wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 01:50 AM EST

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 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 (i) 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 (i)) were used in the production of this report:

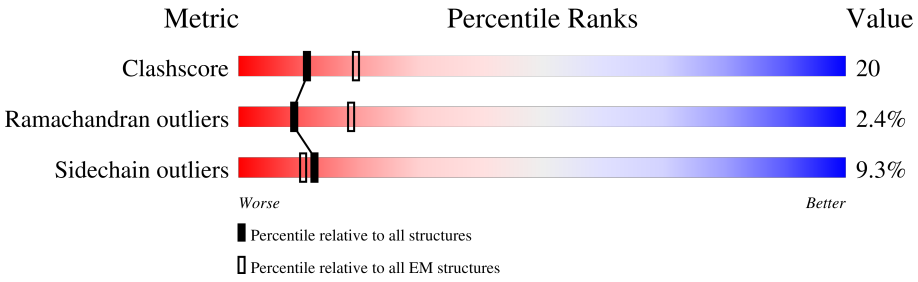
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	626	78% 54% 36% 8% •
1	C	626	82% 59% 33% 7% •
1	D	626	76% 58% 34% 8% •
1	E	626	77% 58% 34% 6% •
1	F	626	81% 58% 32% 8% •
1	G	626	90% 59% 33% 7% •
1	H	626	81% 60% 32% 7% •
1	I	626	77% 58% 34% 8% •

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Mol	Chain	Length	Quality of chain
1	J	626	79% 57% 35% 7%
1	K	626	93% 58% 34% 7%
1	L	626	89% 59% 33% 8%
1	M	626	94% 55% 36% 8%

2 Entry composition (i)

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.

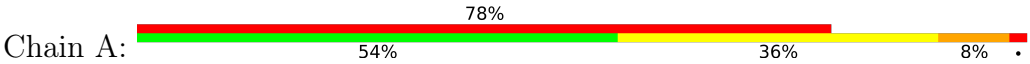
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	C	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	D	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	E	626	Total	C	H	N	O	S	0	0
			6184	3199	1123	877	961	24		
1	F	626	Total	C	H	N	O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

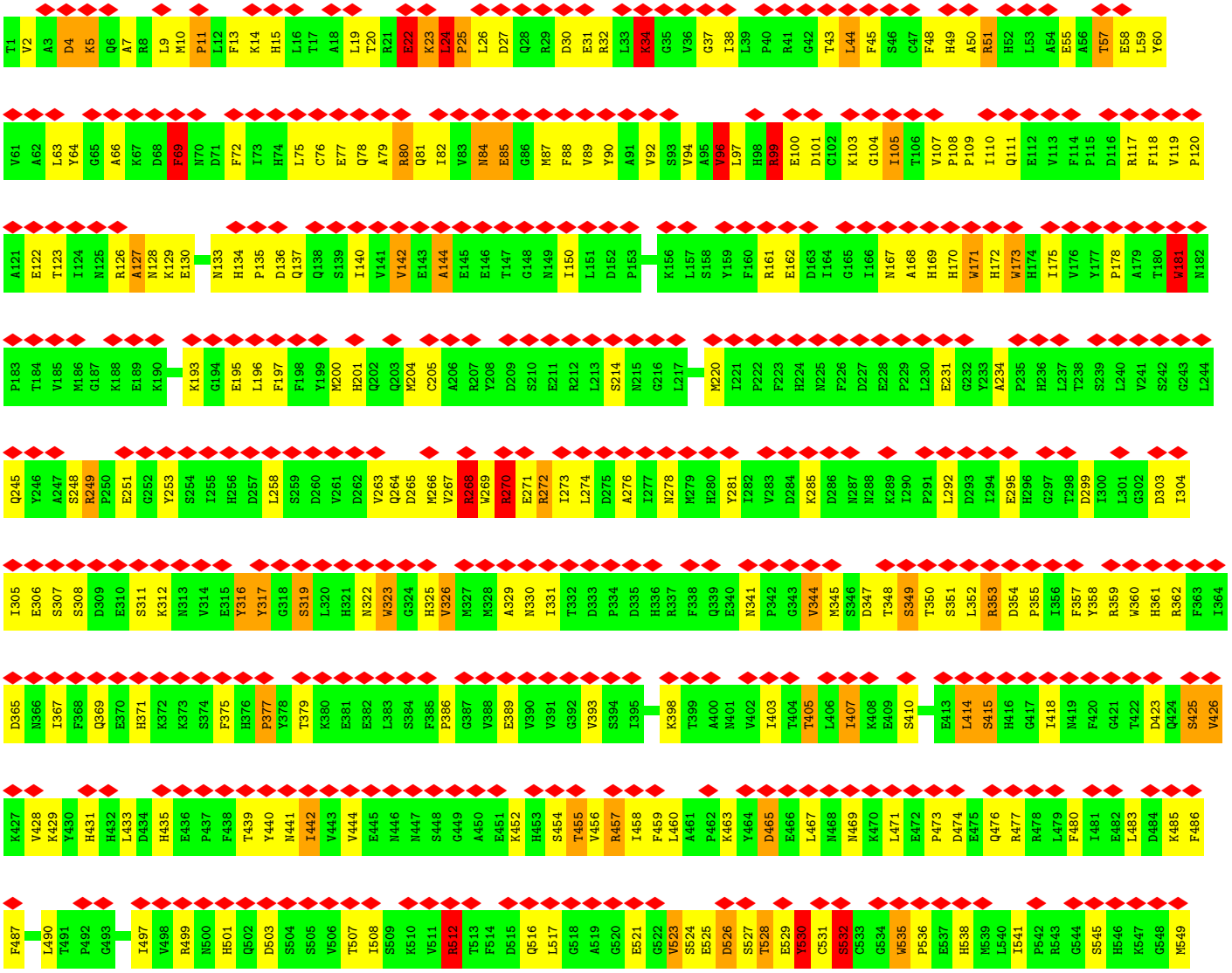
3 Residue-property plots (i)

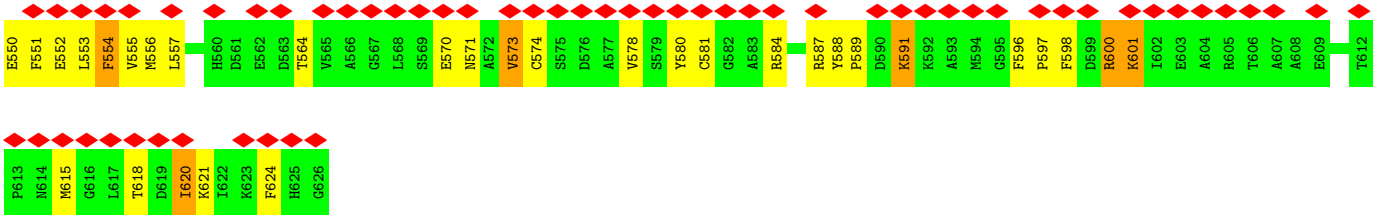
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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

Chain A:

