chain L: 59% 33% 8% •



• Molecule 1: Hemocyanin AA6 chain

Chain M: 55% 36% 8% •



I541	D465	B376	L292
S545	E466	P377	E295
M549	L467	Y378	
E550	N468	T379	D299
F551	K470	P386	
E552	L471	E389	I304
L553	E472		I305
F554	P473	V393	E306
V555	D474		S307
M556		K398	S308
L557	R477		
	F480	I403	S311
T564		T404	
E570	L483	T405	E315
N571	D484	L406	Y316
A572	K485	I407	Y317
V573	F486		G318
C574	F487	S410	S319
A577	L490	L414	N322
V578		S415	N323
S579	K494		G324
Y580	N495	I418	H325
C581	T496		Y326
	I497	D423	
R584	V498	Q424	A329
	R499	S425	N330
	N500	V426	I331
R587	H501	K427	
K591	H502	V428	R337
	D503	K429	
		Y430	N341
P597	V506	H431	
F598	T507	H432	Y344
F599	I508	L433	K345
R600		D434	S346
K601	R512	H435	D347
L602			T348
E603	Q516	T439	S349
A604	L517	Y440	T350
R605		N441	S351
		I442	L352
M615	V523	V443	R353
	S524	V444	
	E525	E445	F357
T618	D526		Y358
D619	S527	K452	R359
I620	T528	H453	I360
K621	E529	S454	H361
	Y530	T455	R362
F624	C531	V456	
H625	S532	R457	D365
G626	C533	I458	
	Q534	F459	Q369
	H535	L460	E370
	F536		H371
	E537	K463	
	H538	Y464	F375

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C	Depositor
Number of images	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	41
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	10	52
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	7	45
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	8	49
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	6	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	7	45
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	6	43
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	8	48
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	7	45
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	11	53
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	10	52
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	7	45
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	12	47

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%)	8	35
1	C	556/556 (100%)	508 (91%)	48 (9%)	13	47
1	D	556/556 (100%)	503 (90%)	53 (10%)	11	41
1	E	556/556 (100%)	506 (91%)	50 (9%)	12	44
1	F	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	G	556/556 (100%)	508 (91%)	48 (9%)	13	47
1	H	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	I	556/556 (100%)	504 (91%)	52 (9%)	11	42
1	J	556/556 (100%)	503 (90%)	53 (10%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	556/556 (100%)	505 (91%)	51 (9%)	11	43
1	L	556/556 (100%)	504 (91%)	52 (9%)	11	42
1	M	556/556 (100%)	504 (91%)	52 (9%)	11	42
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	16	42

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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.