



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 01:14 am GMT

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.

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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.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

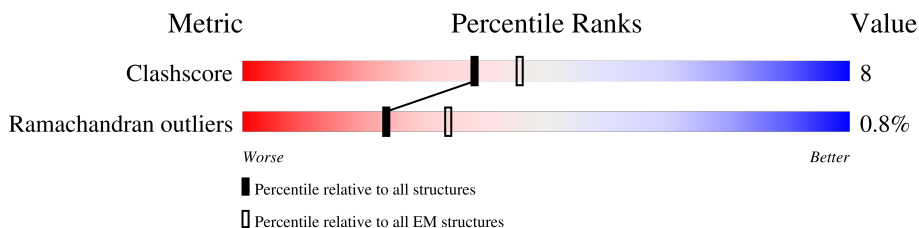
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 $\leq 5\%$. 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	10a	3314	
1	1a	3314	
1	2a	3314	
1	3a	3314	
1	4a	3314	
1	5a	3314	
1	6a	3314	
1	7a	3314	
1	8a	3314	

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Mol	Chain	Length	Quality of chain
1	9a	3314	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a red segment on the left labeled '31%' and a green segment on the right labeled '98%'. A small grey square is visible at the far right end of the bar.</p>

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.

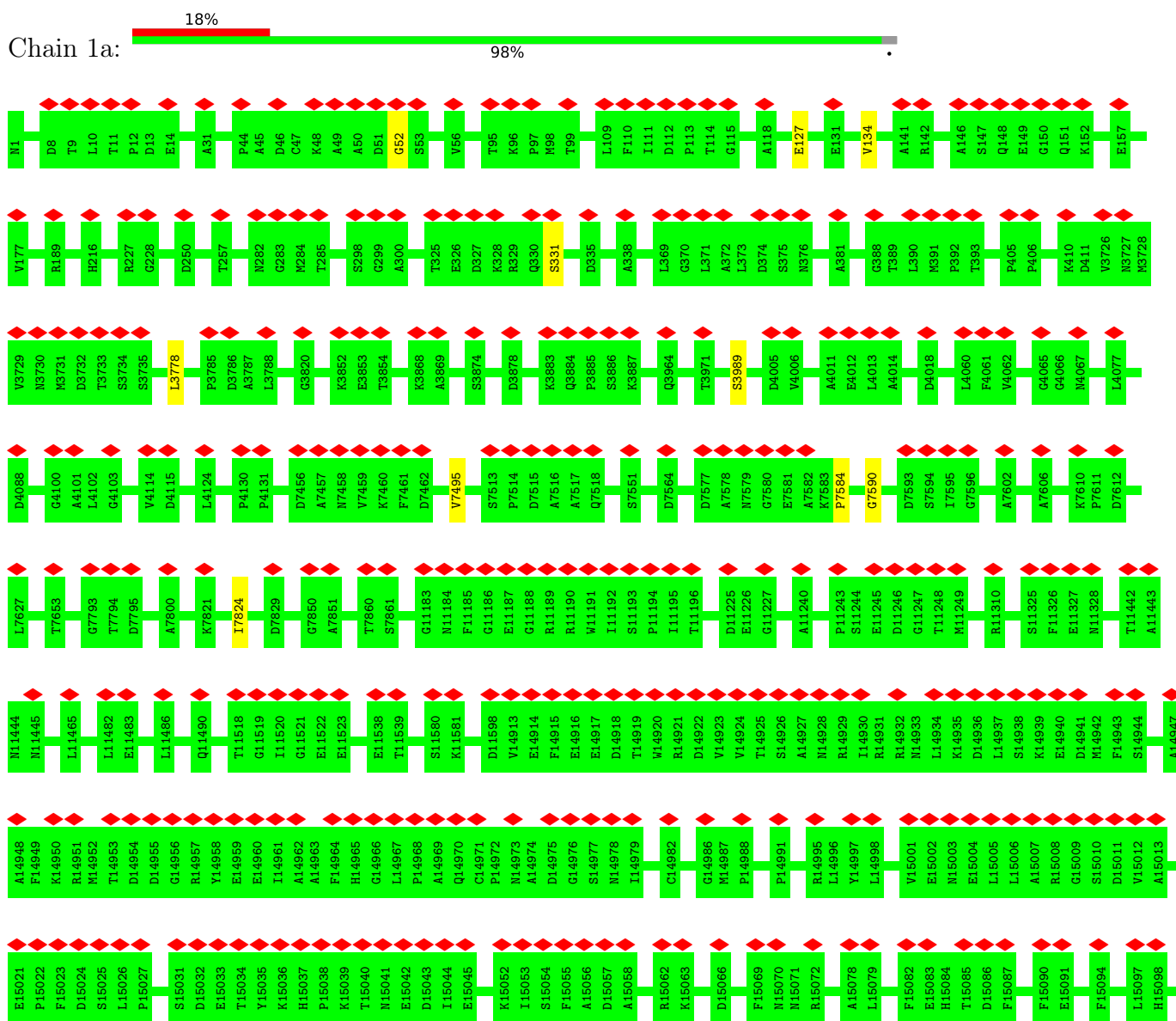
- Molecule 1 is a protein called Hemocyanin subunit 1.

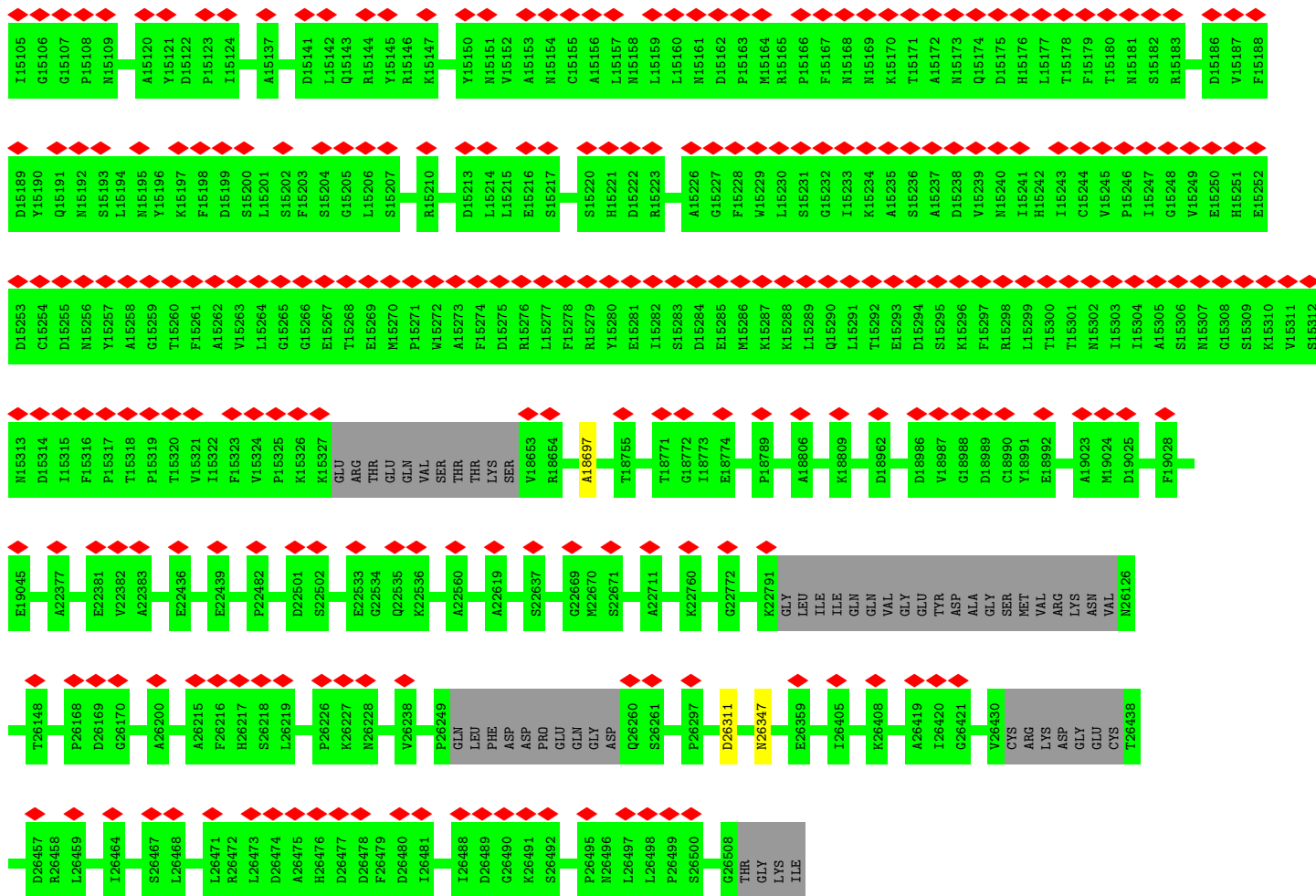
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1a	3262	16130	9606	3262	3262	0	0
1	2a	3262	16130	9606	3262	3262	0	0
1	3a	3262	16130	9606	3262	3262	0	0
1	4a	3262	16130	9606	3262	3262	0	0
1	5a	3262	16130	9606	3262	3262	0	0
1	6a	3262	16130	9606	3262	3262	0	0
1	7a	3262	16130	9606	3262	3262	0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

3 Residue-property plots

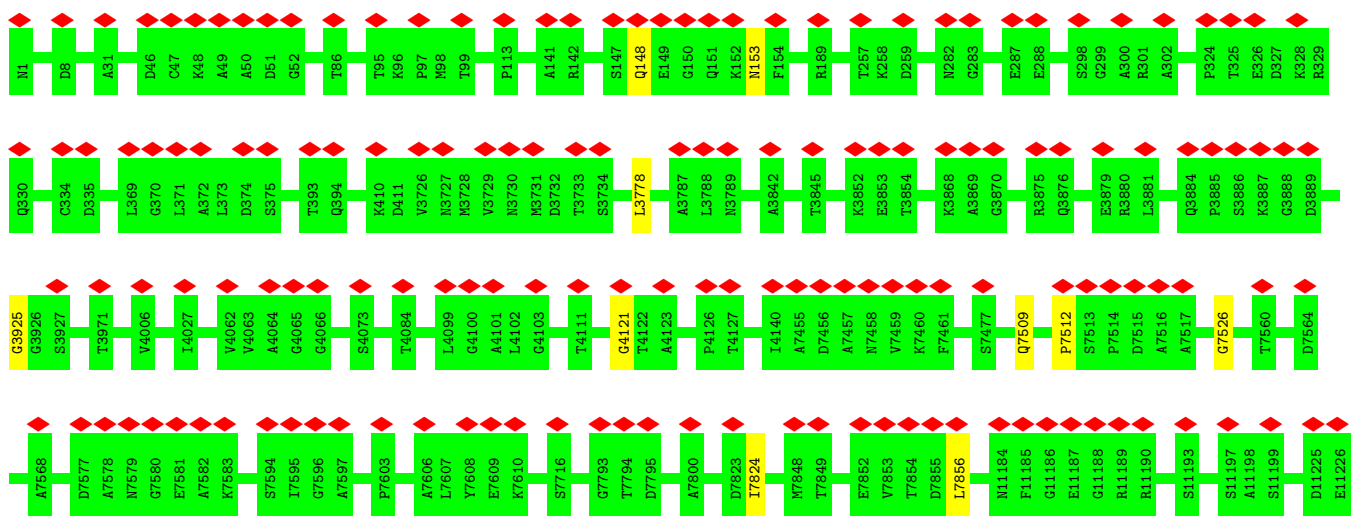
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 subunit 1