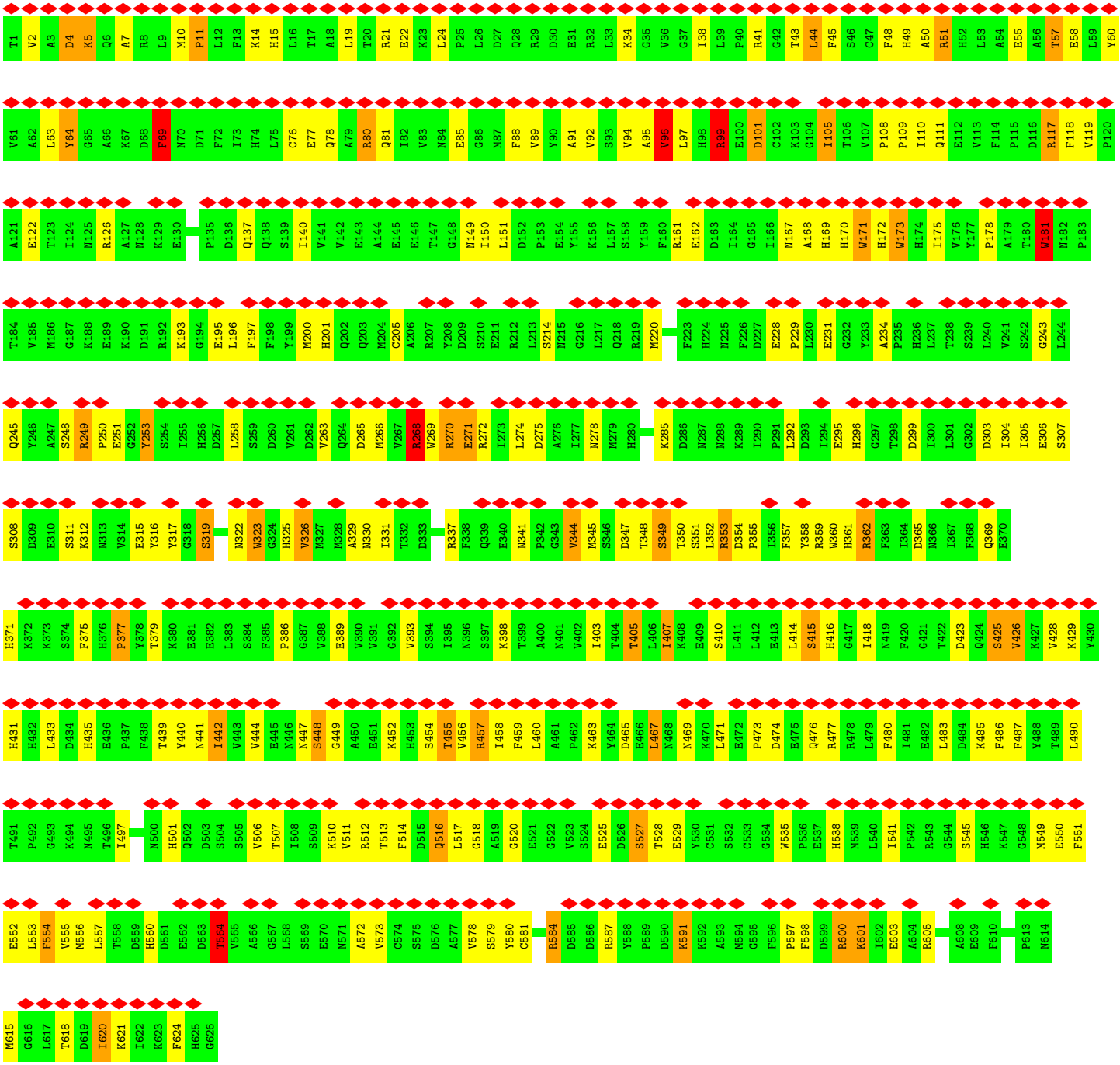






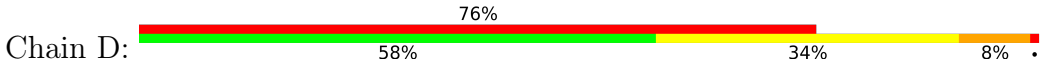
• Molecule 1: Hemocyanin AA6 chain

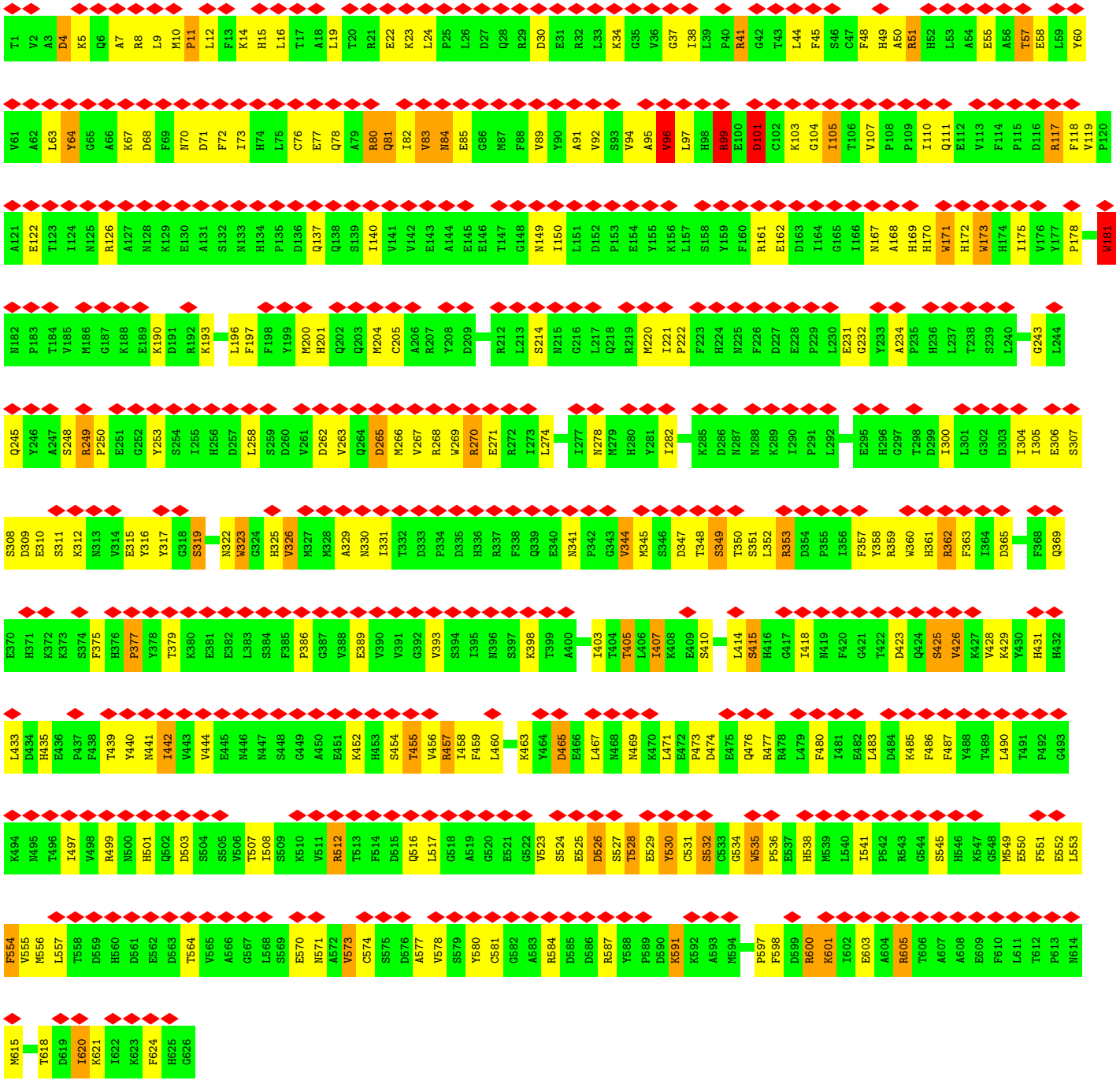
Chain C:



• Molecule 1: Hemocyanin AA6 chain

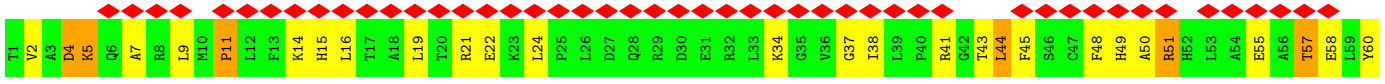
Chain D:

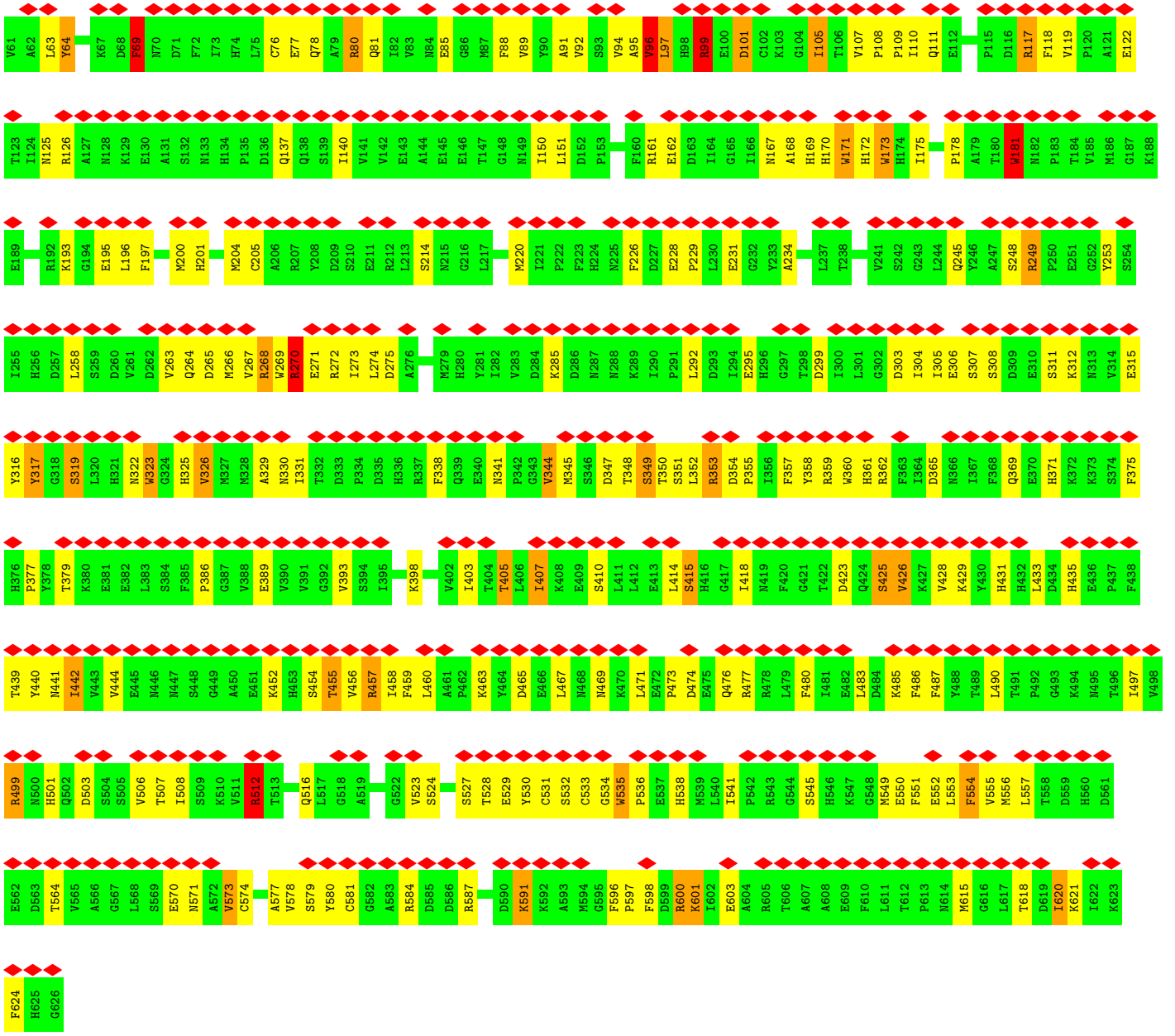




• Molecule 1: Hemocyanin AA6 chain

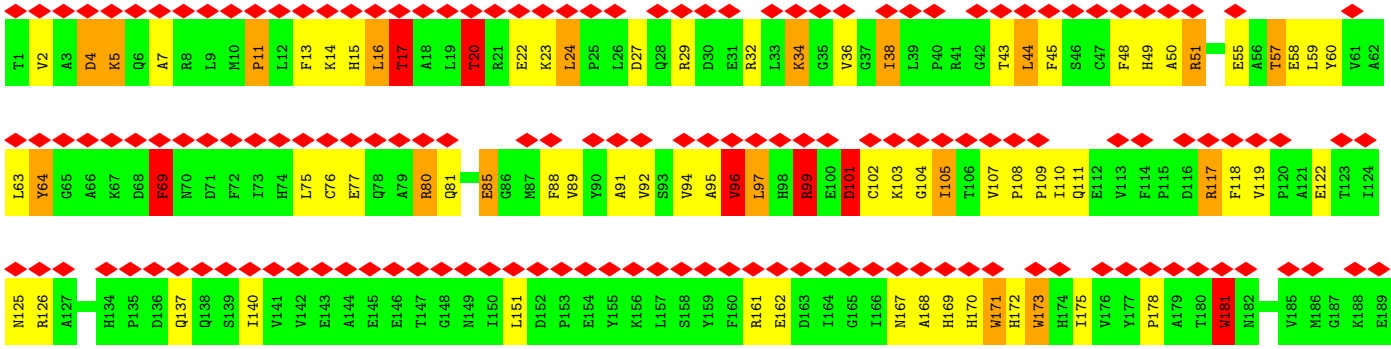
Chain E:

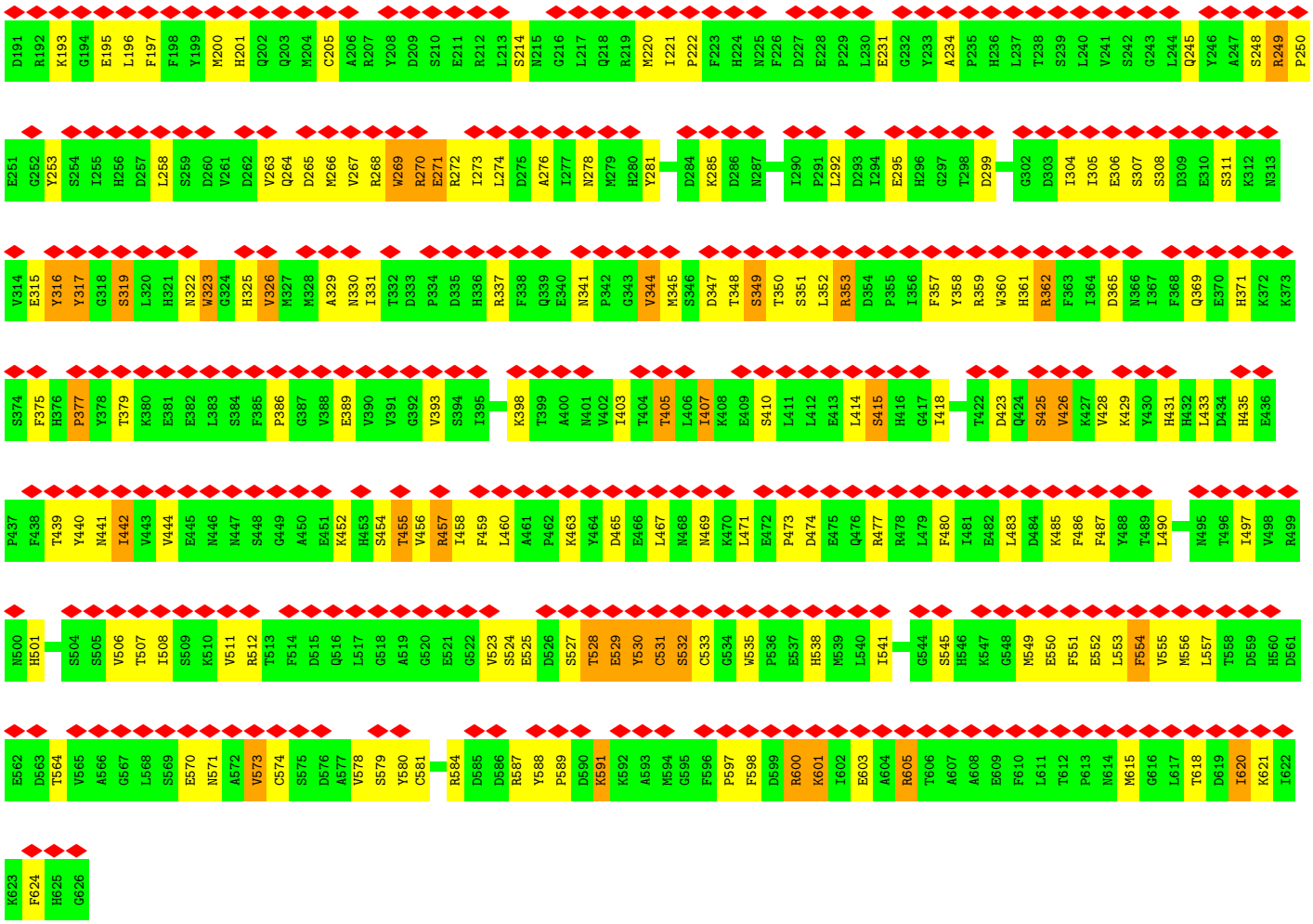




• Molecule 1: Hemocyanin AA6 chain

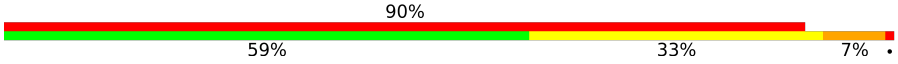
Chain F:

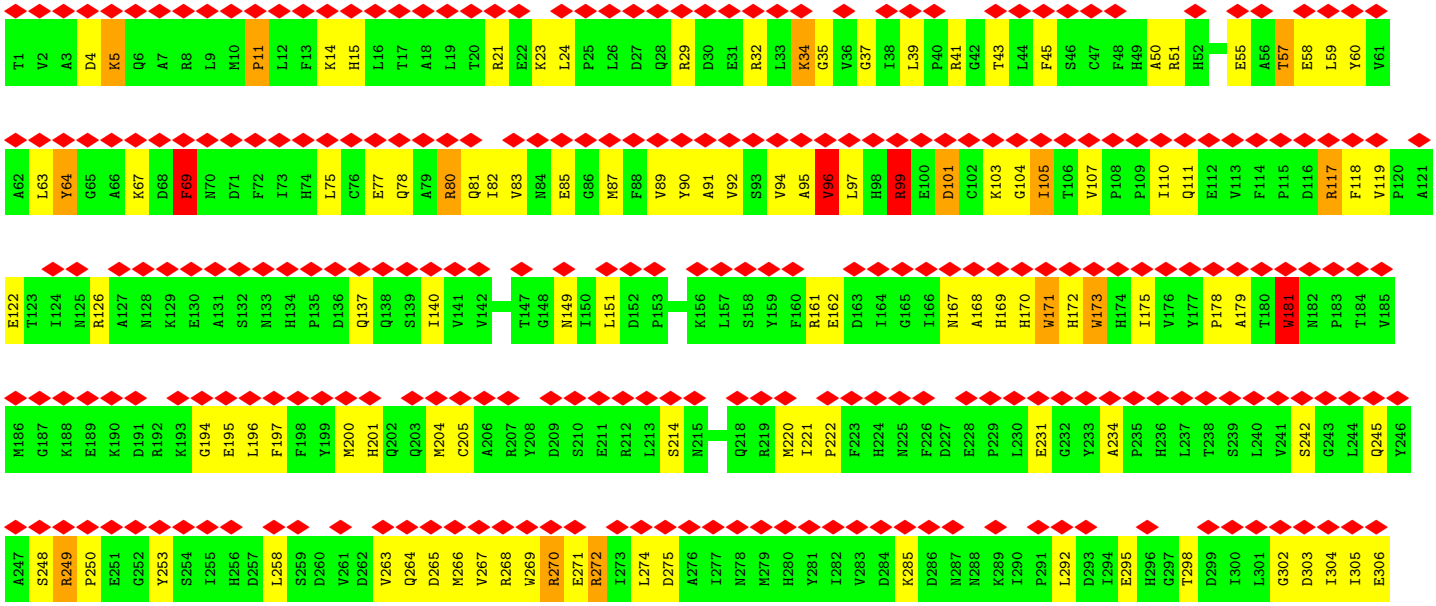


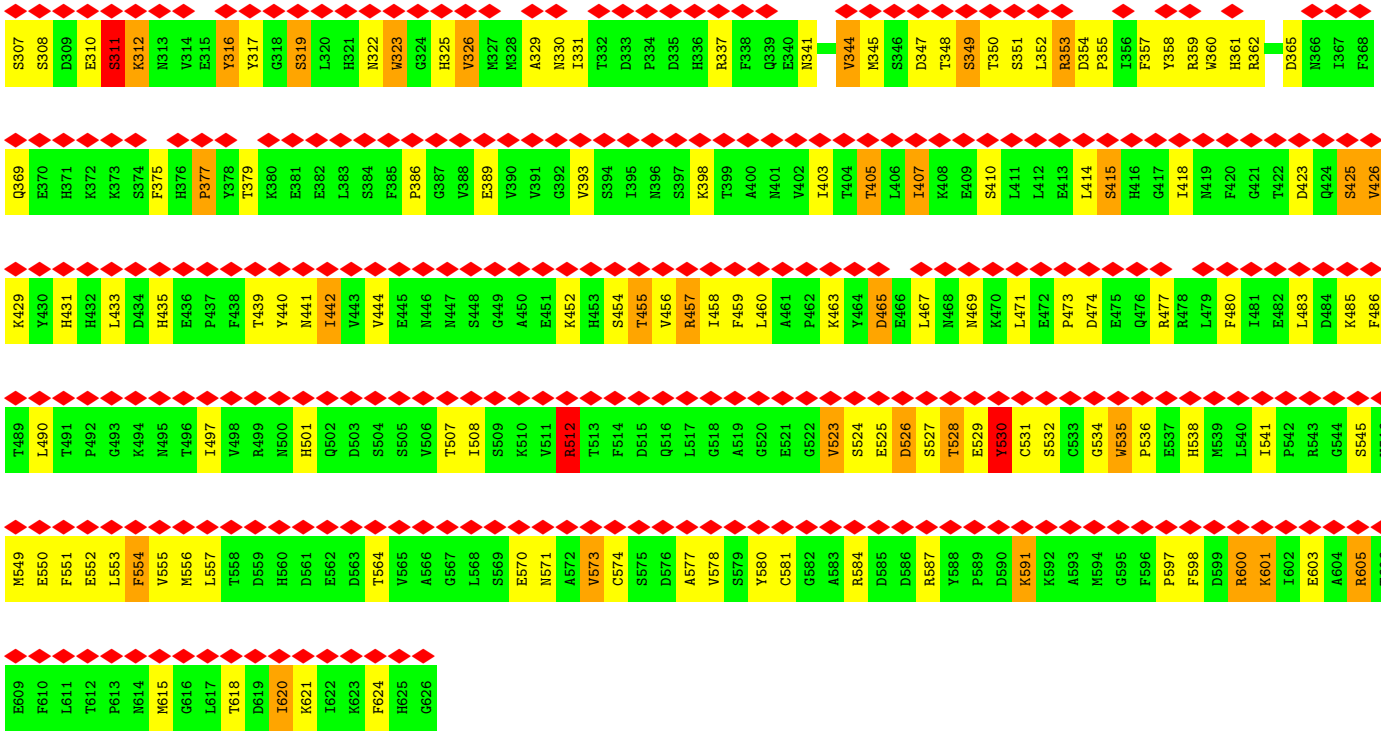


• Molecule 1: Hemocyanin AA6 chain

Chain G:

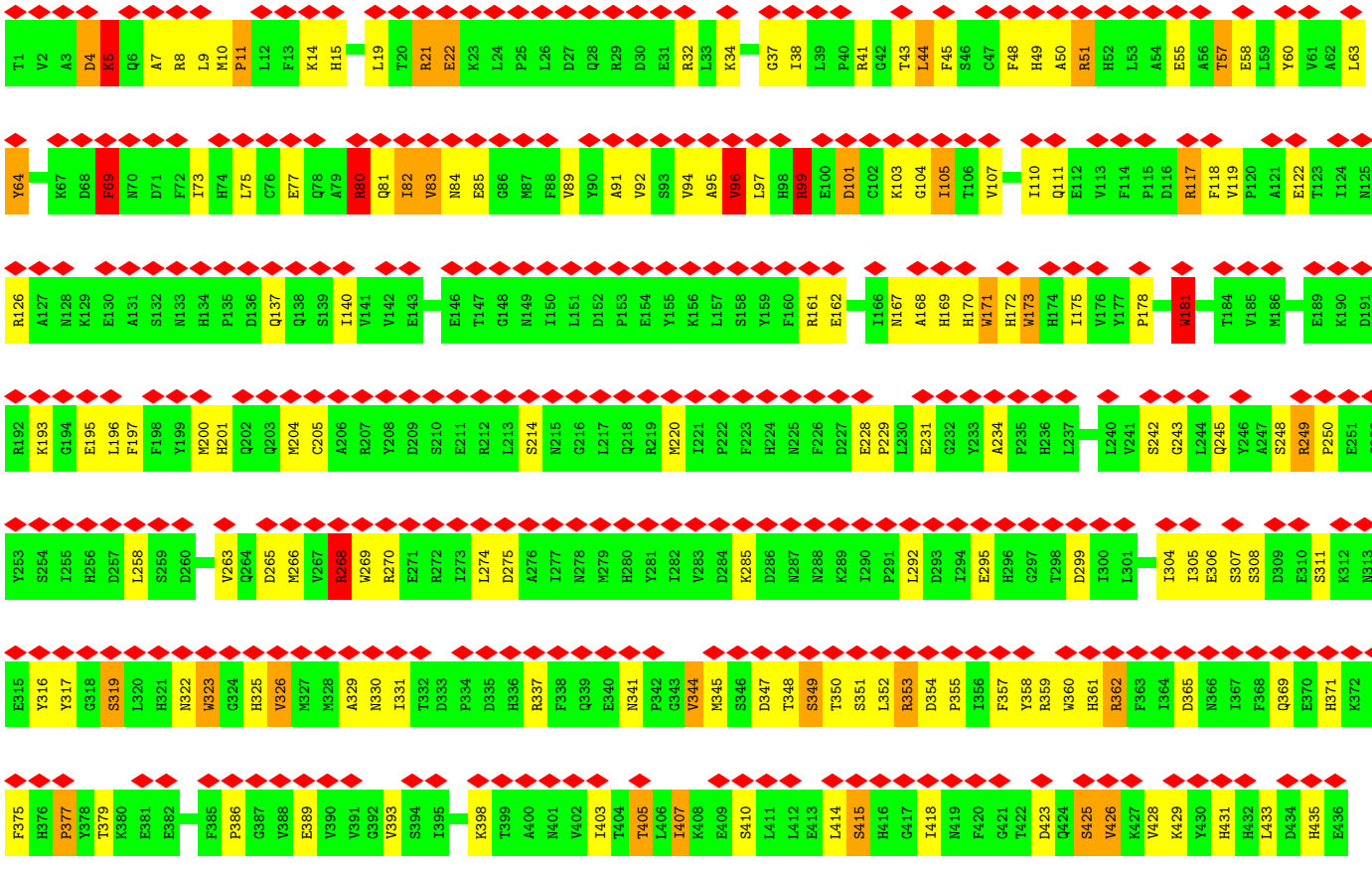






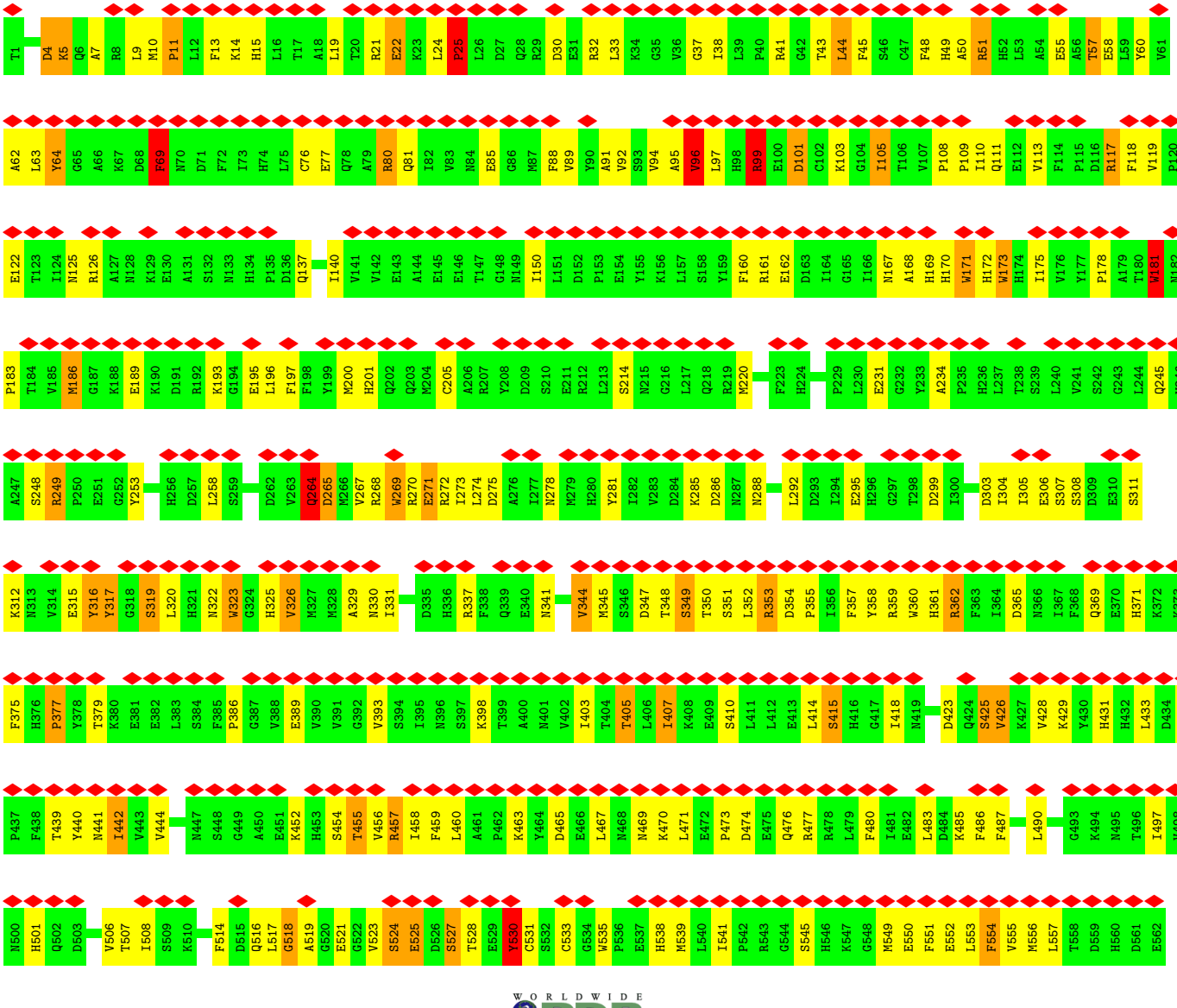
• Molecule 1: Hemocyanin AA6 chain

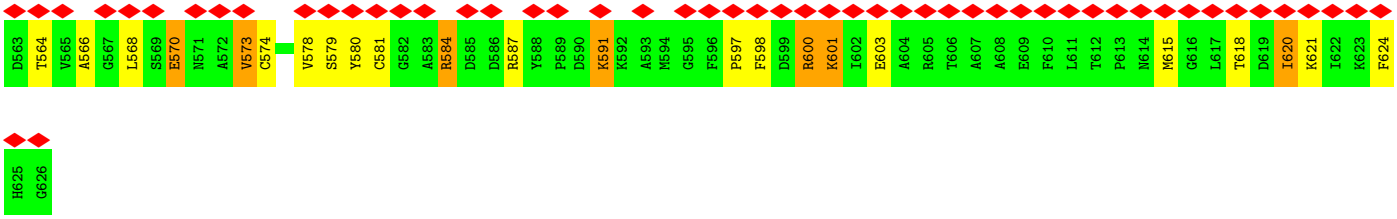
Chain H:



• Molecule 1: Hemocyanin AA6 chain

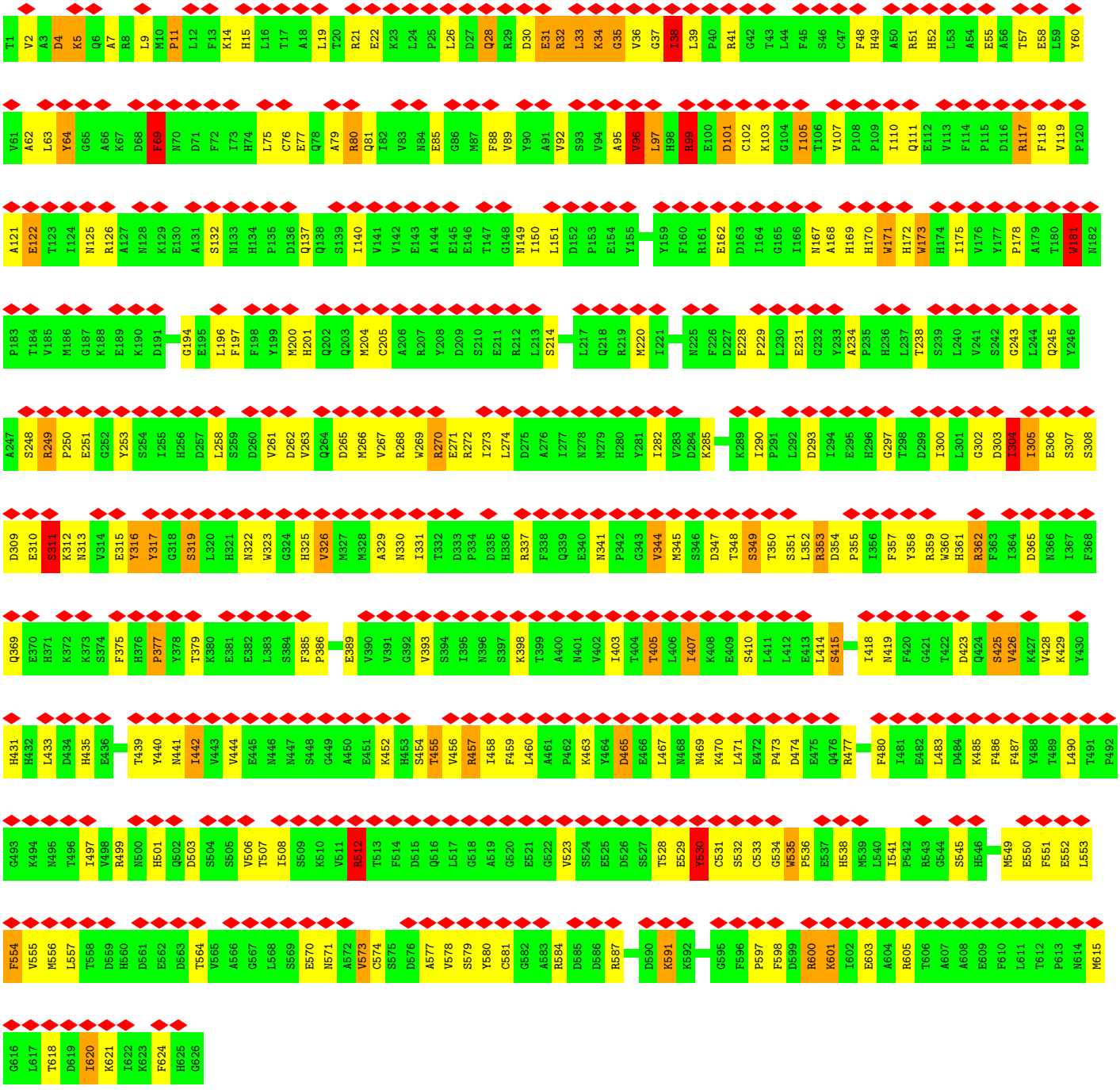
Chain I:





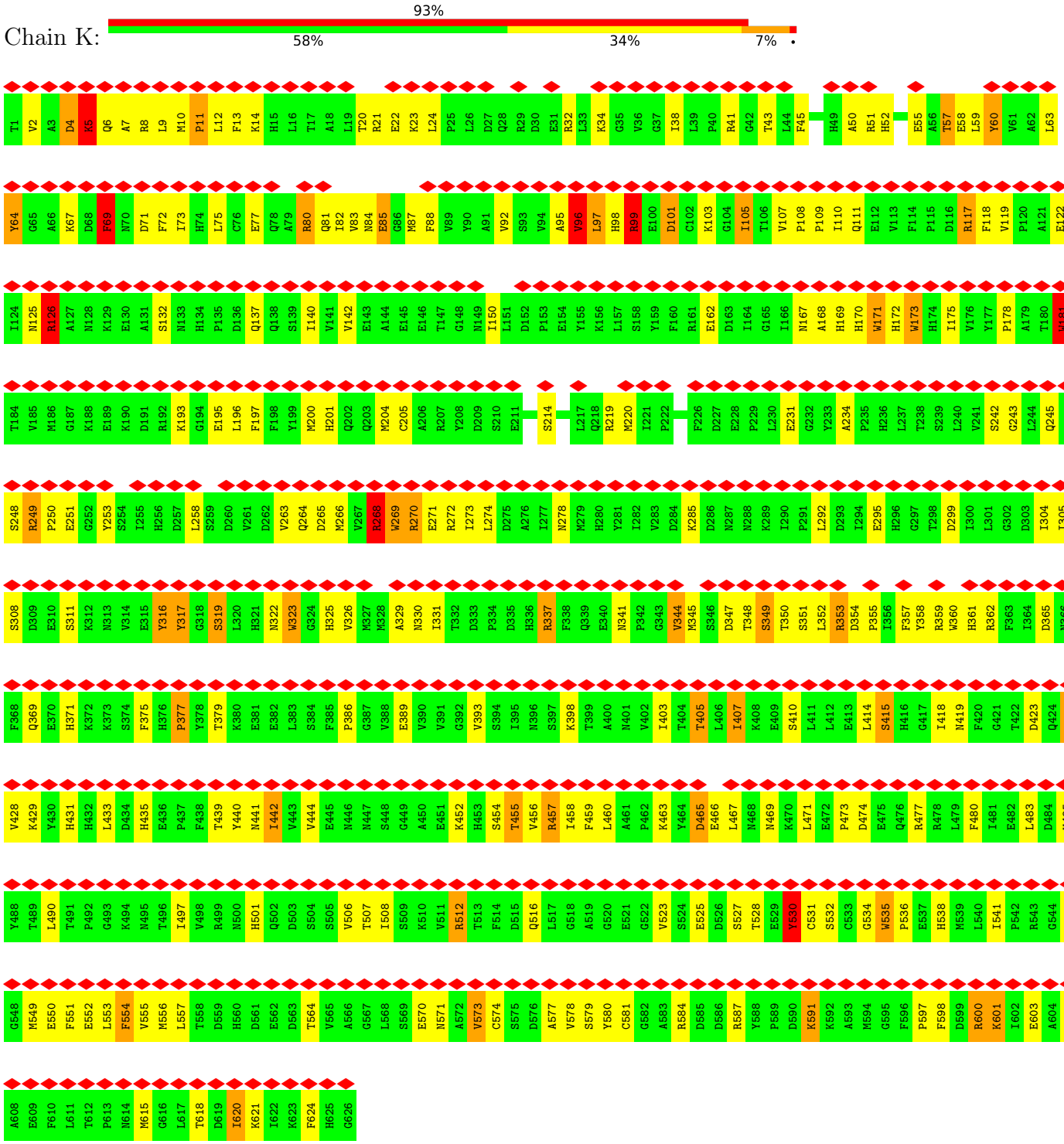
• Molecule 1: Hemocyanin AA6 chain

Chain J:



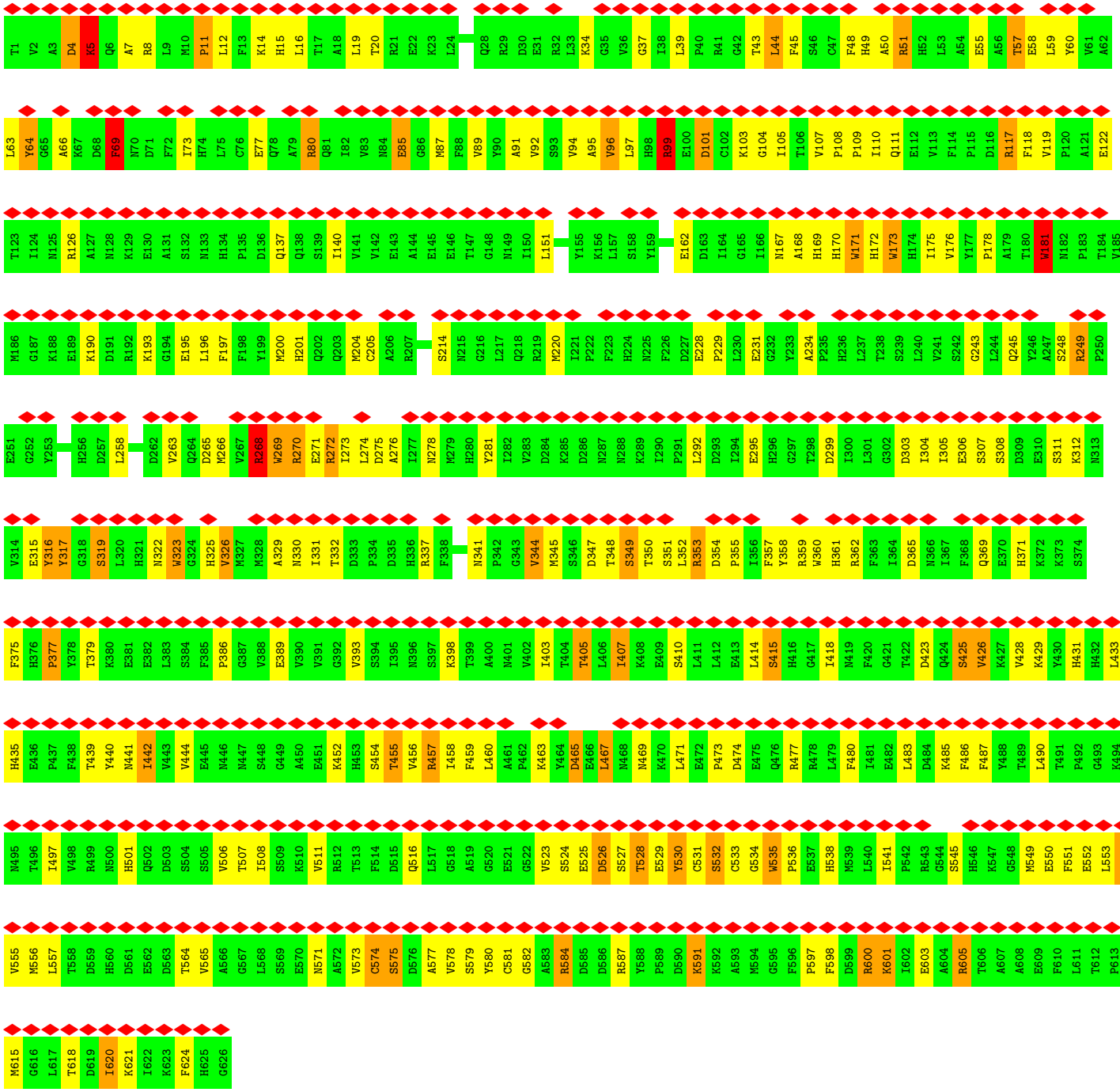
• Molecule 1: Hemocyanin AA6 chain

Chain K:



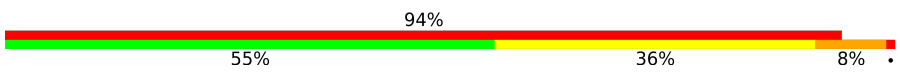
• Molecule 1: Hemocyanin AA6 chain

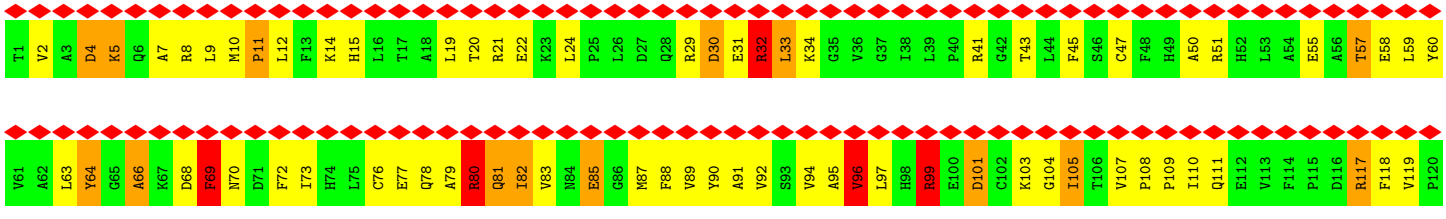
Chain L:

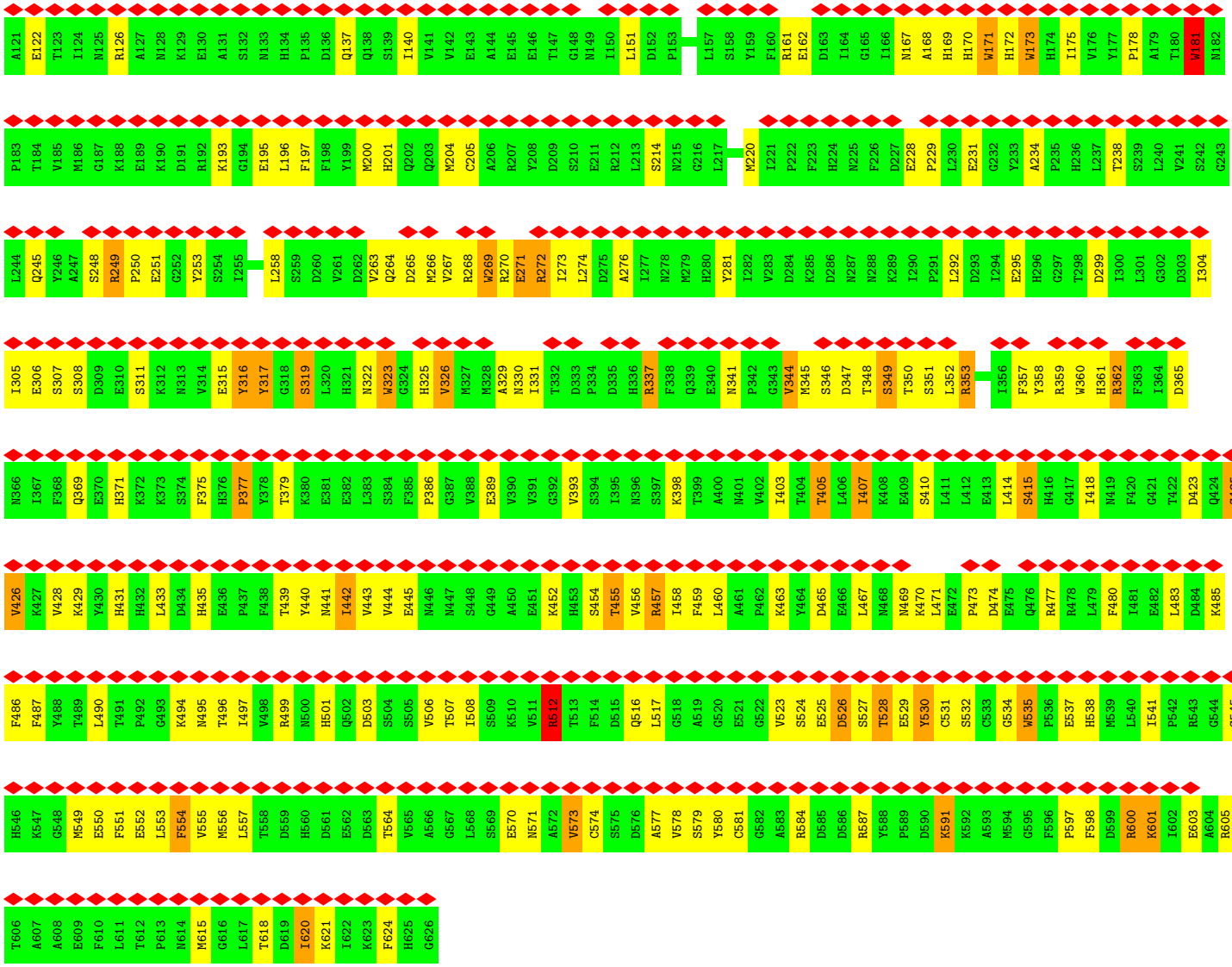


• Molecule 1: Hemocyanin AA6 chain

Chain M:






A121 E122 T123 I124 N125 R126 A127 N128 K129 E130 A131 S132 N133 H134 P135 D136 Q137 Q138 S139 I140 V141 V142 E143 A144 E145 E146 T147 G148 N149 I150 L151 D152 P153 L157 S158 Y159 F160 R161 E162 D163 I164 G165 I166 N167 A168 H169 H170 W171 H172 W173 H174 I175 V176 Y177 P178 A179 T180 W181 N182
P183 T184 V185 M186 G187 K188 E189 K190 D191 R192 K193 G194 E195 L196 F197 F198 Y199 M200 H201 Q202 Q203 M204 C205 A206 R207 Y208 D209 S210 E211 R212 L213 S214 N215 G216 L217 M220 I221 P222 F223 H224 N225 F226 D227 E228 P229 L230 E231 G232 Y233 A234 P235 H236 L237 T238 S239 L240 V241 S242 G243
L244 Q245 Y246 A247 S248 R249 P250 E251 G252 Y253 S254 I255 L258 S259 D260 V261 D262 V263 Q264 D265 M266 V267 R268 W269 R270 E271 R272 I273 L274 D275 A276 I277 N278 M279 H280 Y281 I282 V283 D284 K285 D286 N287 N288 K289 I290 P291 L292 D293 I294 E295 H296 G297 T298 D299 I300 L301 G302 D303 I304
I305 E306 S307 S308 D309 E310 S311 K312 N313 V314 E315 Y316 Y317 G318 S319 L320 H321 N322 W323 G324 H325 V326 M327 M328 A329 N330 I331 T332 D333 P334 D335 H336 R337 F338 Q339 E340 N341 P342 G343 V344 M345 S346 D347 T348 S349 T350 S351 L352 R353 I356 F357 Y358 R359 W360 H361 R362 F363 I364 D365
N366 I367 F368 Q369 E370 H371 K372 K373 S374 F375 H376 P377 Y378 T379 K380 E381 E382 L383 S384 F385 P386 G387 V388 E389 V390 V391 G392 V393 S394 I395 N396 S397 K398 T399 A400 N401 V402 I403 T404 T405 L406 I407 K408 E409 S410 L411 L412 E413 L414 S415 H416 G417 I418 N419 F420 G421 T422 D423 Q424 S425
Y426 K427 V428 K429 Y430 H431 H432 L433 D434 H435 E436 P437 F438 T439 Y440 N441 I442 V443 V444 E445 N446 N447 S448 G449 A450 E451 K452 H453 S454 T455 V456 R457 I458 F459 L460 A461 P462 K463 Y464 D465 E466 L467 N468 N469 K470 L471 E472 P473 D474 E475 Q476 R477 R478 L479 F480 I481 E482 L483 D484 K485
F486 F487 Y488 T489 L490 T491 P492 G493 K494 N495 T496 I497 V498 R499 N500 H501 Q502 D503 S504 S505 V506 T507 I508 S509 K510 V511 R512 T513 F514 D515 Q516 L517 G518 A519 G520 E521 G522 V523 S524 E525 D526 S527 T528 E529 Y530 C531 S532 C533 G534 W535 P536 E537 H538 M539 L540 I541 P542 R543 G544 S545
H546 K547 G548 M549 E550 F551 E552 L553 F554 V555 M556 L557 T558 D559 H560 D561 E562 D563 T564 V565 A566 G567 L568 S569 E570 N571 A572 V573 C574 S575 D576 A577 V578 S579 Y580 C581 G582 A583 R584 D585 D586 R587 Y588 P589 D590 K591 K592 A593 M594 G595 F596 P597 F598 D599 R600 K601 I602 E603 A604 R605
T606 A607 A608 E609 F610 L611 T612 P613 N614 M615 G616 L617 T618 D619 I620 K621 I622 K623 F624 H625 G626

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	13400	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.663	Depositor
Minimum map value	-0.473	Depositor
Average map value	0.074	Depositor
Map value standard deviation	0.264	Depositor
Recommended contour level	1.16	Depositor
Map size (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.8, 1.8, 1.8	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	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(^{o})	Ideal(^{o})
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 (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	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:CE1	1:K:69:PHE:CZ	1.94	1.55
1:G:69:PHE:CD2	1:G:69:PHE:CE2	1.96	1.54
1:G:69:PHE:CD1	1:G:69:PHE:CE1	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 (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 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%)	4 26
1	C	622/626 (99%)	526 (85%)	84 (14%)	12 (2%)	8 38
1	D	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	5 31
1	E	624/626 (100%)	529 (85%)	81 (13%)	14 (2%)	6 35
1	F	624/626 (100%)	529 (85%)	77 (12%)	18 (3%)	4 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	624/626 (100%)	532 (85%)	76 (12%)	16 (3%)	5 31
1	H	624/626 (100%)	528 (85%)	78 (12%)	18 (3%)	4 29
1	I	622/626 (99%)	529 (85%)	79 (13%)	14 (2%)	6 34
1	J	624/626 (100%)	533 (85%)	75 (12%)	16 (3%)	5 31
1	K	624/626 (100%)	532 (85%)	81 (13%)	11 (2%)	8 40
1	L	624/626 (100%)	531 (85%)	81 (13%)	12 (2%)	8 38
1	M	624/626 (100%)	526 (84%)	82 (13%)	16 (3%)	5 31
All	All	7484/7512 (100%)	6348 (85%)	953 (13%)	183 (2%)	9 33

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 (i)

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%)	6 23
1	C	556/556 (100%)	508 (91%)	48 (9%)	10 32
1	D	556/556 (100%)	503 (90%)	53 (10%)	8 27
1	E	556/556 (100%)	506 (91%)	50 (9%)	9 30
1	F	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	G	556/556 (100%)	508 (91%)	48 (9%)	10 32
1	H	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	I	556/556 (100%)	504 (91%)	52 (9%)	8 28
1	J	556/556 (100%)	503 (90%)	53 (10%)	8 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	556/556 (100%)	505 (91%)	51 (9%)	9 29
1	L	556/556 (100%)	504 (91%)	52 (9%)	8 28
1	M	556/556 (100%)	504 (91%)	52 (9%)	8 28
All	All	6672/6672 (100%)	6051 (91%)	621 (9%)	12 28

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

Mol	Chain	Res	Type
1	J	601	LYS
1	M	85	GLU
1	K	101	ASP
1	J	591	LYS
1	L	57	THR

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

Mol	Chain	Res	Type
1	H	169	HIS
1	M	81	GLN
1	I	288	ASN
1	L	431	HIS
1	L	81	GLN

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 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	I	2
1	C	2
1	A	1
1	E	1
1	F	1
1	H	1
1	L	1

The worst 5 of 9 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	34:LYS	C	35:GLY	N	4.15
1	C	519:ALA	C	520:GLY	N	2.61
1	A	44:LEU	C	45:PHE	N	1.71
1	C	44:LEU	C	45:PHE	N	1.71
1	E	44:LEU	C	45:PHE	N	1.71

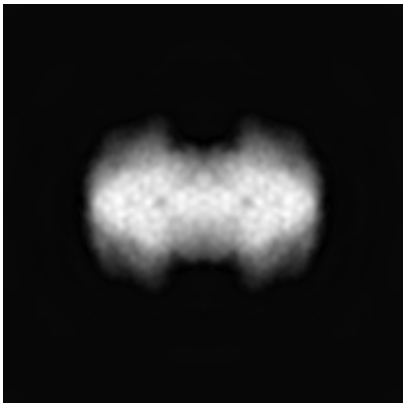
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-5101. 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.

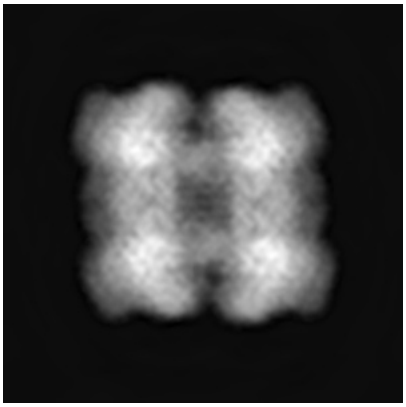
6.1 Orthogonal projections

6.1.1 Primary map



X

Y

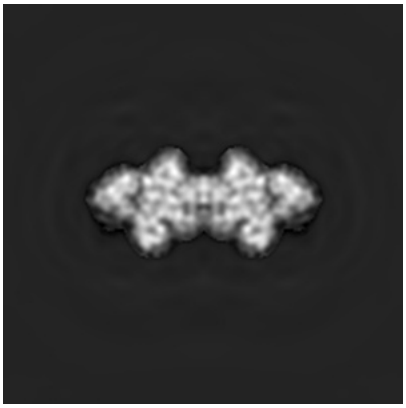


Z

The images above show the map projected in three orthogonal directions.

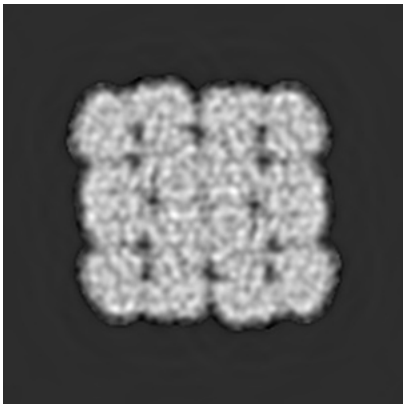
6.2 Central slices

6.2.1 Primary map



X Index: 104

Y Index: 104

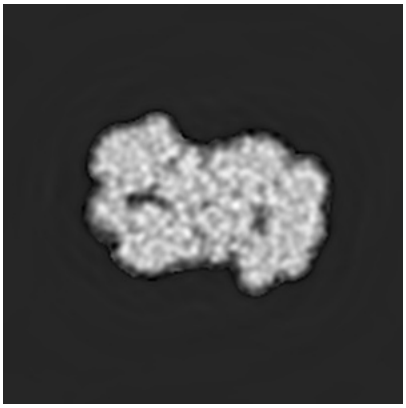


Z Index: 104

The images above show central slices of the map in three orthogonal directions.

