wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 06:22 pm GMT

PDB ID	:	4BED
EMDB ID	:	EMD-1569
Title	:	Keyhole limpet hemocyanin (KLH): 9A cryoEM structure and molecular model of the KLH1 didecamer reveal the interfaces and intricate topology of the 160 functional units
Authors	:	Gatsogiannis, C.; Markl, J.
Deposited on	:	2013-03-08
Resolution	:	9.00 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:

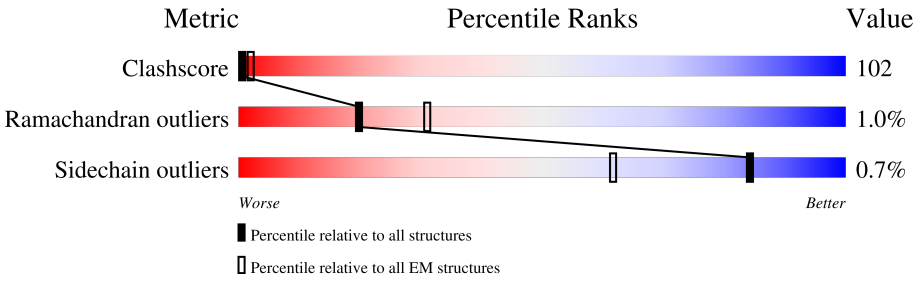
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.00 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	1664	28% 28% 72% ·
1	C	1664	27% 27% 72% ·
2	B	1734	33% 28% 69% ·
2	D	1734	29% 28% 69% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CUO	B	9008	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CUO	D	9008	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 55292 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 KLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1664	Total	C	N	O	S	0	0
			13530	8611	2347	2515	57		
1	C	1664	Total	C	N	O	S	0	0
			13530	8611	2347	2515	57		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ASP	GLY	conflict	UNP Q53IP9
A	139	VAL	ALA	conflict	UNP Q53IP9
A	162	ALA	PRO	conflict	UNP Q53IP9
A	178	ALA	PRO	conflict	UNP Q53IP9
A	259	ASN	-	insertion	UNP Q53IP9
A	260	GLU	-	insertion	UNP Q53IP9
A	261	HIS	-	insertion	UNP Q53IP9
A	262	SER	-	insertion	UNP Q53IP9
A	263	THR	-	insertion	UNP Q53IP9
A	264	PRO	-	insertion	UNP Q53IP9
A	265	ALA	-	insertion	UNP Q53IP9
A	266	ASP	-	insertion	UNP Q53IP9
A	267	LEU	-	insertion	UNP Q53IP9
A	268	PHE	-	insertion	UNP Q53IP9
A	269	ASP	-	insertion	UNP Q53IP9
A	270	TYR	-	insertion	UNP Q53IP9
A	271	CYS	-	insertion	UNP Q53IP9
A	272	GLU	-	insertion	UNP Q53IP9
A	273	LEU	-	insertion	UNP Q53IP9
A	274	HIS	-	insertion	UNP Q53IP9
A	275	TYR	ASN	conflict	UNP Q53IP9
A	?	-	TYR	deletion	UNP Q53IP9
A	?	-	TRP	deletion	UNP Q53IP9
A	?	-	GLY	deletion	UNP Q53IP9
A	?	-	LEU	deletion	UNP Q53IP9
A	?	-	PRO	deletion	UNP Q53IP9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q53IP9
A	?	-	LYS	deletion	UNP Q53IP9
A	?	-	LEU	deletion	UNP Q53IP9
A	?	-	ASN	deletion	UNP Q53IP9
A	?	-	ARG	deletion	UNP Q53IP9
C	129	ASP	GLY	conflict	UNP Q53IP9
C	139	VAL	ALA	conflict	UNP Q53IP9
C	162	ALA	PRO	conflict	UNP Q53IP9
C	178	ALA	PRO	conflict	UNP Q53IP9
C	259	ASN	-	insertion	UNP Q53IP9
C	260	GLU	-	insertion	UNP Q53IP9
C	261	HIS	-	insertion	UNP Q53IP9
C	262	SER	-	insertion	UNP Q53IP9
C	263	THR	-	insertion	UNP Q53IP9
C	264	PRO	-	insertion	UNP Q53IP9
C	265	ALA	-	insertion	UNP Q53IP9
C	266	ASP	-	insertion	UNP Q53IP9
C	267	LEU	-	insertion	UNP Q53IP9
C	268	PHE	-	insertion	UNP Q53IP9
C	269	ASP	-	insertion	UNP Q53IP9
C	270	TYR	-	insertion	UNP Q53IP9
C	271	CYS	-	insertion	UNP Q53IP9
C	272	GLU	-	insertion	UNP Q53IP9
C	273	LEU	-	insertion	UNP Q53IP9
C	274	HIS	-	insertion	UNP Q53IP9
C	275	TYR	ASN	conflict	UNP Q53IP9
C	?	-	TYR	deletion	UNP Q53IP9
C	?	-	TRP	deletion	UNP Q53IP9
C	?	-	GLY	deletion	UNP Q53IP9
C	?	-	LEU	deletion	UNP Q53IP9
C	?	-	PRO	deletion	UNP Q53IP9
C	?	-	GLY	deletion	UNP Q53IP9
C	?	-	LYS	deletion	UNP Q53IP9
C	?	-	LEU	deletion	UNP Q53IP9
C	?	-	ASN	deletion	UNP Q53IP9
C	?	-	ARG	deletion	UNP Q53IP9