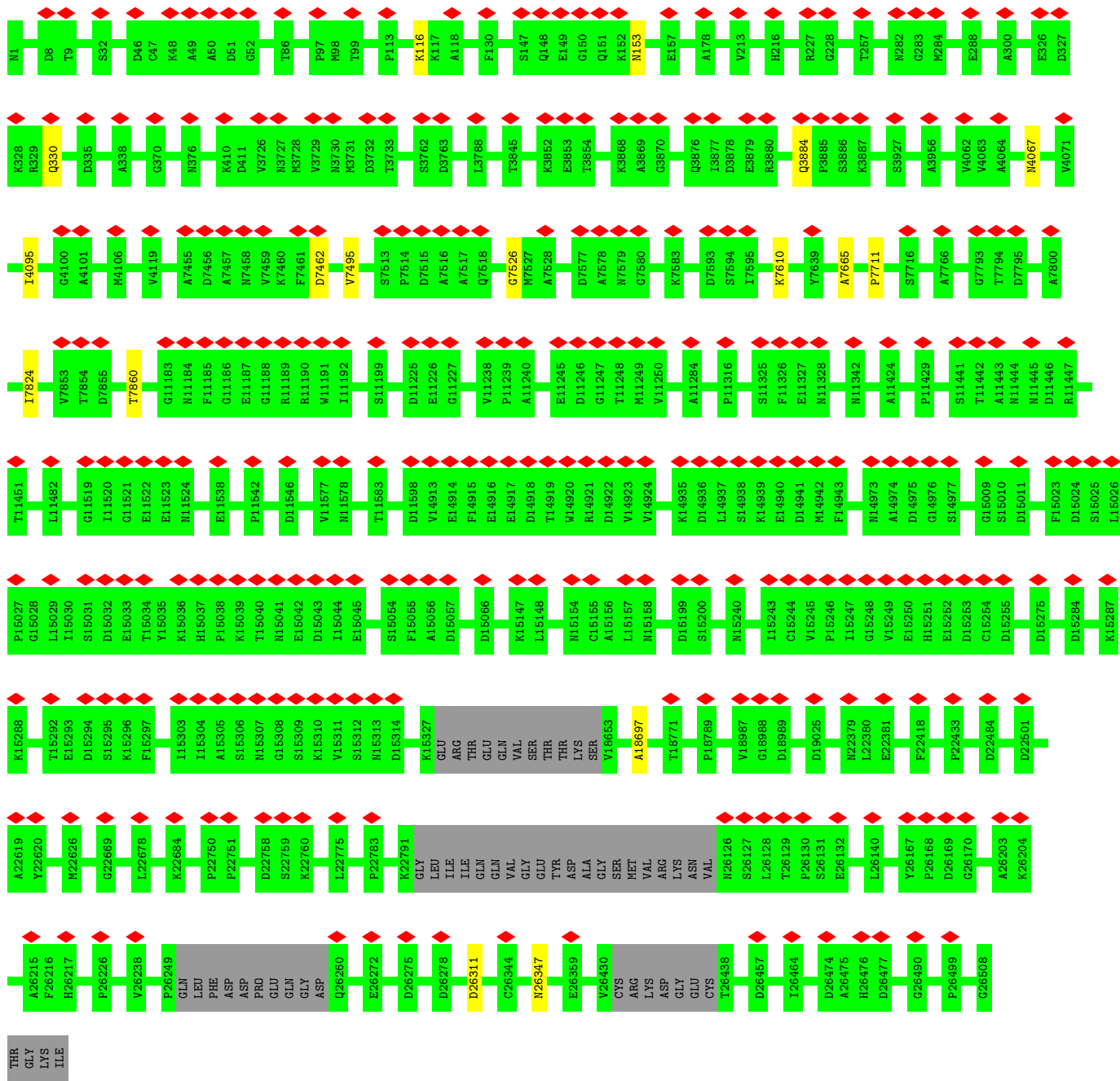
• Molecule 1: Hemocyanin subunit 1



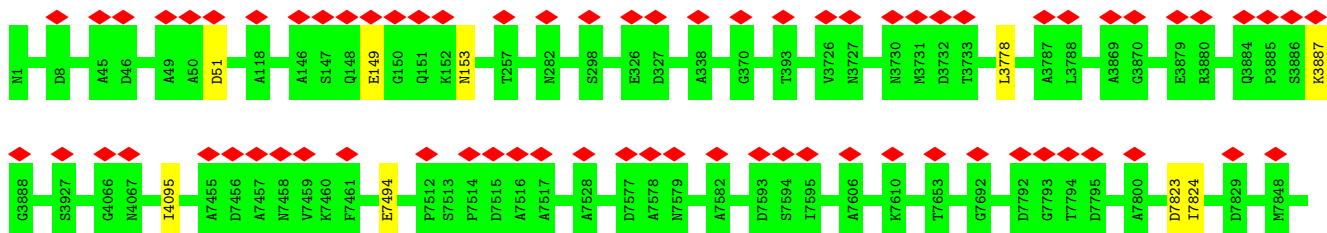
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L14945	R14946	A14947	A14948	F14949	K14950	R14951	M14952	T14953	D14954	D14955	G14956	R14957	Y14958	E14959	E14960	I14961	A14962	A14963	L14967	P14968	A14969	Q14970	D14975	G14976	S14977	N14978	I14979	H14985	G14986	M14987	P14988	Y14997	L14998	S14999	L15000	V15001	E15002	N15003	E15004	A14927	L15005	R14929	A15007	R15008	G15009	S15010	D15011	V15012	A15013	V15014	D15024	D15032	E15033	T15034
Y15035	K15036	H15037	P15038	N15039	T15040	N15041	E15042	T15043	I15044	E15045	N15046	G15051	K15052	I15053	S15054	F15055	A15056	D15057	A15058	V15059	T15060	V15061	K15062	K15063	D15066	P15108	N15109	F15110	H15111	S15112	Y15121	A15153	M15154	C15155	L15156	L15157	M15158	L15159	L15160	M15161	D15162	F15167	N15168	M15169	K15170	V15171	V15172	M15173	Q15174	E15267	H15175	L15176	L15177	T15178
F15179	T15180	M15181	S15182	R15183	D15186	V15187	F15188	D15189	M15192	S15193	L15194	N15195	D15199	S15204	G15205	F15228	M15229	L15230	S15231	G15232	I15233	K15234	A15235	S15236	A15237	D15238	C15244	V15245	P15246	I15247	G15248	V15249	E15250	H15251	E15252	D15253	C15254	D15255	M15256	Y15257	T15260	F15261	A15262	V15263	L15264	G15265	V15266	E15267	T15268	E15269	M15270	P15271		
M15272	A15273	F15274	D15275	R15276	E15281	D15284	E15285	M15286	K15287	K15288	L15289	Q15290	L15291	T15292	E15293	D15294	S15295	K15296	F15297	M15302	I15303	I15304	A15305	S15306	N15307	G15308	S15309	V15310	S15311	S15312	D15313	D15314	I15315	F15316	T15317	P15318	P15319	V15320	V15321	K15327	ARG	THR	GLU	GLN	VAL	SER	THR	LYS	ASN	VAL	SER	V18653	R18654	A18697
K18708	I18742	T18765	T18771	G18772	I18773	E18774	P18789	E18790	R18795	E18796	V18797	A18806	A18895	E18958	D18986	V18987	G18988	D18989	C18990	Y18991	G18992	S19002	A19023	M19024	F19028	K19035	T19036	K19037	G19043	T19044	E19045	A22377	E22381	V22382	A22383	S22395	L22396	E22397	E22415															
E22533	G22534	Q22535	E22551	A22560	S22637	G22669	M22670	S22671	A22677	K22684	A22685	D22686	A22711	D22712	G22717	V22718	T22741	D22742	K22745	K22746	R22747	M22748	D22758	S22759	A22790	K22791	GLY	LEU	ILE	ILE	GLN	VAL	PRO	GLU	GLN	GLY	TYR	ASP	ALA	GLY	SER	MET	VAL	ARG	LYS	ASN	VAL	N26126						
S26127	L26128	T26129	E26132	T26148	D26149	Q26166	T26167	P26168	D26169	G26170	K26199	A26200	K26201	K26204	T26214	A26215	P26216	H26217	S26218	L26219	P26220	V26223	T26224	E26225	P26226	K26227	N26228	D26237	V26238	P26249	GLN	LEU	PHE	ASP	ASP	PRO	GLU	GLN	GLY	GLY	ASP	Q26260	F26263	Y26264	R26265	Q26266	I26267	A26270	L26271					
E26272	Q26273	R26274	D26275	F26276	C26277	E26280	I26281	K26403	Q26404	I26405	Q26406	E26407	K26408	D26409	R26410	V26411	F26412	A26413	G26414	F26415	L26416	A26419	I26420	V26426	N26427	F26428	D26429	V26430	CYS	ARG	LYS	ASP	GLY	CYS	F26438	F26439	G26440	G26441	T26442	L26446	M26452	T26453	W26454	A26455	F26456	D26457	R26458	L26459	F26460	L26461	I26464	S26465	K26466	
S26467	L26468	V26469	H26470	D26471	R26472	D26473	D26474	A26475	H26476	D26477	D26478	D26479	D26480	I26481	K26482	V26483	L26484	M26485	M26486	I26488	D26489	G26490	K26491	S26492	L26493	P26494	P26495	N26496	L26497	L26498	P26499	S26500	T26501	T26502	L26503	L26504	F26505	P26506	P26507	G26508	THR	GLY	LYS	ILE										