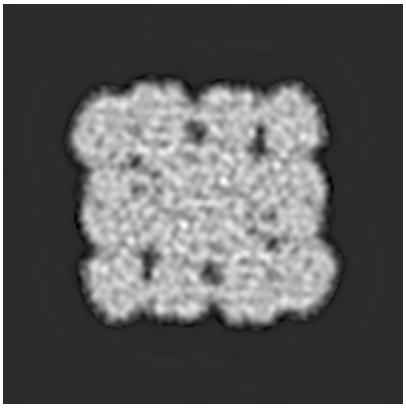
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 75

Y Index: 133

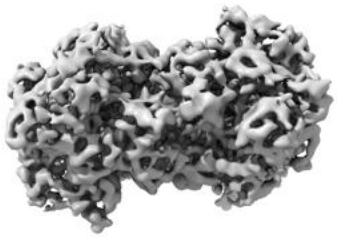


Z Index: 107

The images above show the largest variance slices of the map in three orthogonal directions.

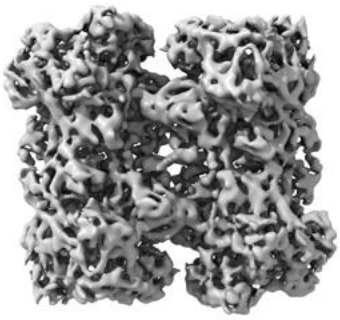
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

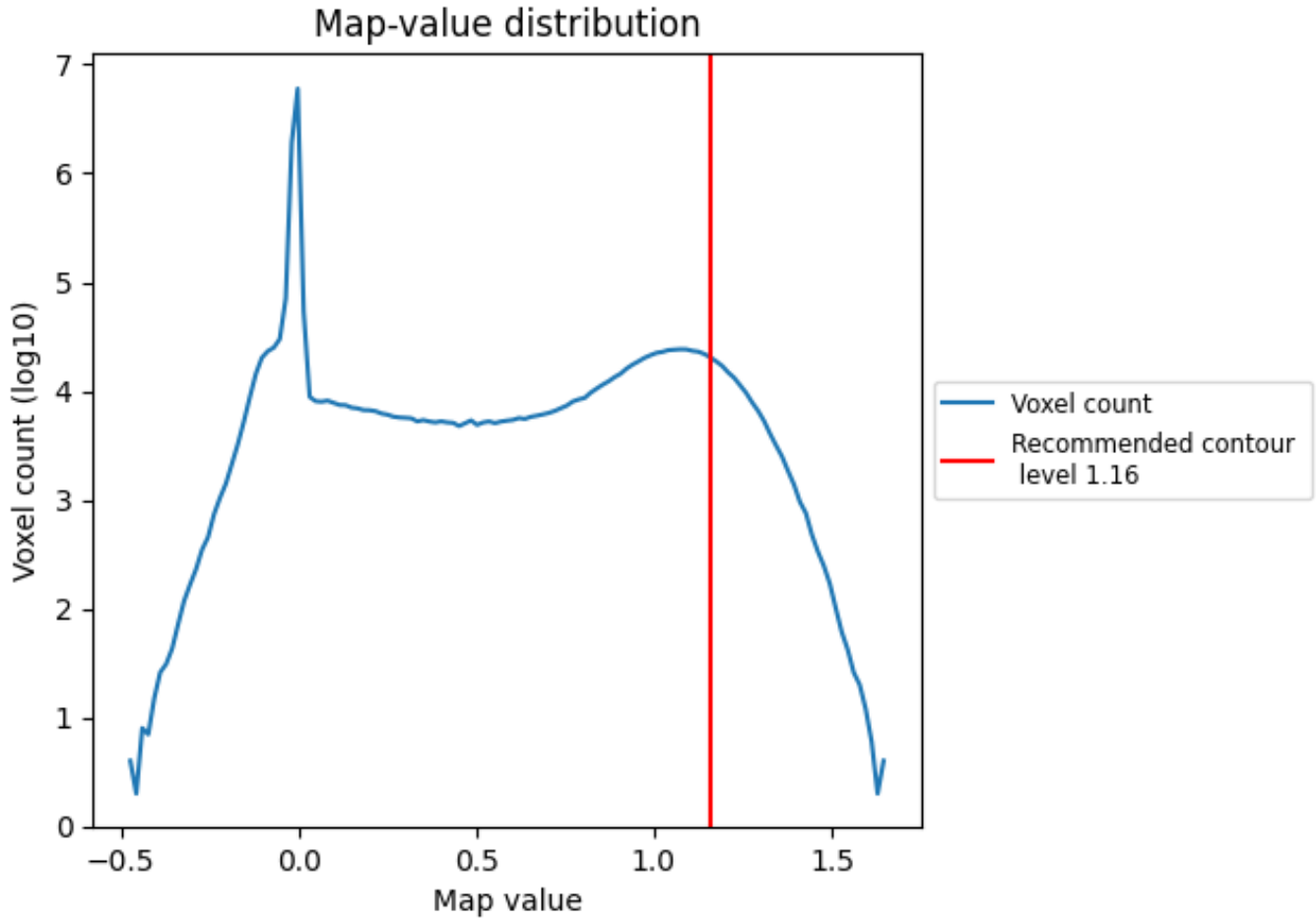
6.5 Mask visualisation (i)

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

7 Map analysis

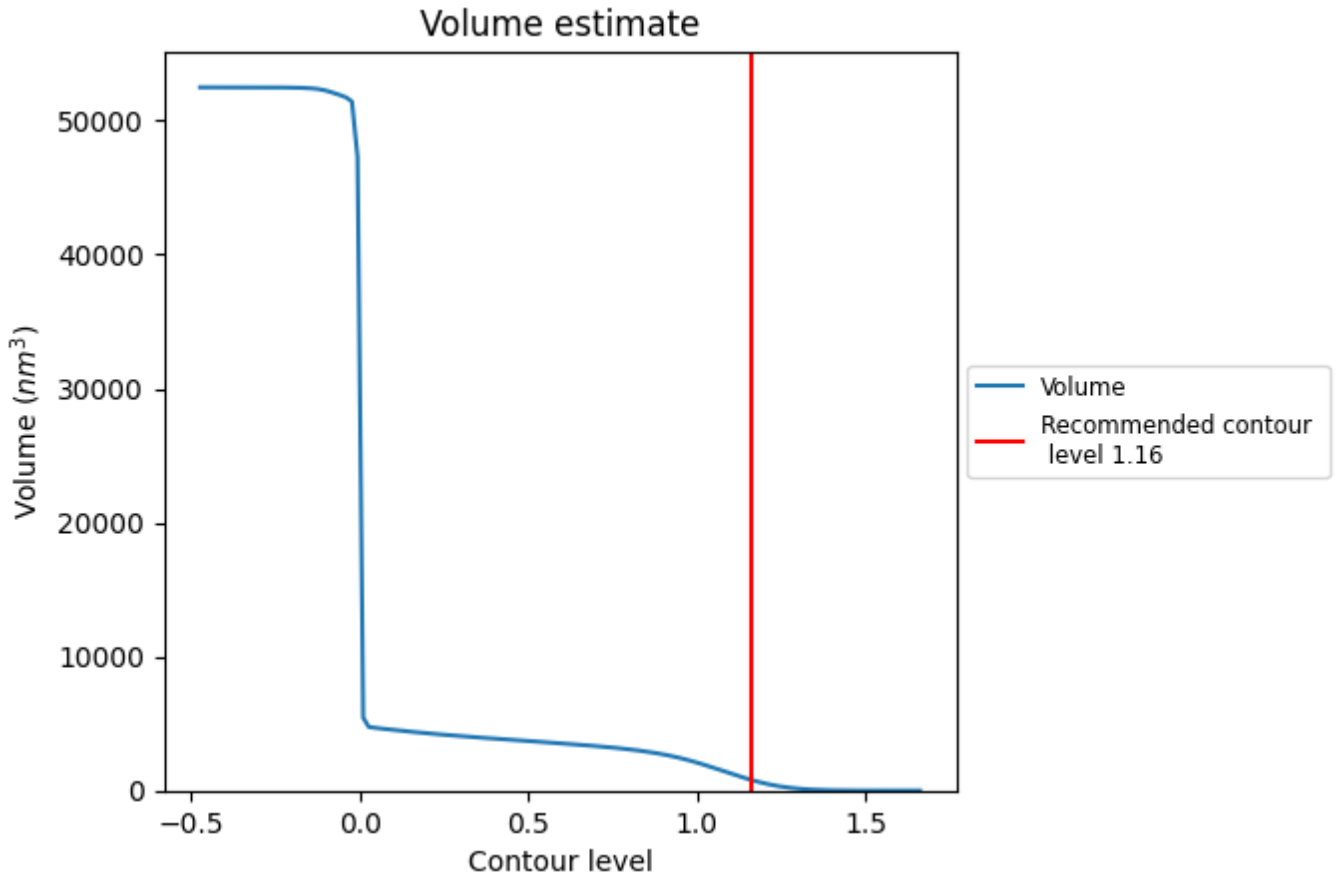
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

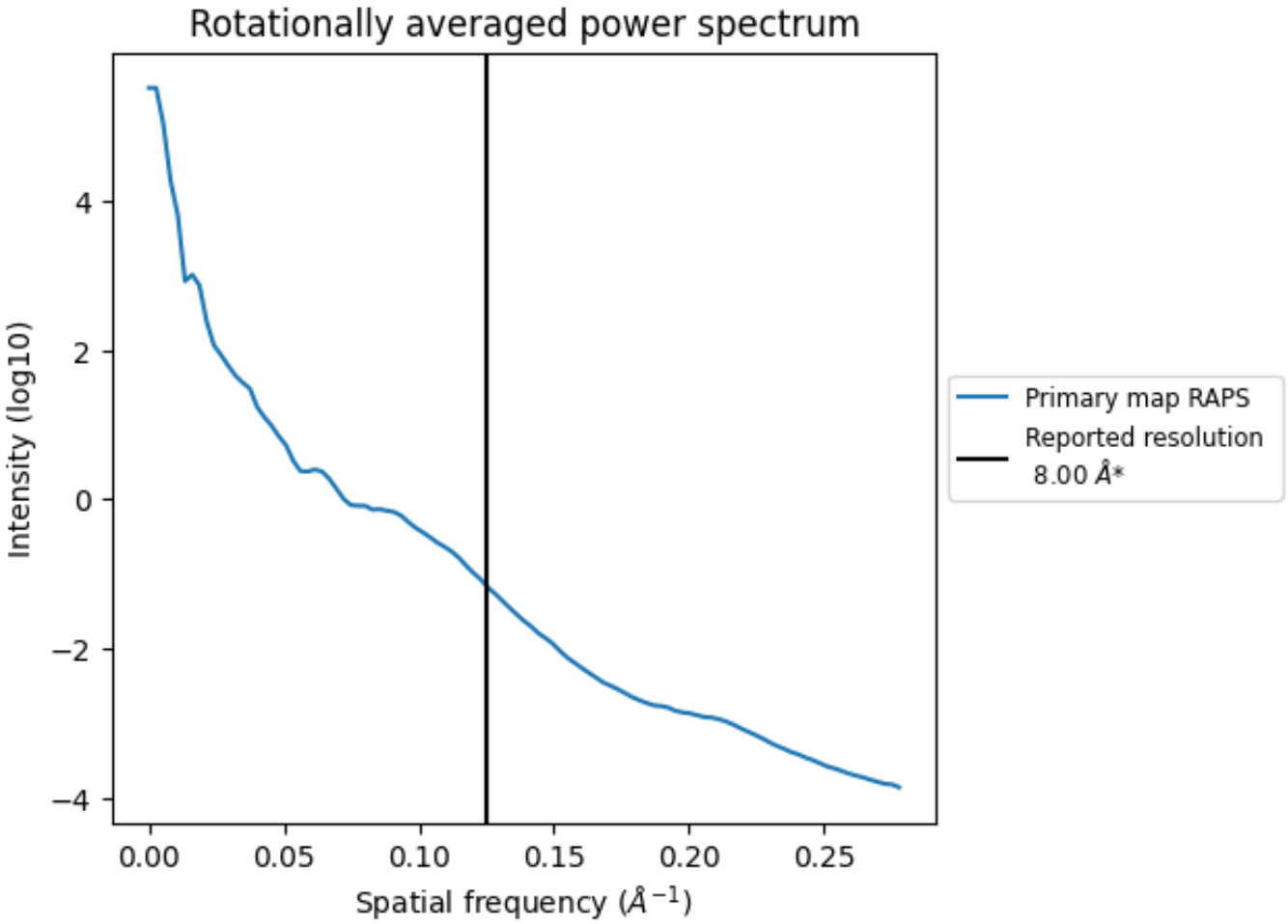
7.2 Volume estimate (i)