- Molecule 2 is a protein called HEMOCYANIN KLH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1734	Total	C	N	O	S	0	0
			14084	8985	2438	2594	67		

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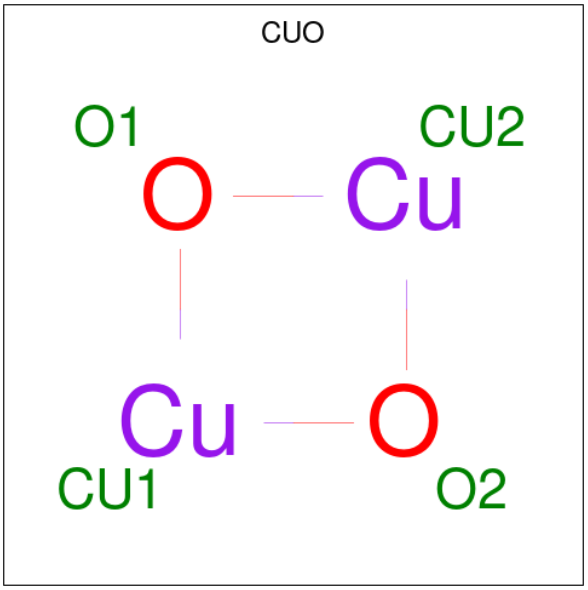
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	1734	Total	C	N	O	S	0	0
			14084	8985	2438	2594	67		

- Molecule 3 is CU2-O2 CLUSTER (three-letter code: CUO) (formula: Cu_2O_2).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	Cu	O		0
			16	8	8		
3	A	1	Total	Cu	O		0
			16	8	8		
3	A	1	Total	Cu	O		0
			16	8	8		
3	A	1	Total	Cu	O		0
			16	8	8		
3	B	1	Total	Cu	O		0
			16	8	8		
3	B	1	Total	Cu	O		0
			16	8	8		
3	B	1	Total	Cu	O		0
			16	8	8		
3	B	1	Total	Cu	O		0
			16	8	8		
3	C	1	Total	Cu	O		0
			16	8	8		
3	C	1	Total	Cu	O		0
			16	8	8		

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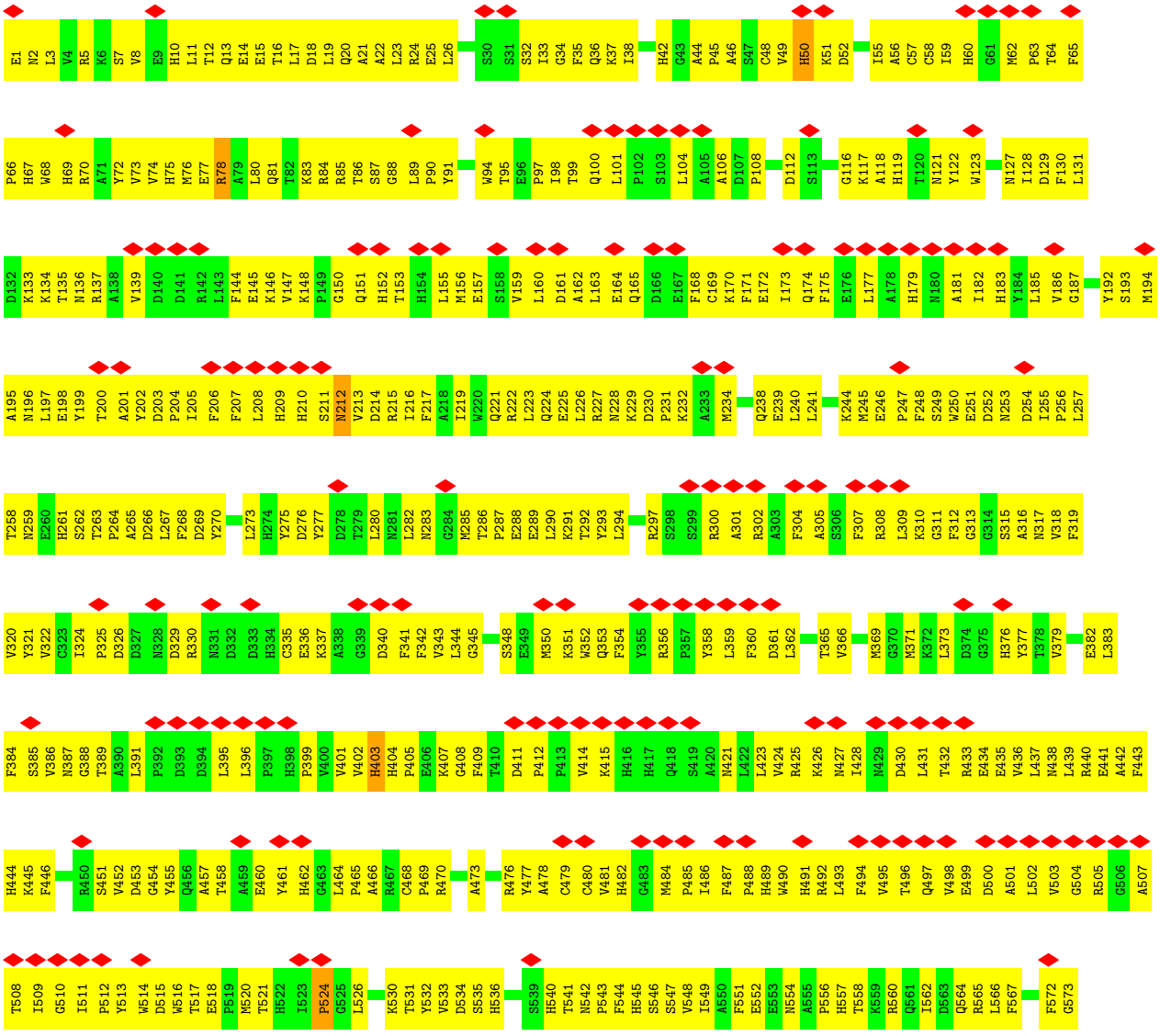
Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	Cu	O	0
			16	8	8	
3	C	1	Total	Cu	O	0
			16	8	8	
3	D	1	Total	Cu	O	0
			16	8	8	
3	D	1	Total	Cu	O	0
			16	8	8	
3	D	1	Total	Cu	O	0
			16	8	8	
3	D	1	Total	Cu	O	0
			16	8	8	