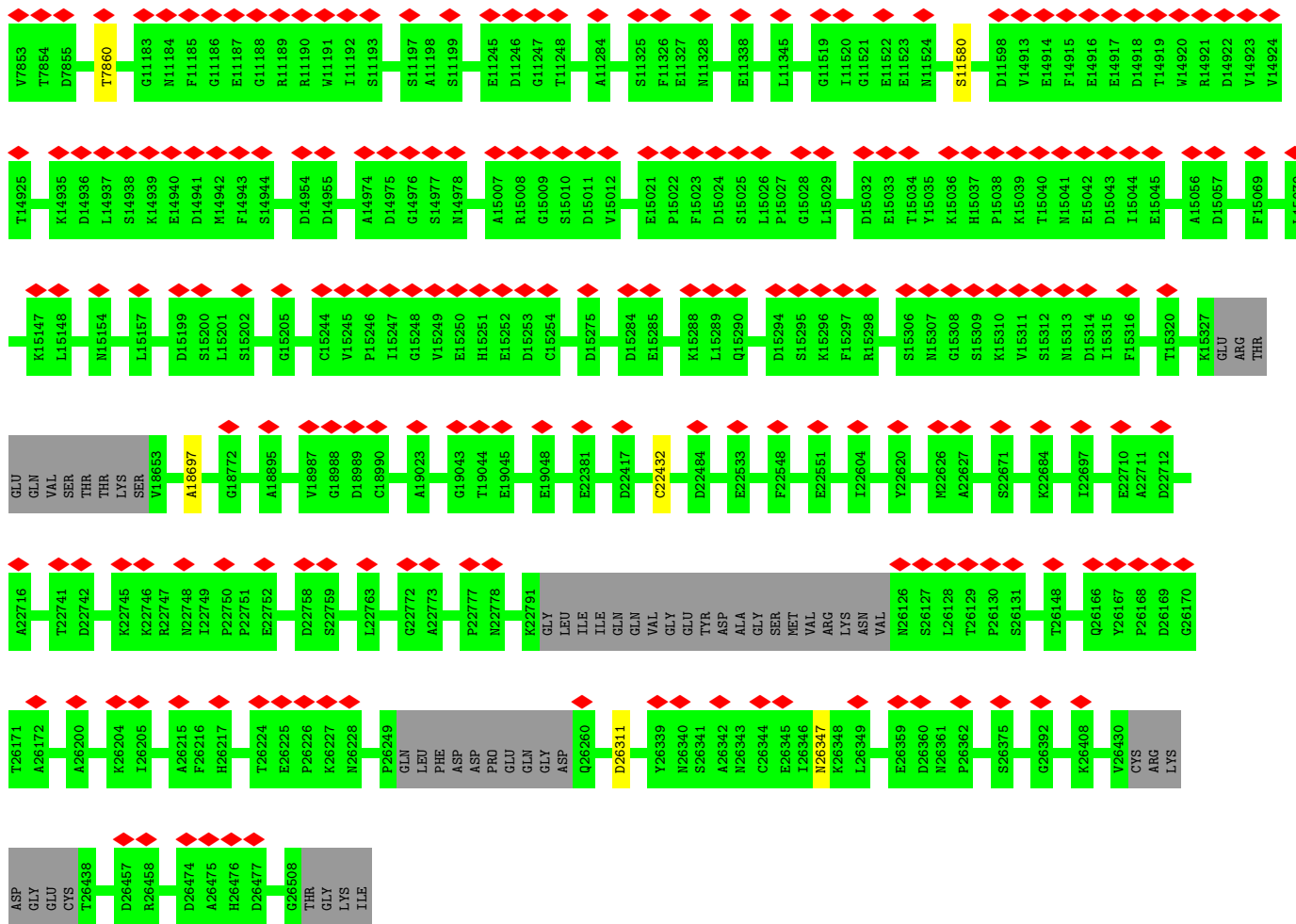
● Molecule 1: Hemocyanin subunit 1



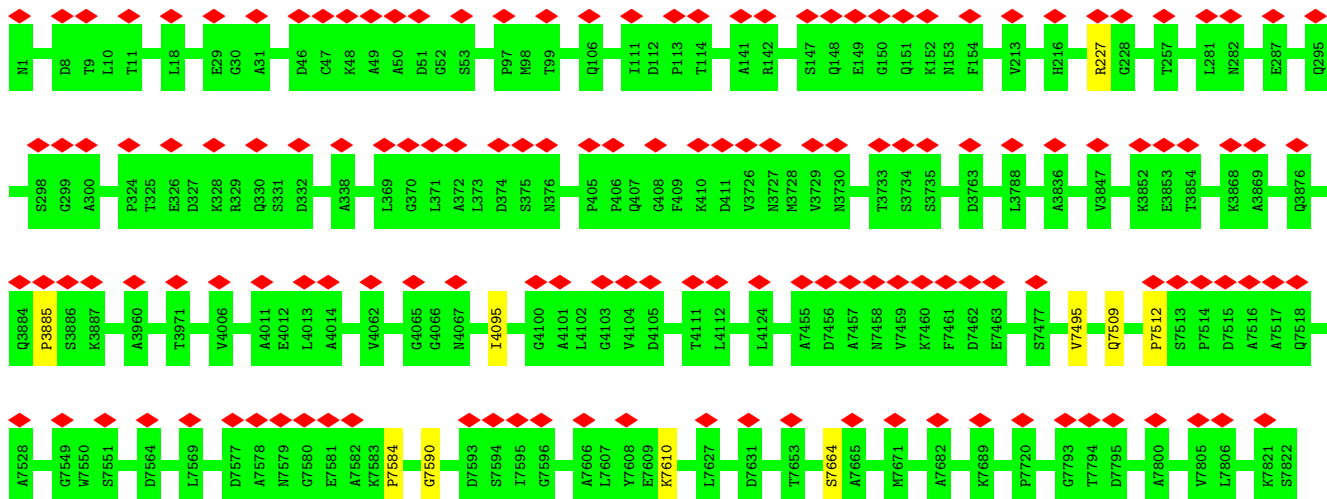


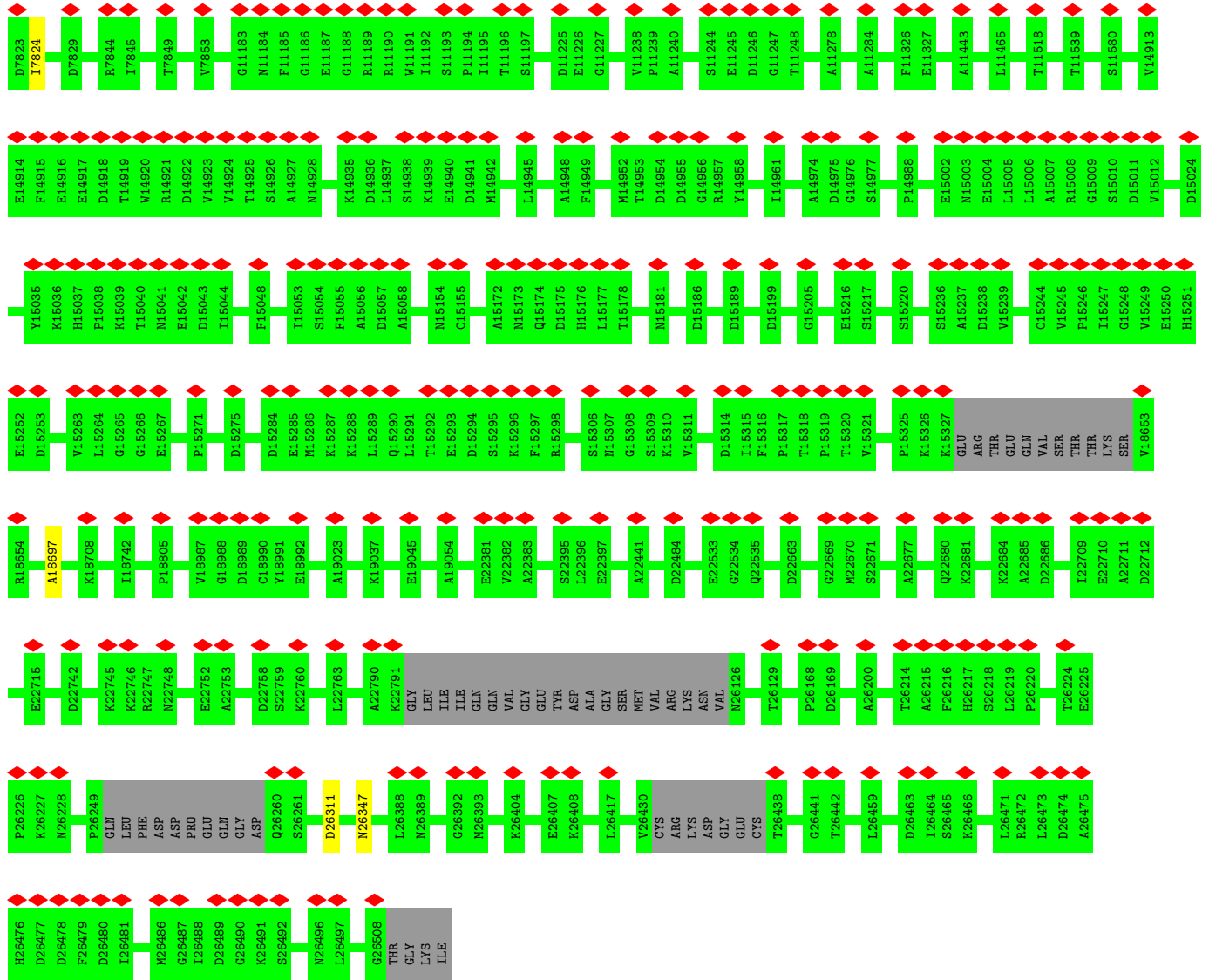
• Molecule 1: Hemocyanin subunit 1



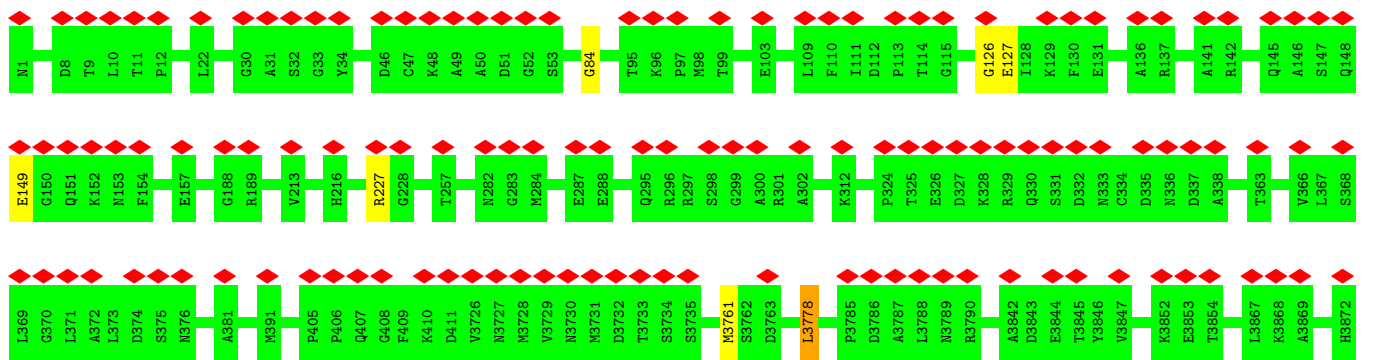


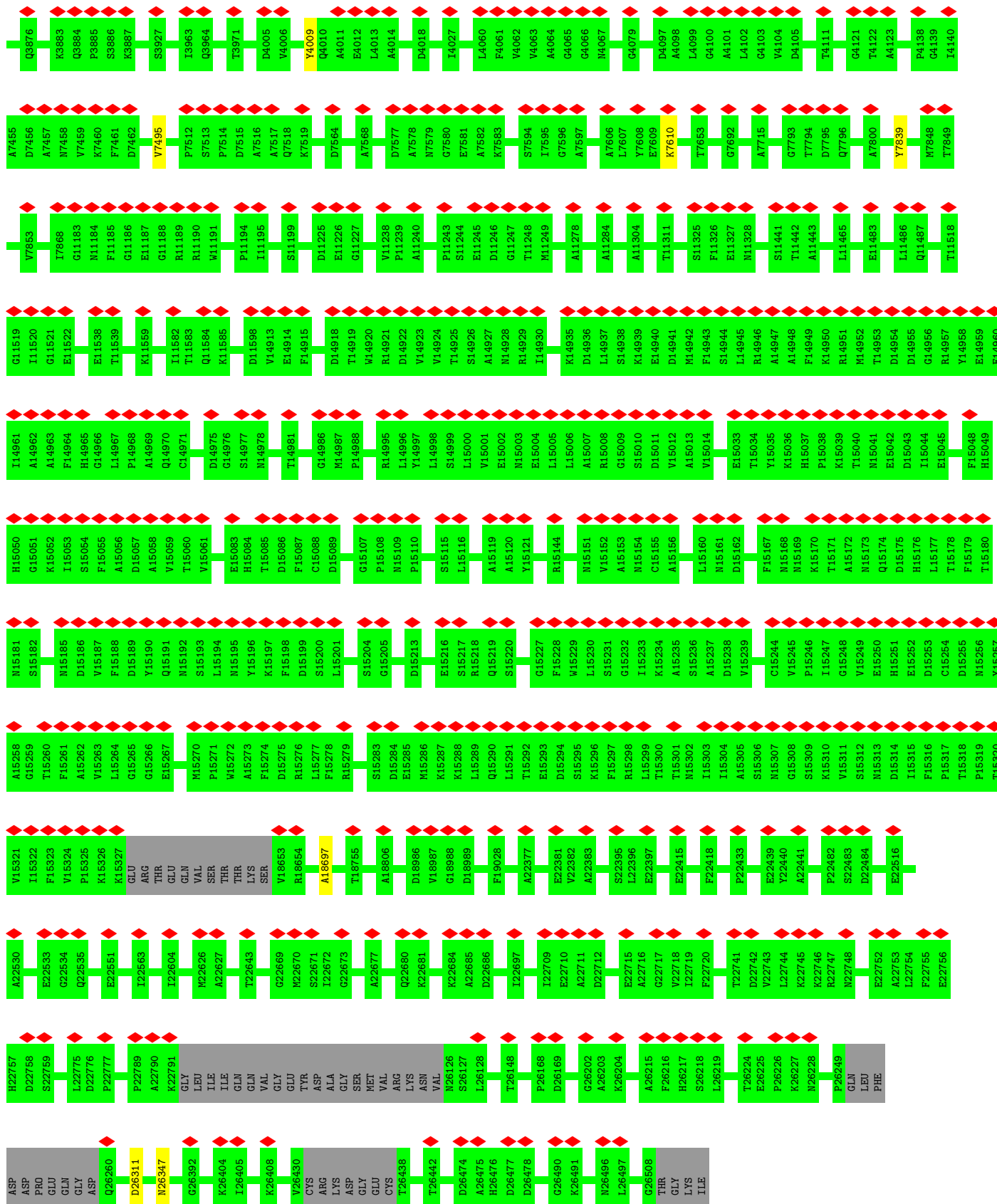
• Molecule 1: Hemocyanin subunit 1





● Molecule 1: Hemocyanin subunit 1



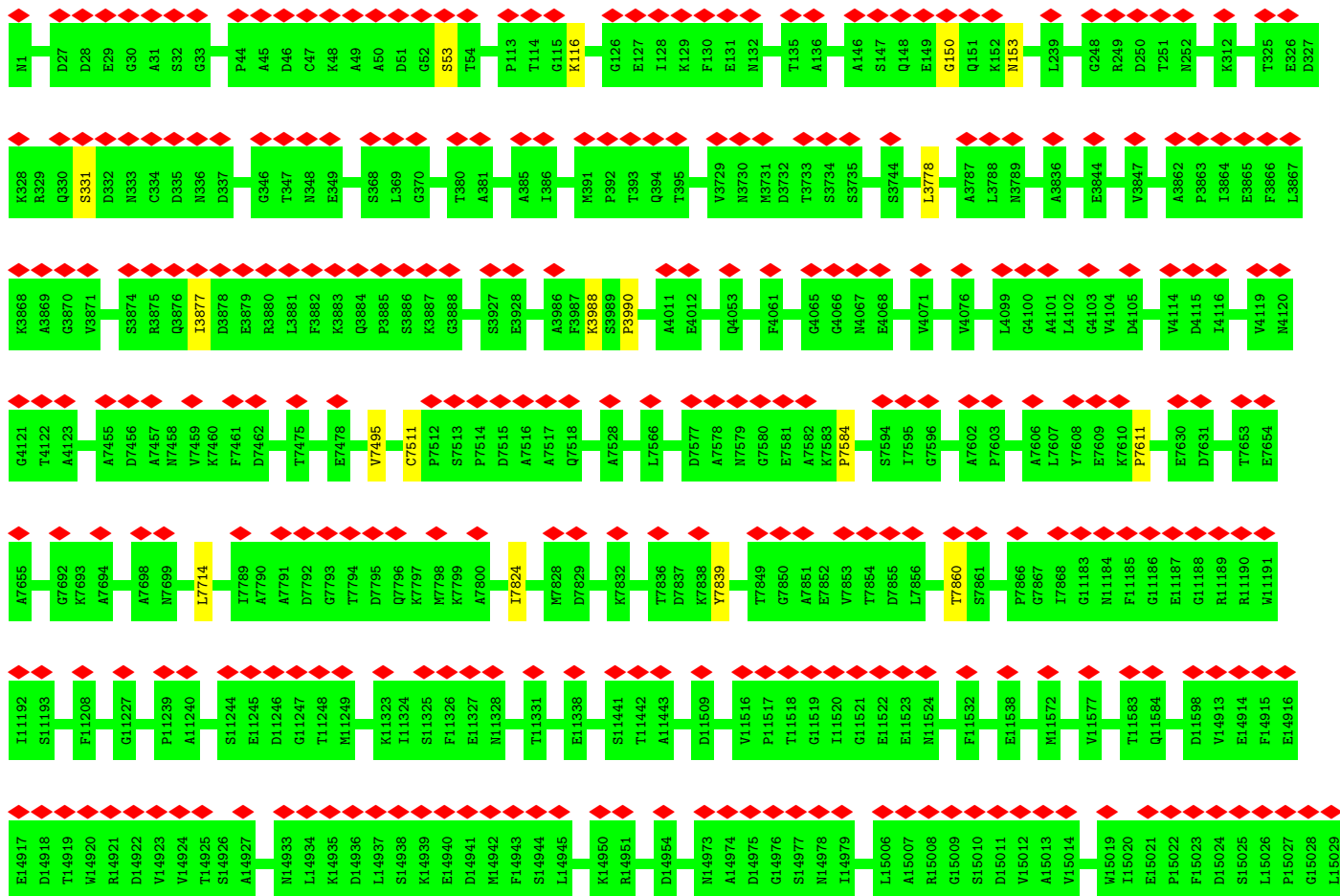


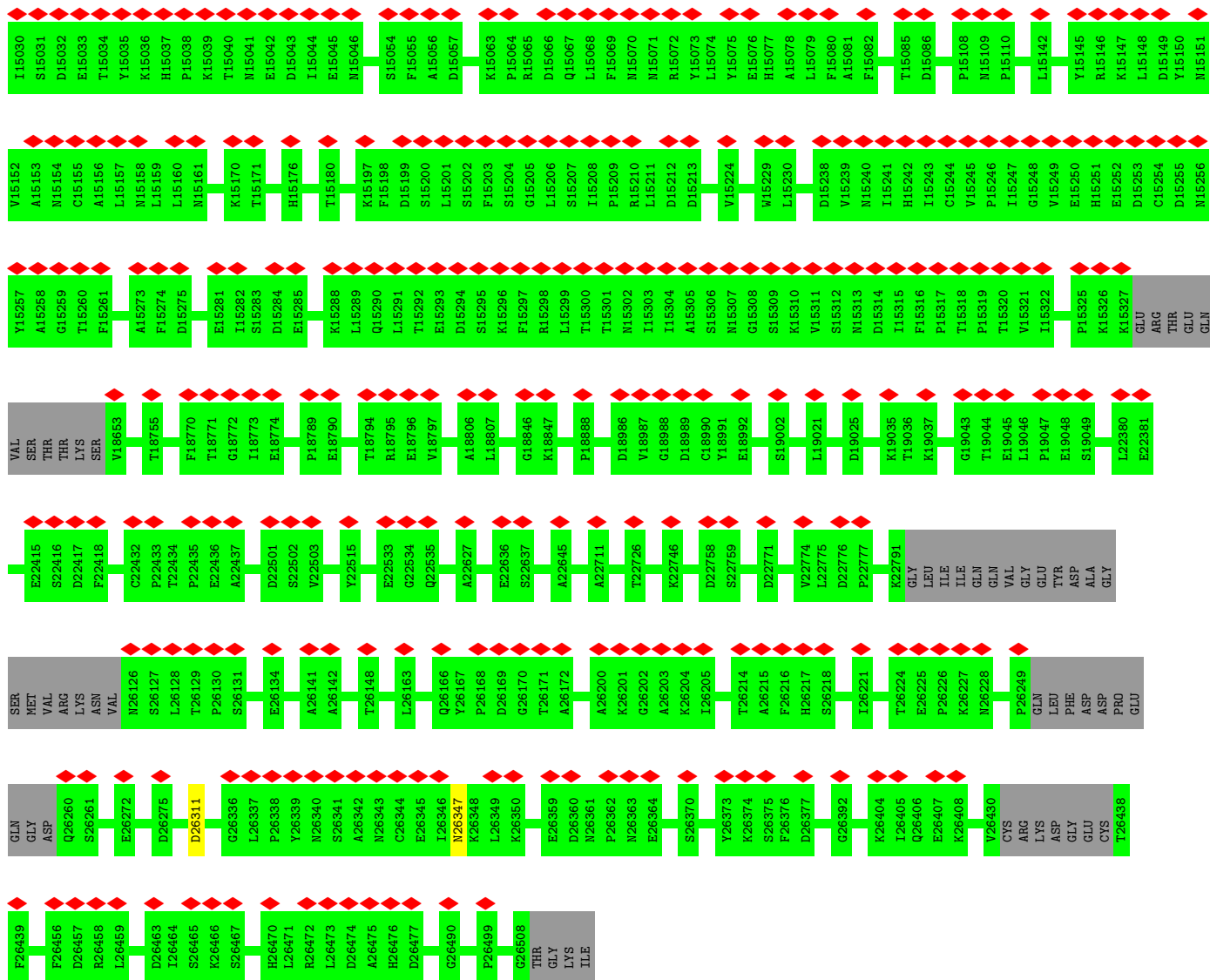
● Molecule 1: Hemocyanin subunit 1



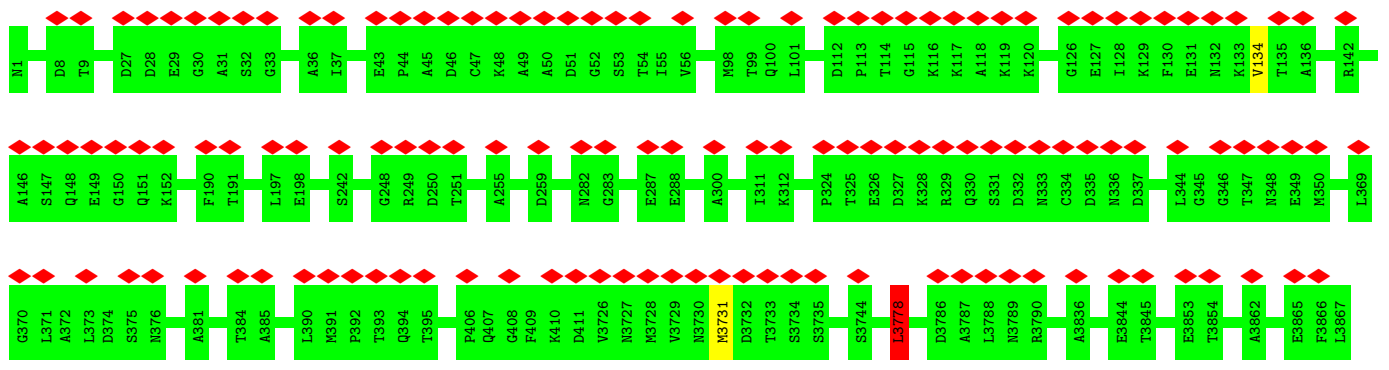


• Molecule 1: Hemocyanin subunit 1