The volume at the recommended contour level is 811 nm^3; this corresponds to an approximate mass of 733 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.125 Å^{-1}

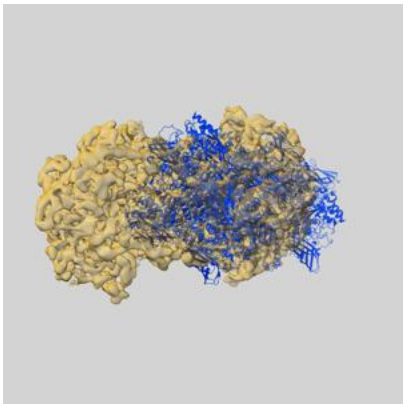
8 Fourier-Shell correlation (i)

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

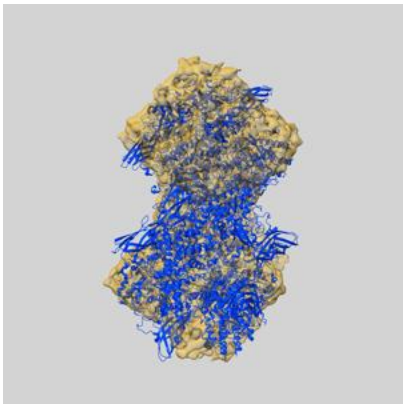
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-5101 and PDB model 3IXW. Per-residue inclusion information can be found in section 3 on page 5.

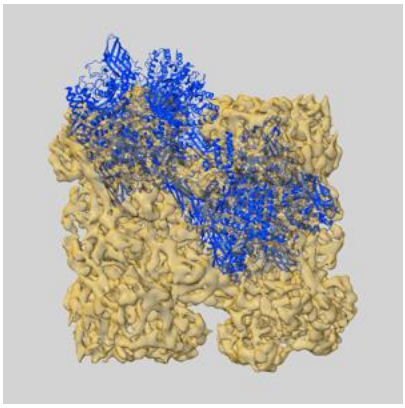
9.1 Map-model overlay



X



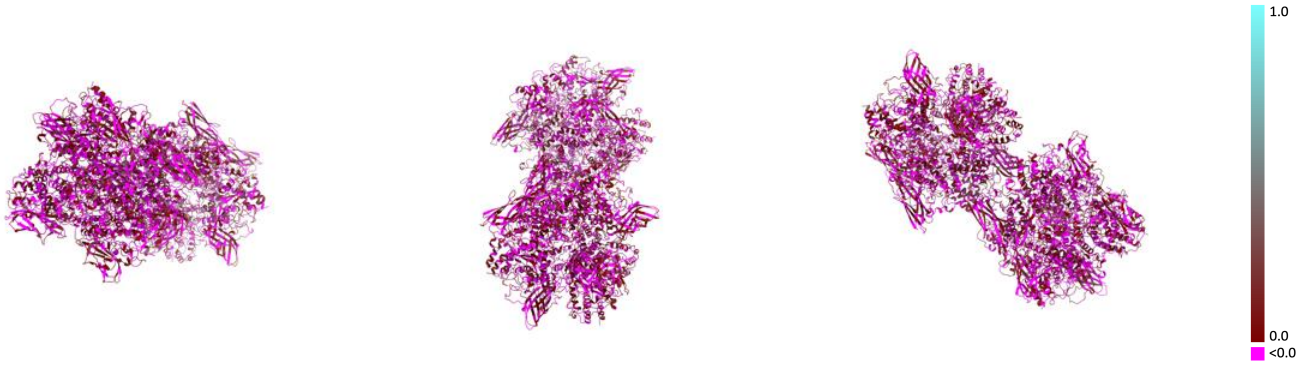
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

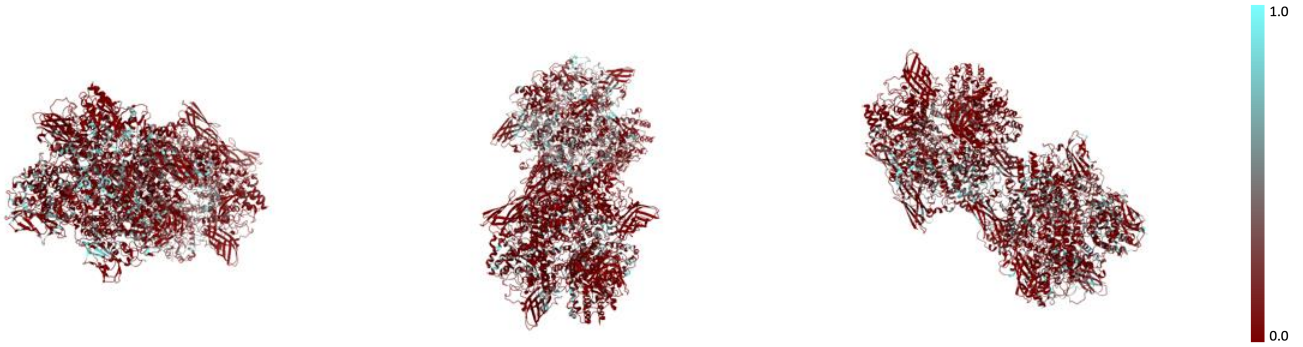
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

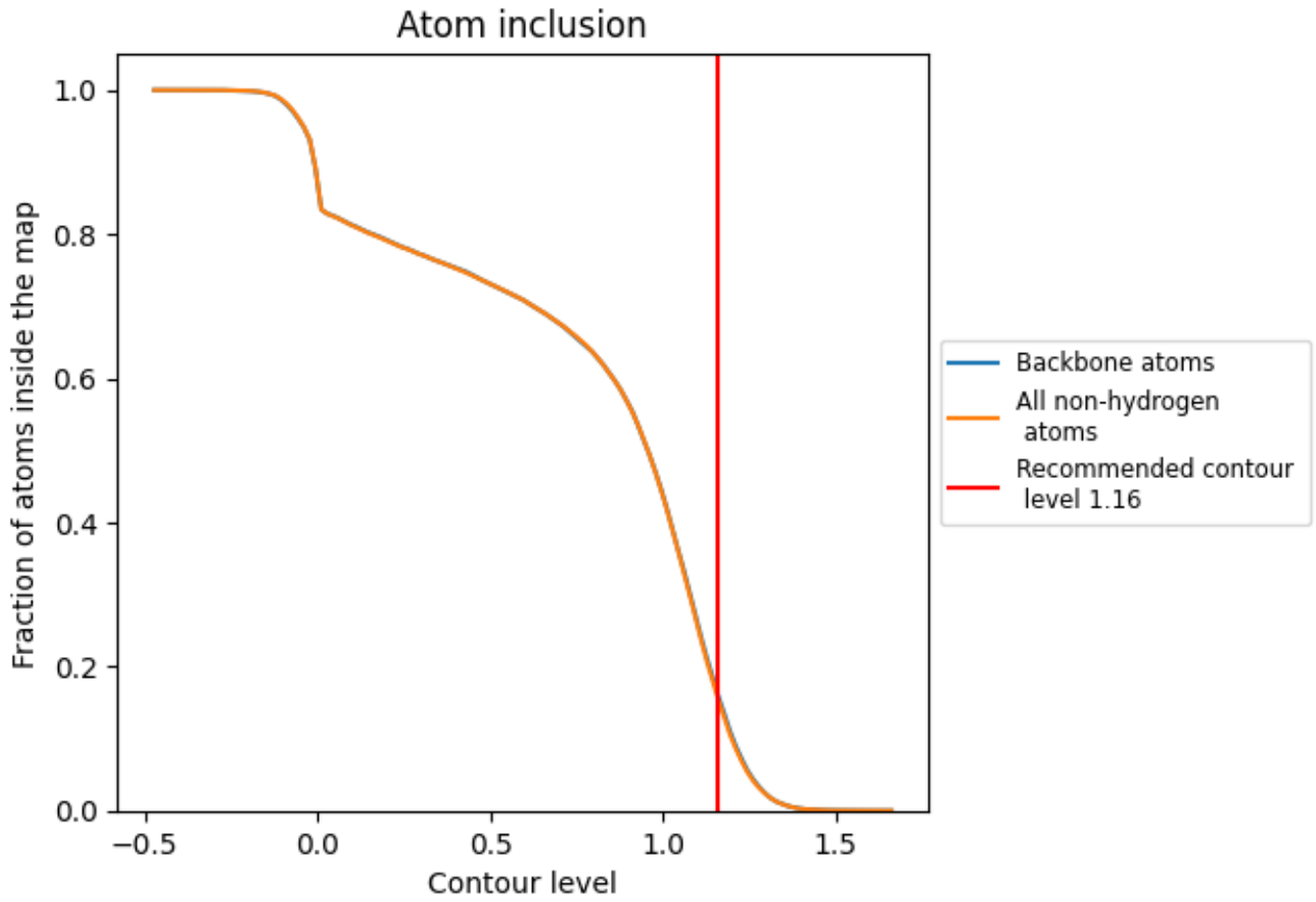
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.16).

9.4 Atom inclusion (i)



At the recommended contour level, 16% of all backbone atoms, 16% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (1.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.1556	0.0080
A	0.2052	-0.0000
C	0.1646	0.0050
D	0.2167	0.0110
E	0.2153	0.0120
F	0.1752	0.0040
G	0.0886	0.0030
H	0.1672	0.0100
I	0.2075	0.0090
J	0.1960	0.0100
K	0.0610	0.0080
L	0.0959	0.0110
M	0.0576	0.0090