3 Residue-property plots (i)

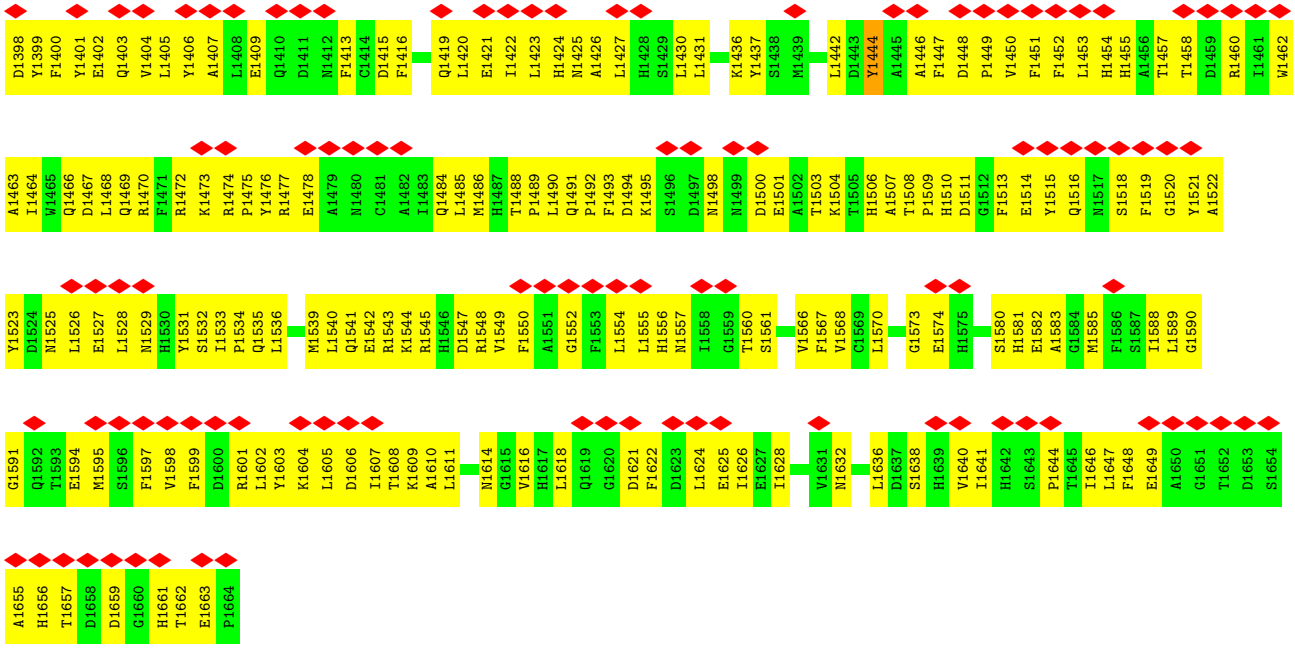
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 KLH1

Chain A:

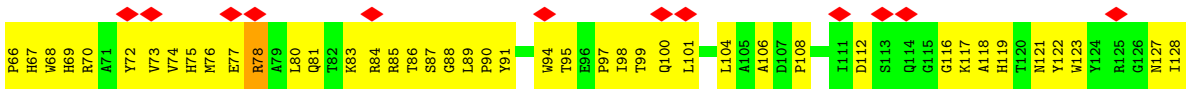


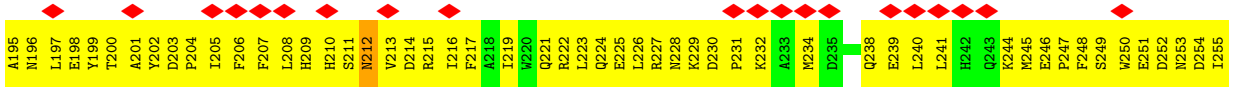

H574 H575 T576 D577 L578 F579 N580 Q581 I582 L583 Y584 A585 F586 E587 Q588 E589 D590 Y591 C592 D593 F594 E595 V596 Q597 F598 E599 I600 T601 H602 W603 T604 I605 H606 A607 W608 T609 G610 E613 H614 F615 S616 M617 S618 S619 L620 H621 Y622 T623 A624 F625 D626 P627 L628 F629 Y630 F631 H632 H633 S634
N635 V636 D637 R638 L639 W640 A641 V642 W643 Q644 A645 L646 Q647 M648 R649 R650 H651 K652 P653 Y654 R655 A656 H657 C658 A659 I660 S661 L662 E663 H664 M665 H666 L667 K668 P669 F670 S673 S674 P675 L676 N677 N678 N679 E680 K681 T682 N685 A686 M687 P688 M689 K690 I691 Y692 D693 Y694 E695 W696
V697 L698 H699 Y700 T701 Y702 E703 D704 L705 T706 F707 G708 G709 I710 S711 L712 E713 N714 I715 E716 K717 M718 I719 H720 E721 N722 Q723 Q724 R727 I728 Y729 A730 G731 F732 L733 L734 A735 G736 I737 N742 V743 D744 I745 F746 I747 K748 T749 T750 D751 S752 V753 Q754 H755 K756 A757 G758 T759 F760
G765 S766 K767 E768 M769 K770 W771 G772 F773 D774 R775 V776 F777 K778 F779 D780 I781 T782 H783 V784 L785 K786 D787 L788 D789 L790 T791 A792 D793 G794 D795 F796 E797 V798 T799 V800 D801 I802 T803 E804 V805 D806 G807 T808 K809 L810 A811 S812 S813 L814 I815 P816 H817 A818 S819 V820 I821 R822 E823
R826 V827 K828 F829 D830 K831 V832 P833 R834 S835 R836 L837 I838 R839 K840 N841 V842 D843 R844 L845 E848 E849 M850 N851 E852 L853 R854 L857 L860 K861 K864 S865 A866 F869 Q870 Q871 L872 G873 A874 F875 H876 G877 E878 P879 K880 W881 C882 P883 S884 P885 E886 A887 S888 K889
K890 F891 A892 C893 C894 V895 H896 G897 M898 S899 V900 F901 P902 H903 W904 H905 R906 L907 L908 T909 V910 Q911 S912 E913 N914 A915 L916 R917 R918 H919 G920 Y921 D922 G923 A924 L925 P926 Y927 W928 D929 W930 T931 S932 P933 L934 N935 H936 L937 L940 H943 E944 K945 Y946 D951 G952 V953 E954
K955 H956 N957 P958 W959 F960 D961 G962 H963 I964 D965 T966 V967 D968 K969 T970 T971 T972 R973 S974 V975 Q976 N977 F980 E981 Q982 P983 E984 F985 T989 S990 I991 A992 K993 Q994 V995 L996 L997 A998 L999 E1000 Q1001 D1002 N1003 F1004 C1005 D1006 F1007 E1008 I1009 Q1010 Y1011 E1012 I1013 A1014 H1015 N1016 Y1017
I1018 H1019 A1020 L1021 V1022 G1023 Q1026 P1027 Y1028 G1029 M1030 A1031 S1032 L1033 R1034 Y1035 T1036 A1037 F1038 D1039 P1040 L1041 F1042 Y1043 L1044 H1045 H1046 S1047 N1048 T1049 D1050 R1051 I1052 W1053 A1054 I1055 W1056 Q1057 A1058 L1059 Q1060 K1061 Y1062 R1063 G1064 K1065 P1066 Y1067 N1068 V1069 A1070 N1071 C1072 A1073 V1074 T1075 S1076 M1077 R1078
E1079 P1080 L1081 Q1082 P1083 F1084 G1085 L1086 S1087 A1088 N1089 I1090 N1091 T1092 D1093 H1094 V1095 T1096 K1097 E1098 H1099 S1100 V1101 P1102 F1103 N1104 V1105 F1106 D1107 Y1108 K1109 T1110 N1111 F1112 N1113 Y1114 E1115 Y1116 D1117 T1118 L1119 E1120 F1121 N1122 G1123 L1124 S1125 I1126 S1127 Q1128 L1129 N1130 K1131 K1132 L1133 E1134 A1135 I1136 K1137 S1138
Q1139 D1140 R1141 F1142 F1143 A1144 G1145 F1146 L1147 L1148 S1149 G1150 F1151 K1152 K1153 S1154 S1155 L1156 V1157 K1158 F1159 N1160 I1161 C1162 T1163 D1164 C1168 H1169 P1170 A1171 G1172 E1173 F1174 Y1175 L1176 L1177 G1178 D1179 E1180 N1181 E1182 M1183 P1184 W1185 A1186 Y1187 D1188 R1189 V1190 F1191 K1192 Y1193 D1194 I1195 T1196 E1197 K1198 L1199 H1200
D1201 L1202 R1203 L1204 H1205 A1206 E1207 F1210 Y1211 I1212 D1213 Y1214 E1215 V1216 F1217 D1218 L1219 K1220 L1224 G1225 K1226 D1227 L1228 F1229 K1230 Q1231 P1232 S1233 V1234 I1235 H1236 E1237 P1238 R1239 I1240 G1241 H1242 H1243 E1244 G1245 E1246 V1247 Y1248 Q1249 A1250 E1251 V1252 T1253 S1254 A1255 N1256 R1257 I1258 R1259 K1260 N1261 I1262 E1263
N1264 L1265 S1266 L1267 G1268 E1269 L1270 E1271 S1272 L1273 R1274 A1275 A1276 F1277 L1278 E1279 I1280 E1281 N1282 D1283 G1284 T1285 Y1286 E1287 S1288 I1289 A1290 K1291 F1292 H1293 G1294 S1295 P1296 C1299 Q1300 L1301 N1302 G1303 N1304 P1305 I1306 S1307 C1308 C1309 V1310 H1311 G1312 M1313 P1314 T1315 F1316 P1317 H1318 W1319 H1320 R1321 L1322 Y1323 V1324
V1325 V1326 V1327 E1328 N1329 A1330 L1331 L1332 K1333 K1334 V1338 A1339 V1340 P1341 Y1342 W1343 D1344 W1345 I1349 E1350 H1351 L1352 P1353 H1354 L1355 I1356 S1357 D1358 A1359 T1360 Y1361 Y1362 N1363 S1364 R1365 Q1366 H1367 H1368 T1371 N1372 P1373 F1374 I1379 T1380 H1381 E1382 R1388 K1391 D1392 S1393 L1394 F1395 H1396 S1397