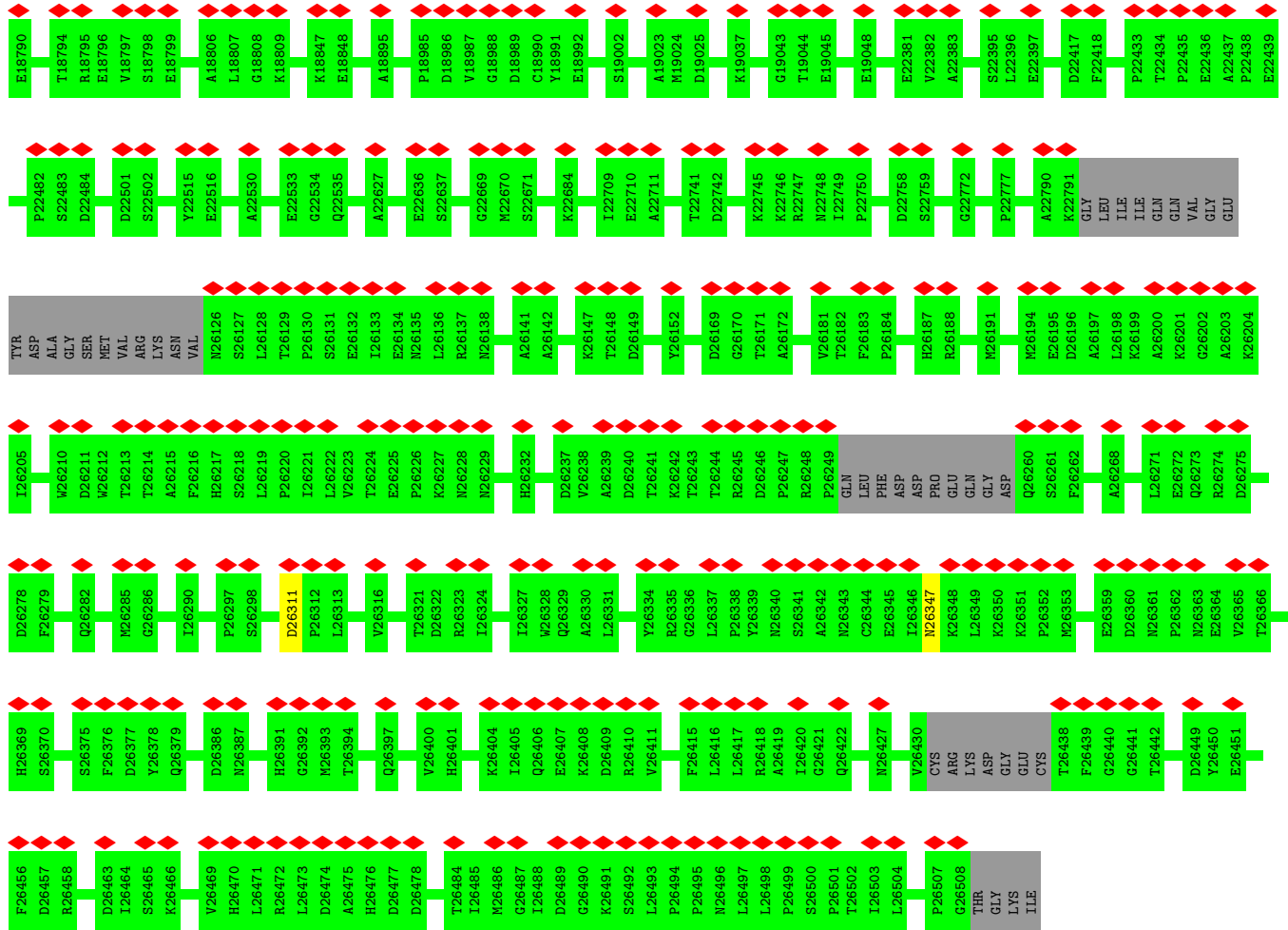




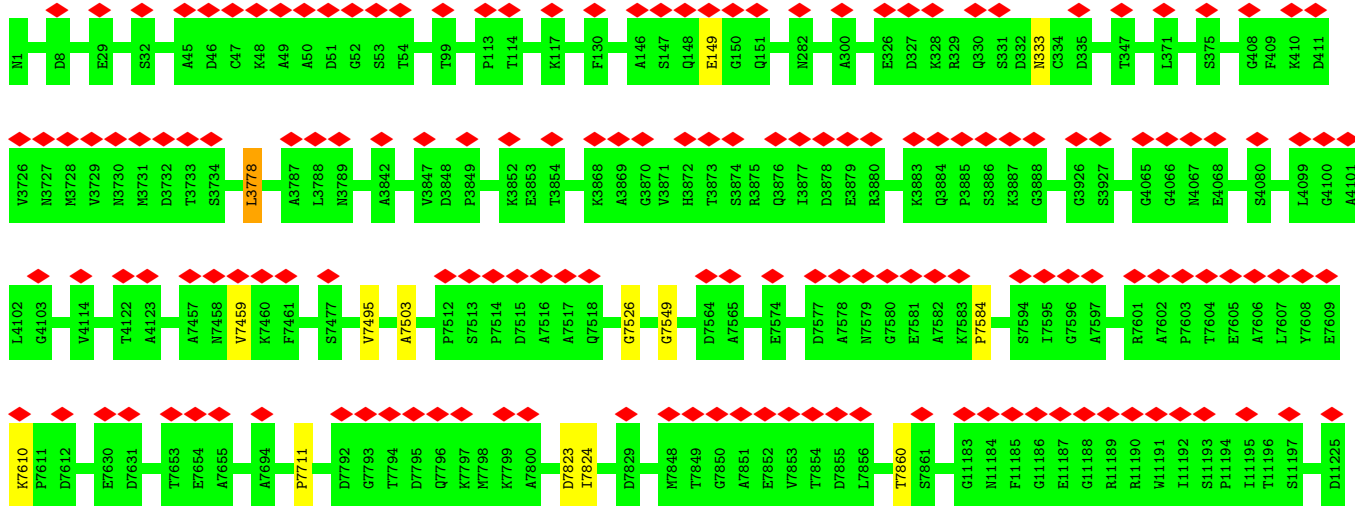
• Molecule 1: Hemocyanin subunit 1



K3868	A3869	G3870	U3871	S3874	R3875	Q3876	L3877	D3878	L3881	F3882	K3883	Q3884	F3885	S3886	K3887	S3927	T3971	L3991	Y4009	Q4010	A4011	E4012	L4013	A4014	L4020	I4027	G4046	L4049	D4059	L4060	F4061	V4062	V4063	A4064	G4065	G4066	M4067	E4068	F4069	F4070	V4071	G4072	S4073	V4076	L4077	E4094													
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G7526	M7527	A7528	R7547	S7551	T7560	D7564	L7569	V7570	T7576	D7577	A7578	M7579	G7580	E7581	A7582	K7583	Y7584	F7587	G7590	D7593	S7594	T7595	G7596	A7597	S7598	A7606	L7607	Y7608	E7609	K7610	P7611	K7615	Y7616	L7627	E7630	D7631	T7653	A7665	M7671	F7690	R7691																		
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E15293	D15294	S15295	K15296	F15297	R15298	L15299	T15300	L15301	M15302	I15303	I15304	A15305	S15306	M15307	G15308	K15309	V15310	S15311	S15312	M15313	D15314	I15315	F15316	P15317	T15318	P15319	T15320	V15321	I15322	F15323	V15324	P15325	K15326	K15327	GLU	ARG	THR	GLU	GLN	VAL	SER	THR	THR	LYS	SER	Y15653	K13708	T13765	E13764	P13769	G13772	I13773	E13774						



● Molecule 1: Hemocyanin subunit 1



P26352	Q26260	D26149	D22742	E22486	M15270	L15206	M15109	A15013	F14915	E11226
S26357	S26261	A26150	K22745	P22482	P15271	S15207	P15110	V15014	E14916	E11226
E26358	F26262	Q26166	R22746	F22482	W15272	I15208	H15111	D15018	E14917	P11239
S26359	F26263	Q26167	R22747	D22501	A15273	P15209	R15144	W15019	D14918	A11240
P26362	Q26265	P26168	N22748	S22502	F15274	F15210	Y15145	W15020	T14919	S11244
N26363	Q26266	D26169	I22749	V22503	D15275	D15212	R15146	E15021	W14920	E11245
E26364	I26267	G26170	P22750	A22530	R15276	D15213	K15147	E15022	R14921	D11246
V26365	A26268	E26267	E22756	E22533	L15277	L15214	L15148	F15023	D14922	G11247
A26368	F26269	V26180	E22757	E22533	F15278	L15215	D15149	D15024	V14923	T11248
Y26373	V26269	V26181	H22758	G22534	E15216	E15216	Y15150	D15024	V14924	V11260
K26374	T26182	T26182	D22758	G22534	S15283	S15217	Y15151	S15025	T14925	T14925
S26375	H26185	H26185	S22759	K22536	E15285	R15218	V15152	S15026	T14926	A11278
F26376	D26196	D26196	K22760	E22537	M15286	Q15219	A15153	P15027	S14926	A11278
D26377	L22763	L22763	E22763	E22551	K15287	H15221	M15154	G15028	A14927	A11284
F26378	G22772	G22772	E22772	E22560	L15288	H15222	A15156	L15029	A14928	A11284
Y26379	A22773	A22773	I18773	A22560	L15289	V15224	L15157	L15030	N14933	S11325
Q26379	E18774	E18774	E18774	I22604	Q15290	F15225	L15158	D15032	L14934	F11326
Q26380	P22777	P22777	P18789	I22604	T15291	A15226	L15159	E15033	K14935	E11327
L26381	P22783	P22783	E18790	L22608	T15292	F15227	L15160	T15034	D14936	M11328
N26382	P22789	P22789	E18790	L22608	E15293	F15228	M15161	K15036	S14938	N11342
F26383	I26205	I26205	R18795	A22619	D15294	F15228	D15162	H15037	K14939	T11349
E26384	G26206	G26206	E18796	A22619	S15295	W15229	D15162	P15038	E14940	T11349
Y26385	Y26209	Y26209	E18803	A22627	K15296	L15230	L15160	K15039	D14941	T11366
D26386	D26210	D26210	D18986	A22645	F15297	S15231	M15168	P15040	M14942	T11366
H26387	D26211	D26211	V18987	V22646	G15232	G15232	M15169	T15040	M14942	S11441
P26397	W26212	W26212	V18987	V22646	I15233	K15234	K15170	E15042	F14943	T11442
S26398	T26213	T26213	G18988	D22663	A15235	K15234	T15171	E15043	L14945	A11443
F26399	G26214	G26214	D18989	D22663	T15300	S15236	A15172	I15044	R14946	N11444
H26399	D26214	D26214	D18989	H22668	T15301	S15236	A15172	E15045	F14949	N11445
G26399	A26215	A26215	C18990	G22668	M15302	A15237	H15176	I15053	G14953	N11446
T26399	F26216	F26216	C18990	G22668	I15303	D15238	L15177	S15054	T14953	R11447
H26401	H26217	H26217	Y18991	G22669	I15304	D15239	F15179	F15055	D14954	E11483
L26402	S26218	S26218	A18992	M22670	A15306	I15243	T15180	F15056	D14955	G11519
K26403	S26218	S26218	E18992	I22672	S15307	C15244	M15181	D15057	G14956	I11520
K26404	GLY	GLY	G18993	I22672	M15308	V15245	R15183	A15058	R14957	I11520
I26405	SER	SER	A19023	G22673	S15309	P15246	R15183	V15059	A14969	G11521
Q26406	VAL	VAL	F19028	A22677	K15310	I15247	P15184	V15059	Q14970	E11522
E26407	ARG	ARG	T19044	L22678	V15311	G15248	P15185	K15063	C14971	E11523
K26408	LVS	LVS	E19045	L22678	S15312	V15249	D15186	P15064	C14971	N11524
D26409	ASN	ASN	E19045	A22684	M15313	E15250	D15186	R15065	P14972	E11538
R26410	VAL	VAL	E19048	A22686	D15314	H15251	F15188	D15066	N14973	E11538
L26411	N26126	N26126	I19048	D22686	I15315	E15252	D15189	Q15067	A14974	T11539
F26411	S26127	S26127	L22380	D22686	I15316	D15253	Y15190	Q15067	D14975	M11572
F26412	S26128	S26128	E22381	A22711	F15317	C15254	Q15191	M15070	G14976	M11572
E26345	T26129	T26129	P15317	D22712	T15318	D15255	M15192	M15071	D14977	V11577
I26346	E26132	E26132	T15318	D22712	P15319	M15256	S15193	R15072	S14977	V11577
N26347	I26133	I26133	P15319	D22712	T15320	N15257	Y15196	Y15073	N14978	V11577
K26348	L26136	L26136	T15320	E22715	V15321	A15258	K15197	E15083	H14980	T11583
L26349	L26140	L26140	V15321	A22716	I15322	G15259	K15198	H15084	M14987	Q11584
K26350	L26148	L26148	I15322	G22717	F15323	T15260	D15199	T15085	M14987	K11585
K26351	T22741	T22741	F15324	V22718	P15325	F15261	S15200	D15086	A15007	I11586
			P15325	D22740	K15326	A15262	L15201	F15087	R15008	D11598
			K15327	I22740	K15327	V15263	S15202	C15088	G15009	V14913
			GLU	T22741	GLU	E15267	F15203	G15107	S15010	E14914
			ARG		ARG	T15268	S15204	S15011	D15011	
			THR		THR			V15012	V15012	
			GLU		GLU					

I26420	G26421	Q26422	S26423	A26424	D26425	V26426	N26427	F26428	D26429	V26430	CYS	ARG	LYS	ASP	GLY	GLU	CYS	T26438	F26439	G26440	G26441	T26442	F26443	C26444	V26445	L26446	G26447	P26453	W26454	A26455	F26456	D26457	R26458	L26459	F26460	L26461	Y26462	D26463	I26464	S26465	K26466	S26467	L26468	V26469	H26470	L26471	R26472	L26473	D26474	A26475	H26476	D26477	D26478	F26479	D26480	I26481	K26482	V26483
T26484	I26485	M26486	G26487	I26488	D26489	G26490	K26491	P26494	P26495	N26496	L26497	L26498	P26499	S26500	P26501	T26502	I26503	L26504	F26505	K26506	P26507	G26508	THR	GLY	LYS	ILE																																

4 Experimental information

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 ($e^-/\text{\AA}^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	513.0, 513.0, 513.0	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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(°)	Ideal(°)
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 [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	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 [i](#)

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

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	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

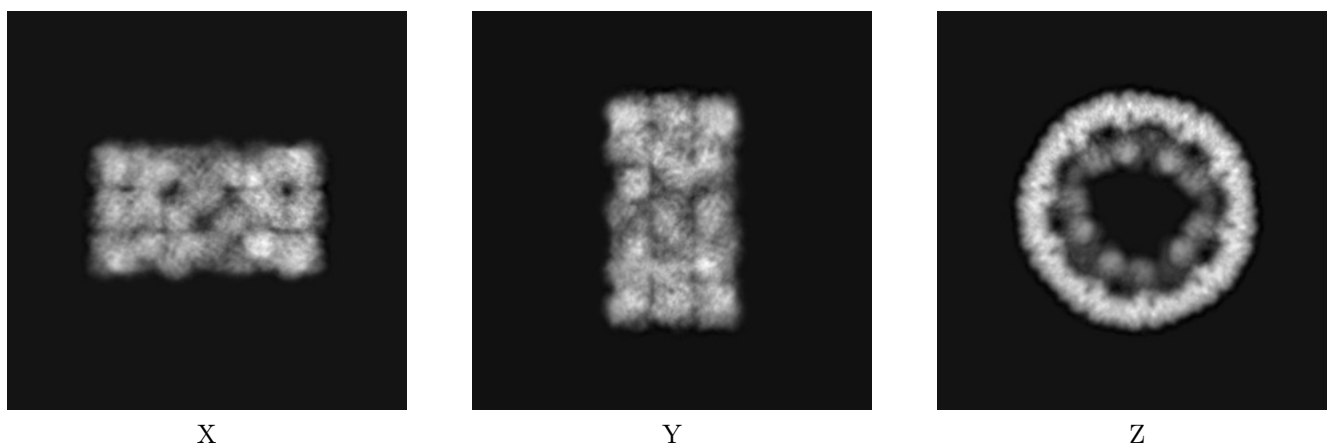
6 Map visualisation [i](#)

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 [i](#)

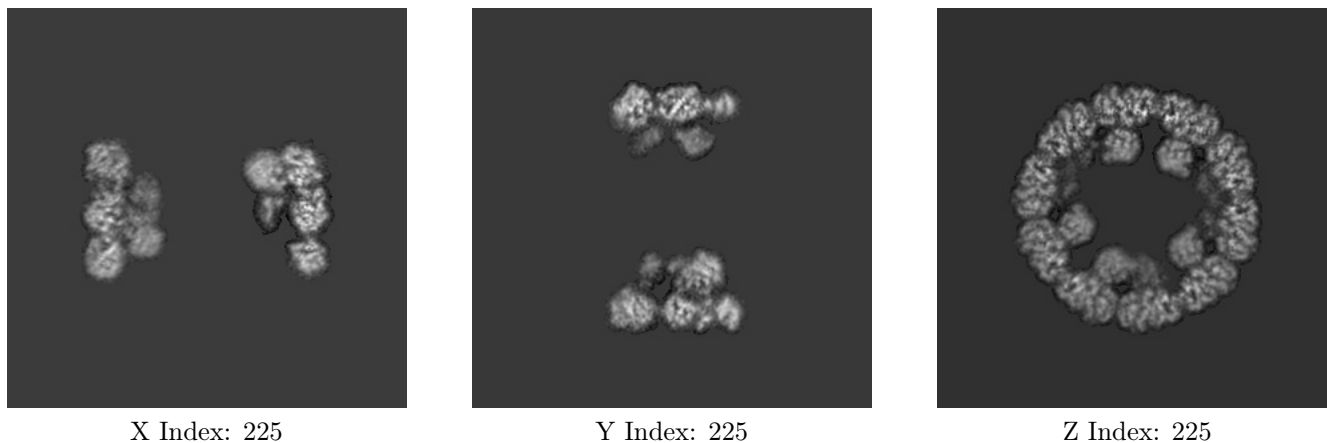
6.1.1 Primary map



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

6.2 Central slices [i](#)

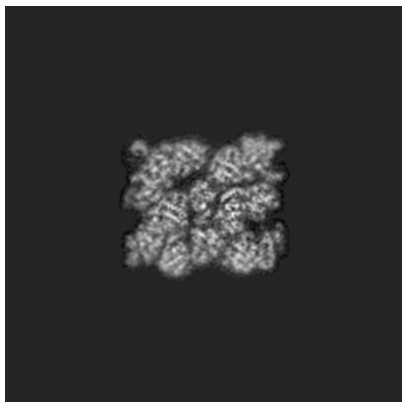
6.2.1 Primary map



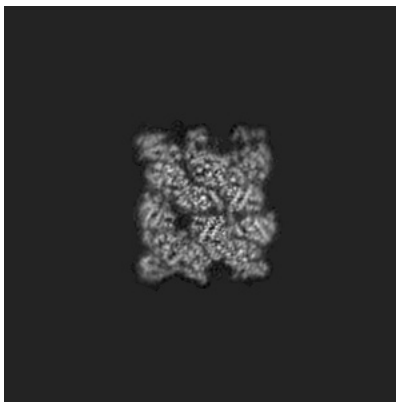
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 331