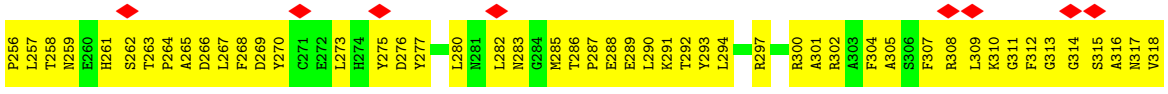


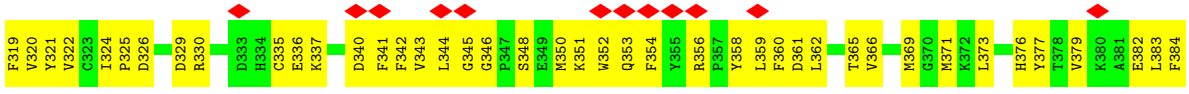
- Molecule 1: HEMOCYANIN KLH1

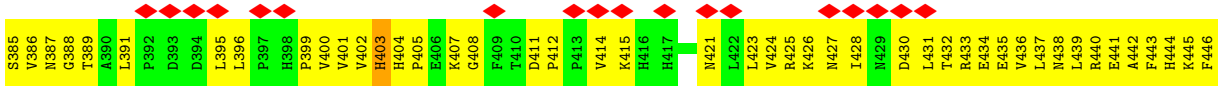
Chain C:

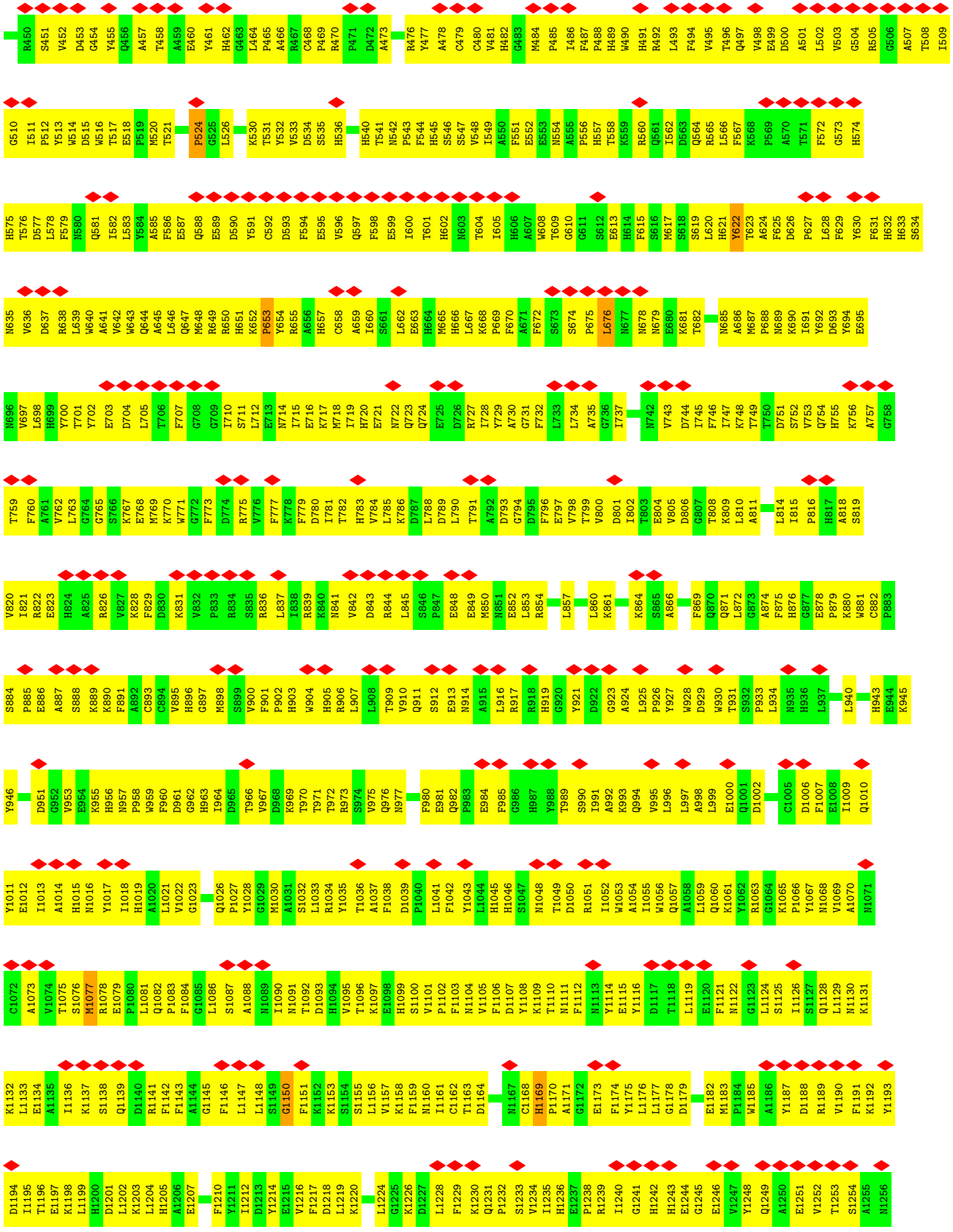








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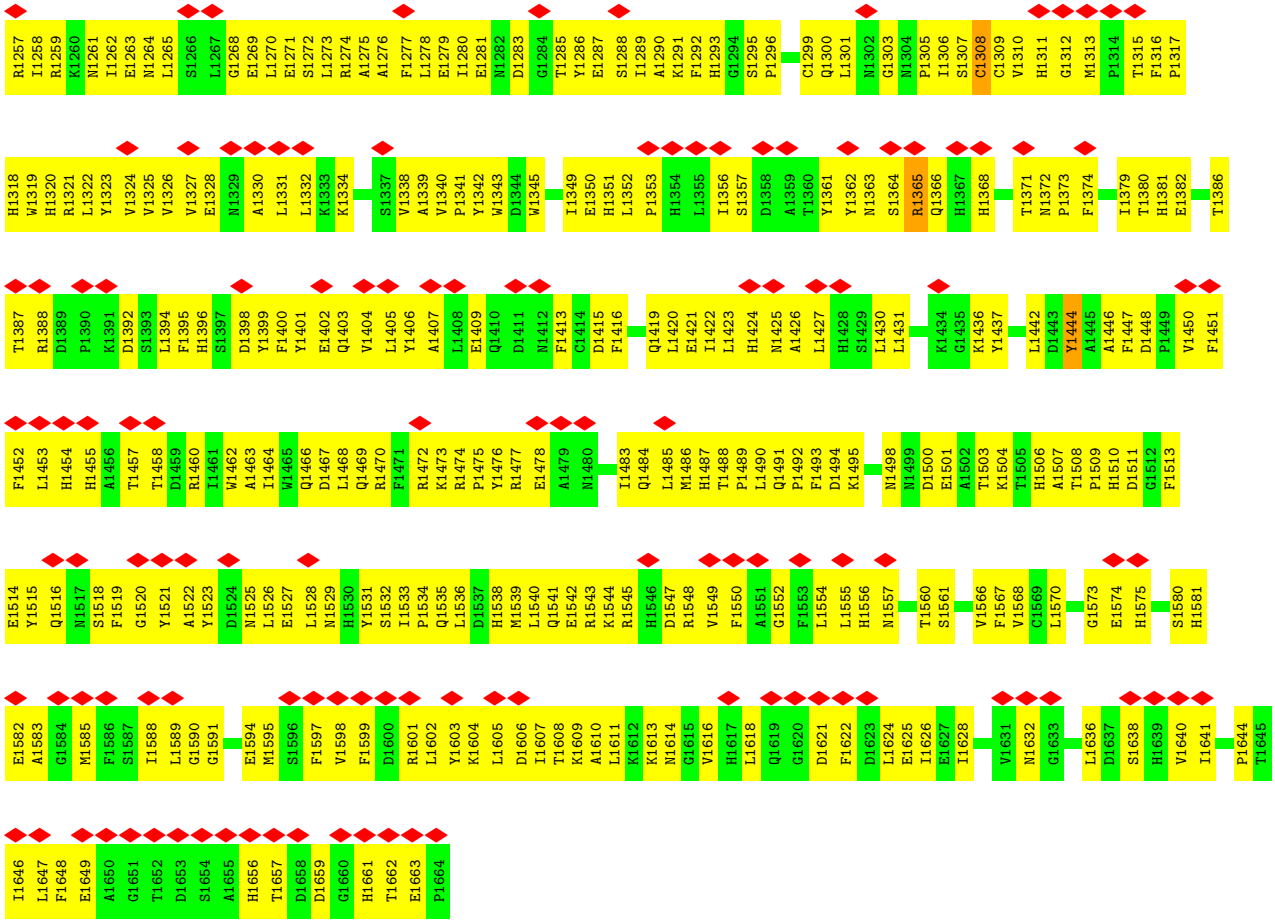
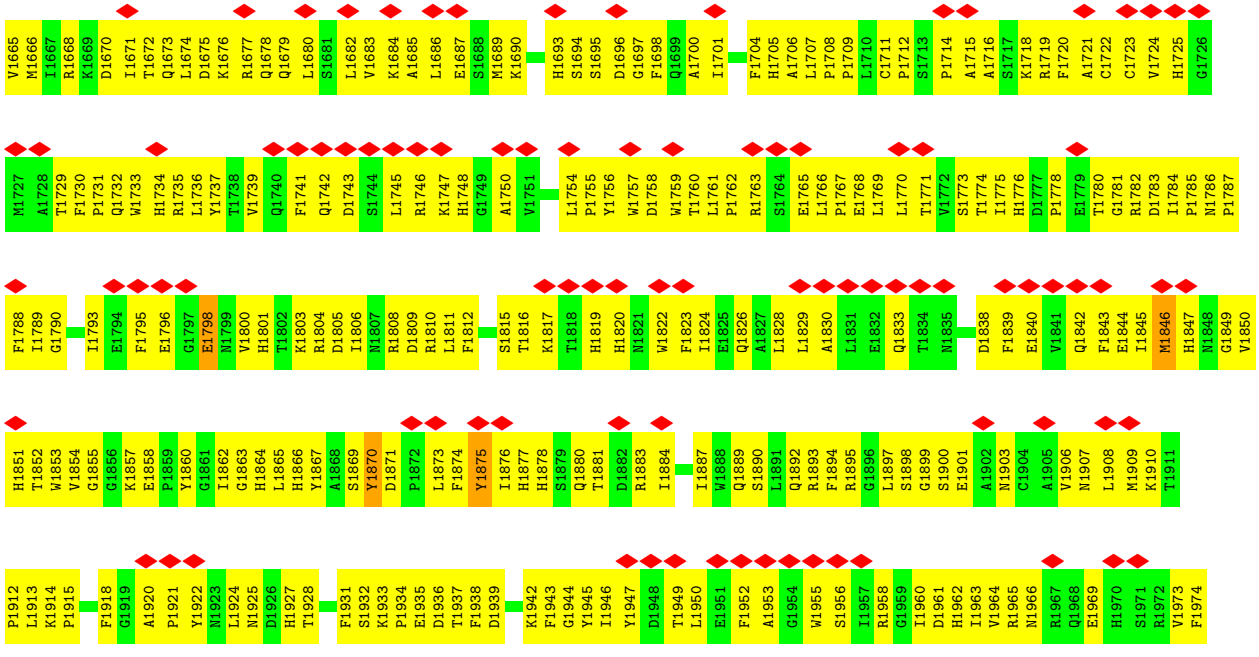
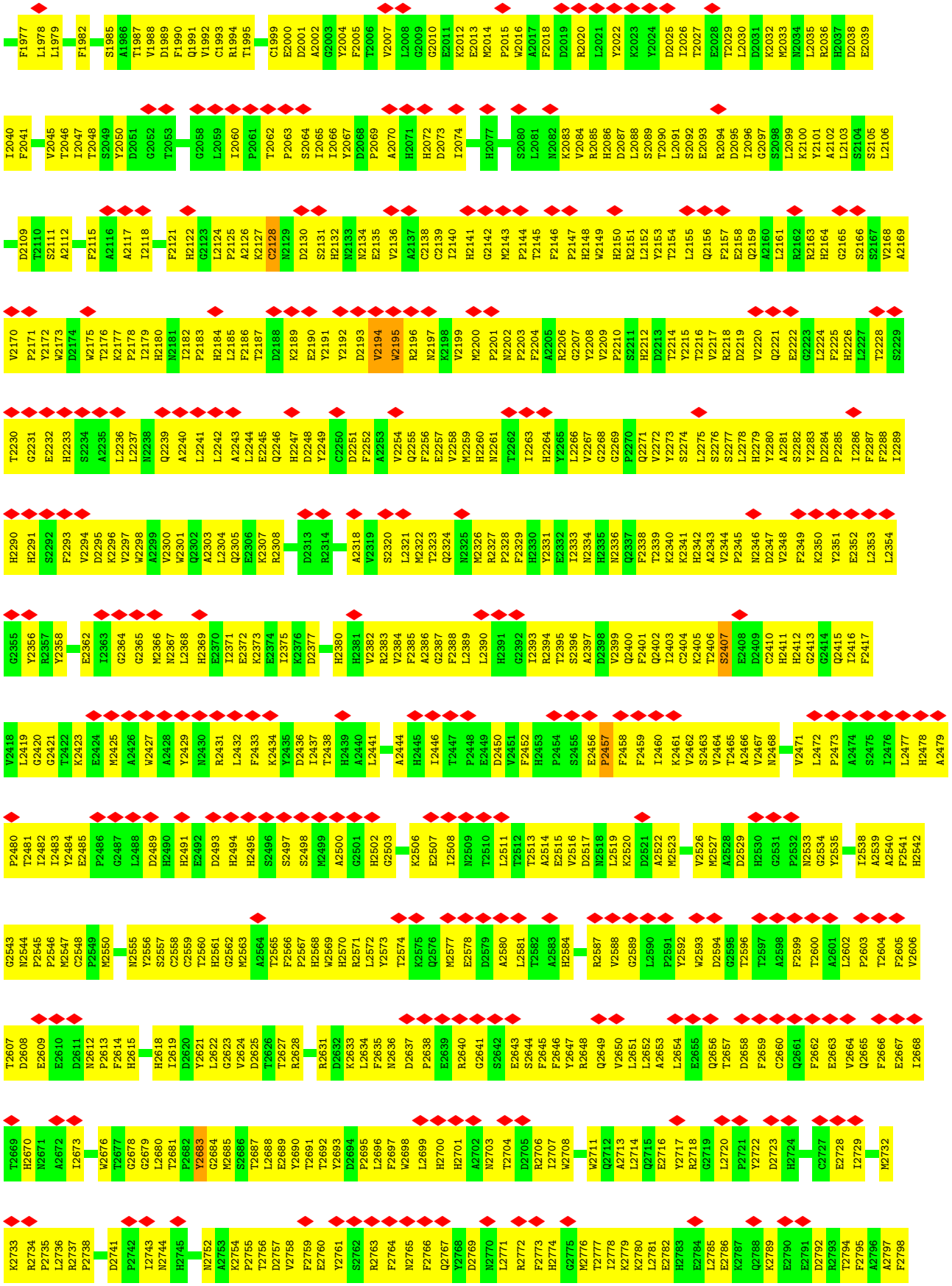
R476 Y477 A478 C479 C480 V481 H482 G483 M484 P485 I486 F487 P488 H489 W490 H491 R492 L493 F494 V495 T496 Q497 V498 E499 D500 A501 L502 V503 G504 R505 G506 A507 T508 I509
G510 I511 P512 Y513 W514 D515 W516 T517 E518 P519 M520 T521
P524 G525 L526
K530 T531 Y532 V533 D534 S535 H536
H540 T541 N542 P543 F544 H545 S546 S547 V548 I549 A550 F551 E552 E553 N554 A555 P556 H557 T558 K559 R560 Q561 I562 D563 Q564 R565 L566 F567 K568 P569 A570 T571 F572 G573 H574