Y Index: 333

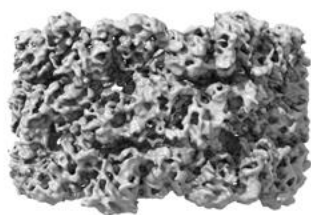


Z Index: 181

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

6.4 Orthogonal surface views [i](#)

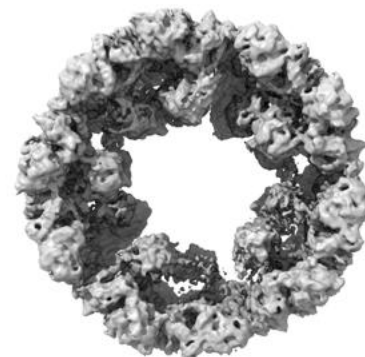
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

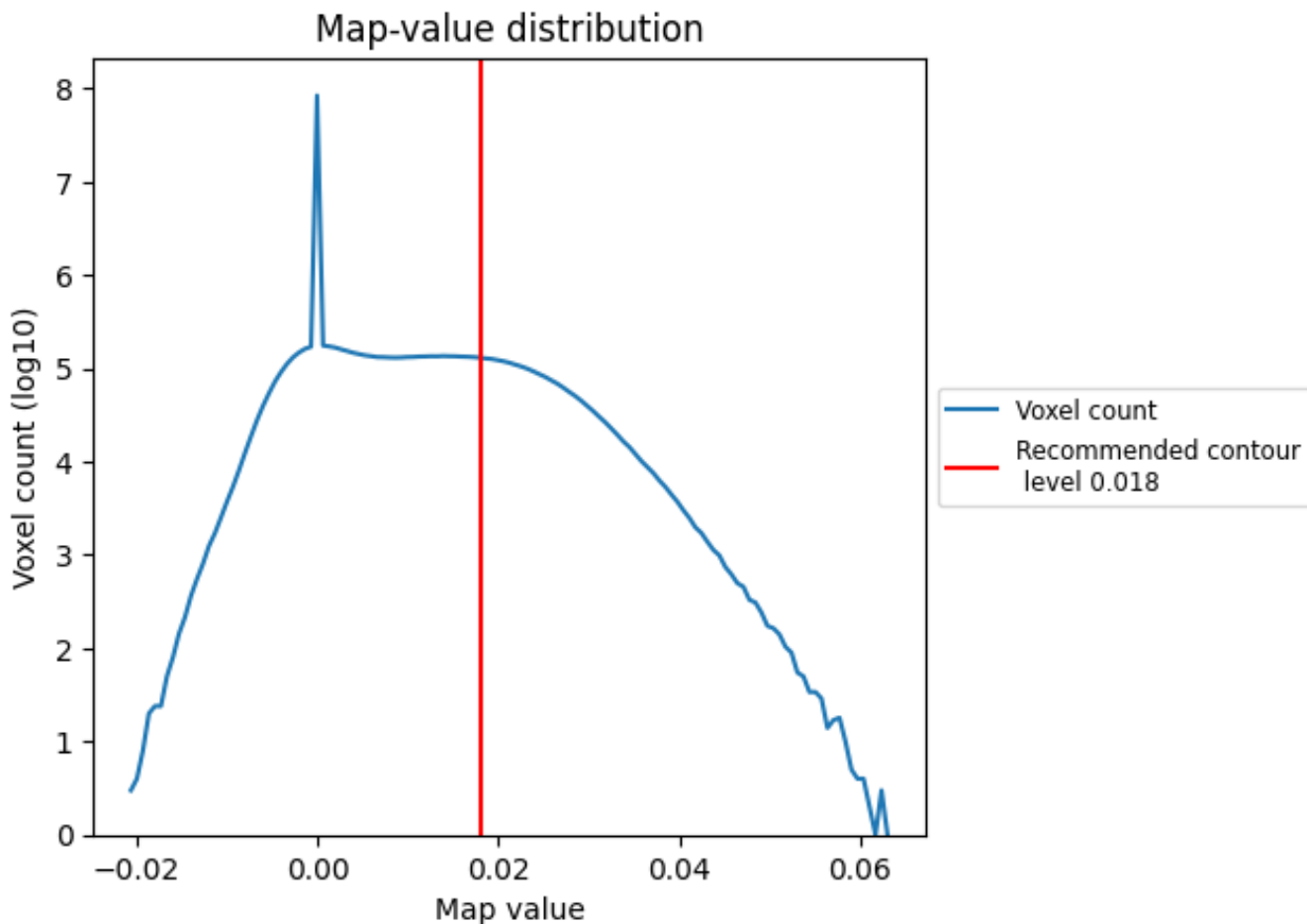
6.5 Mask visualisation

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

7 Map analysis [i](#)

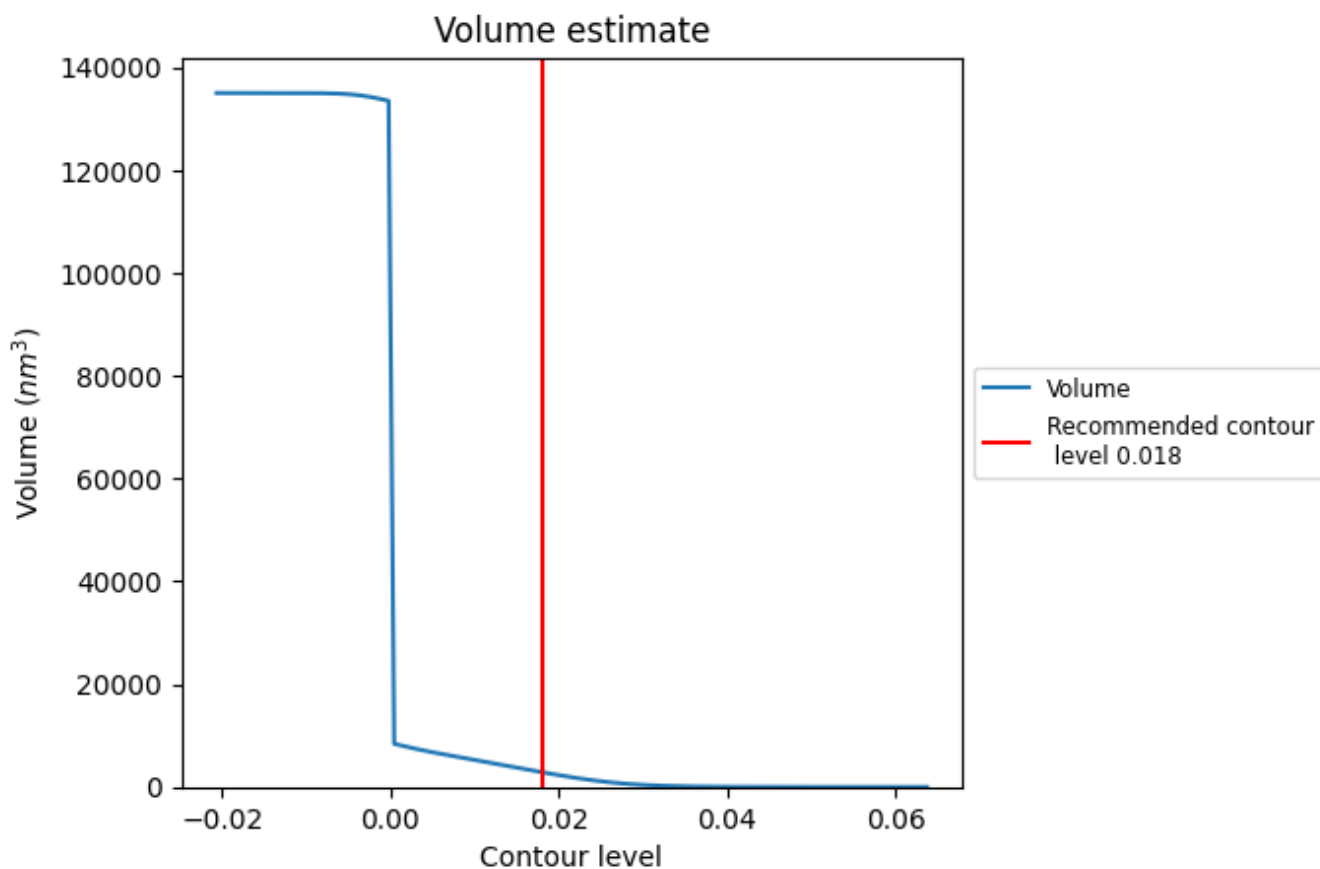
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

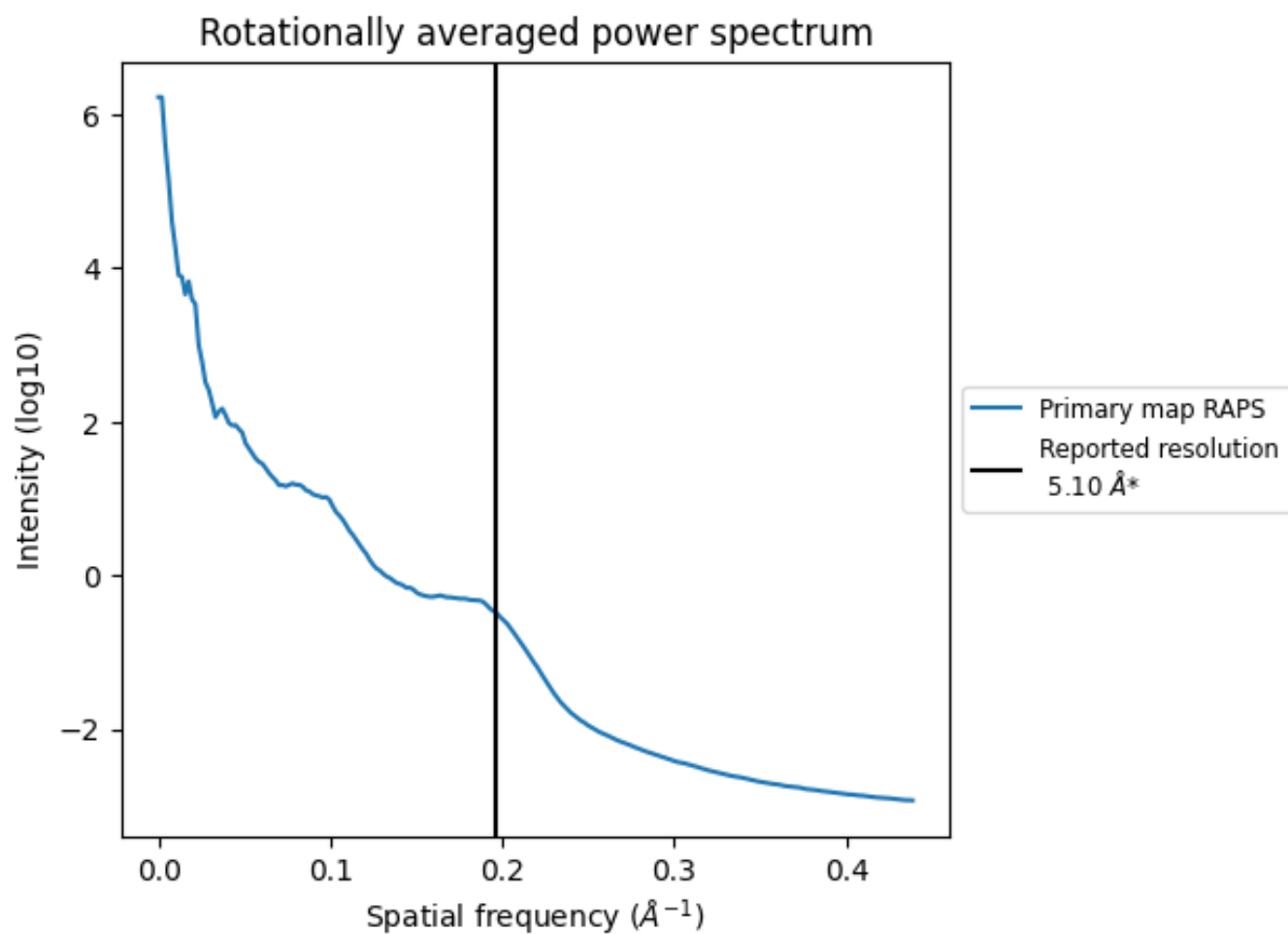
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2864 nm^3 ; this corresponds to an approximate mass of 2587 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 0.196 Å⁻¹

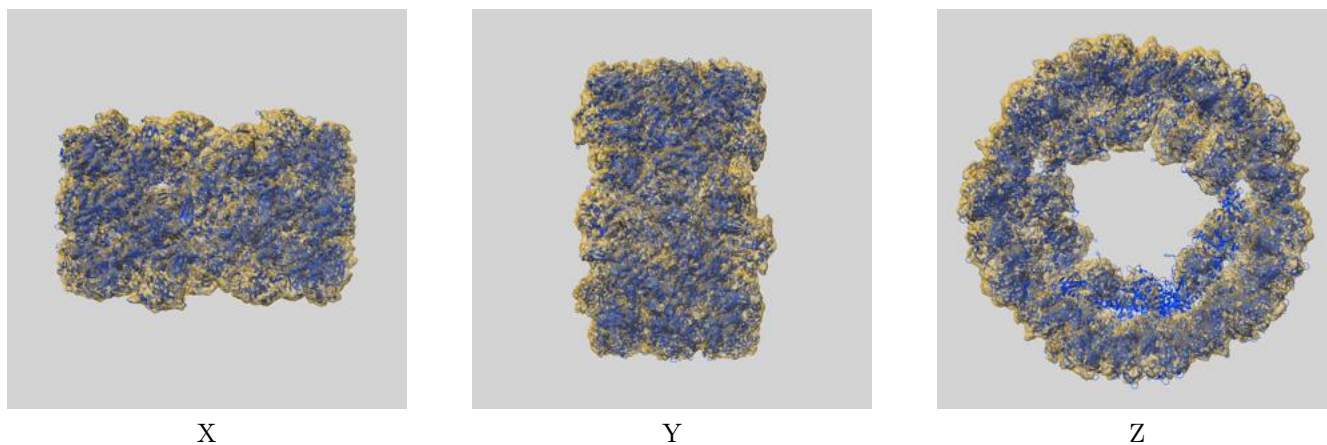
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

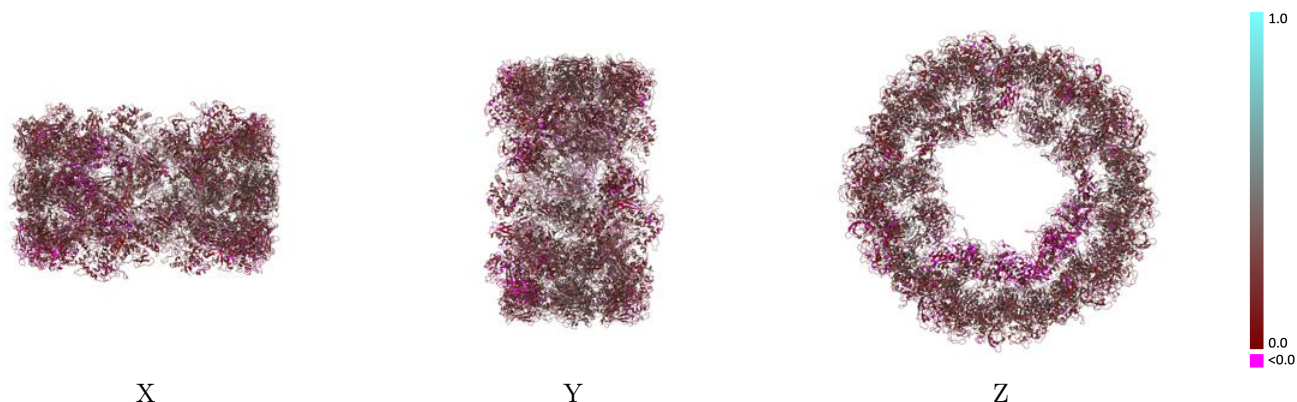
This section contains information regarding the fit between EMDB map EMD-4750 and PDB model 6R83. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



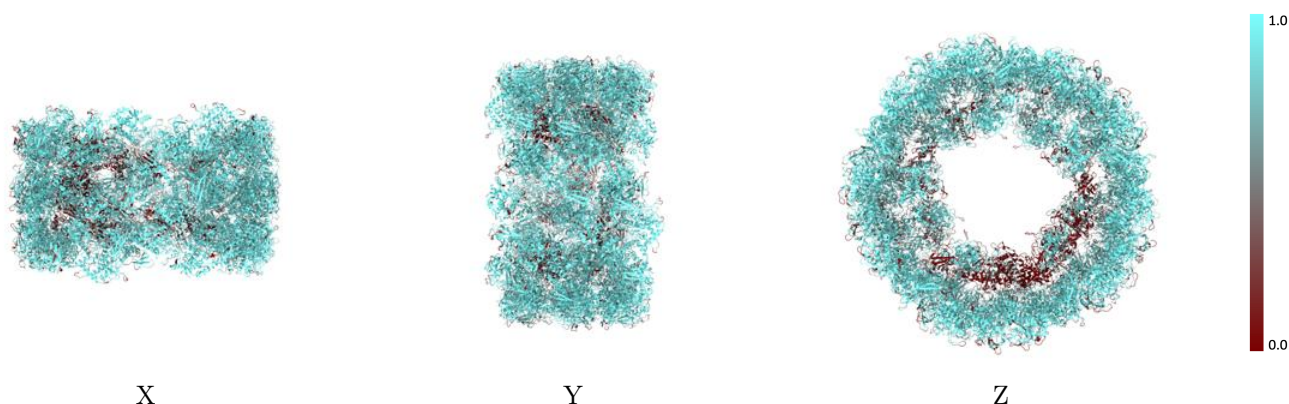
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



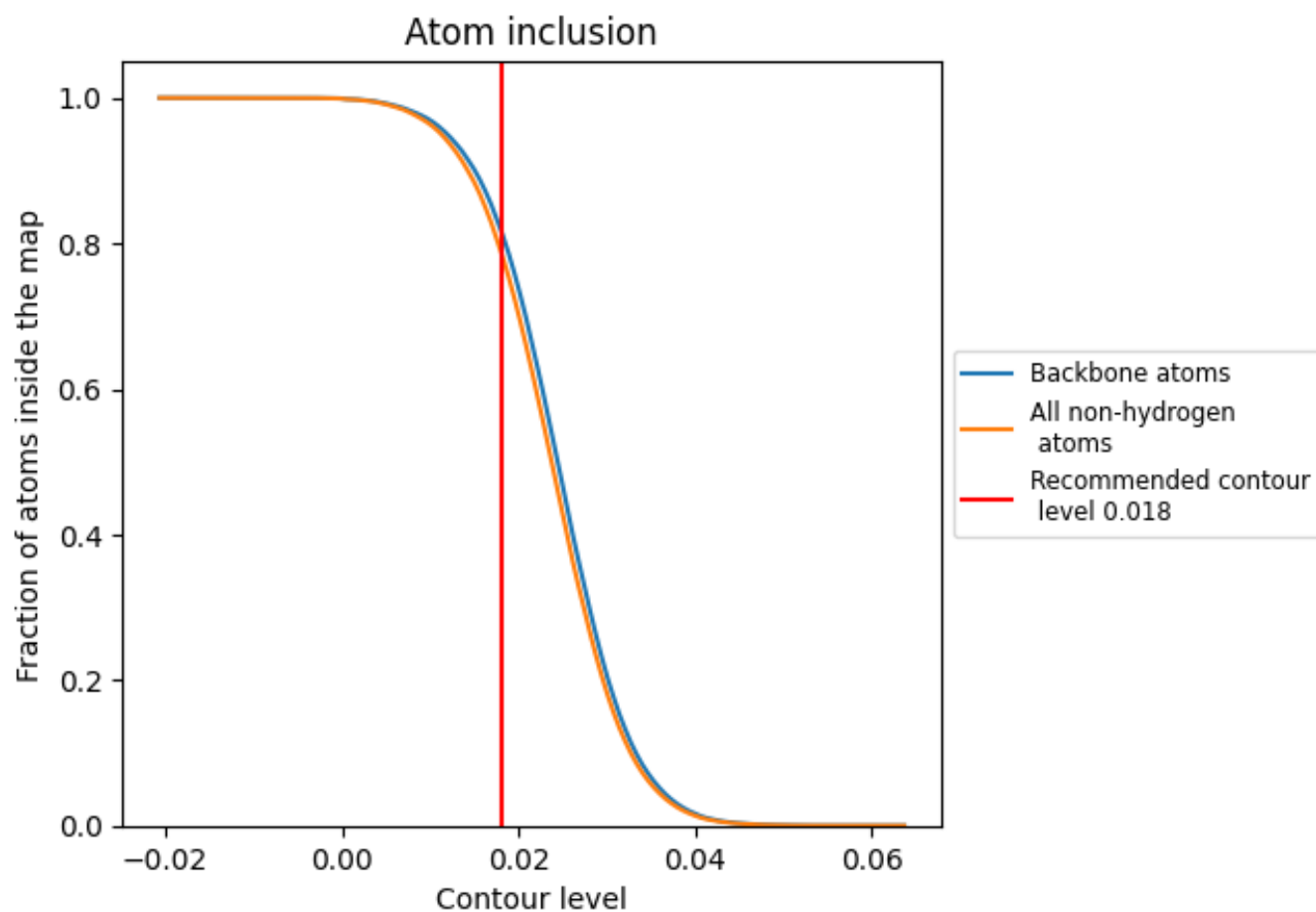
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)



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 (0.018).























9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 79% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7895	 0.2300
10a	 0.7428	 0.2150
1a	 0.7864	 0.2310
2a	 0.7826	 0.2310
3a	 0.8731	 0.2430
4a	 0.8782	 0.2550
5a	 0.8317	 0.2410
6a	 0.7807	 0.2290
7a	 0.7737	 0.2260
8a	 0.7841	 0.2350
9a	 0.6617	 0.1930