H575 T576 D577 L578 F579 N580 Q581 I582 L583 Y584 A585 F586 E587 Q588 E589 D590 Y591 C592 D593 F594 E595 V596 Q597 F598 E599 I600 T601 H602 N603 T604 I605 H606 A607 W608 T609 G610 G611 S612 E613 H614 F615 S616 M617 S618 S619 L620 H621 Y622 T623 A624 F625 D626 P627 L628 F629 Y630 F631 H632 H633 S634
N635 V636 D637 R638 L639 W640 A641 V642 W643 Q644 A645 L646 Q647 M648 R649 R650 H651 K652 P653 Y654 R655 A656 H657 C658 A659 I660 S661 L662 E663 H664 M665 H666 L667 K668 P669 F670 A671 F672 S673 S674 P675 L676 N677 N678 N679 E680 K681 T682
N685 A686 M687 P688 N689 K690 I691 Y692 D693 Y694 E695
N696 V697 L698 H699 Y700 T701 Y702 E703 D704 L705 T706 F707 G708 G709 I710 S711 L712 E713 N714 I715 E716 K717 M718 I719 H720 E721 N722 Q723 Q724 E725 D726 R727 I728 Y729 A730 G731 F732 L733 L734 A735 G736 I737 N742 V743 D744 I745 F746 I747 K748 T749 T750 D751 S752 V753 Q754 H755 K756 A757 G758
T759 F760 A761 V762 L763 G764 G765 S766 K767 E768 M769 K770 W771 G772 F773 D774 R775 V776 F777 K778 F779 D780 I781 T782 H783 V784 L785 K786 D787 L788 D789 L790 T791 A792 D793 G794 D795 F796 E797 V798 T799 V800 D801 I802 T803 E804 V805 D806 G807 T808 K809 L810 A811 L814 I815 P816 H817 A818 S819
V820 I821 R822 E823 H824 A825 R826 V827 K828 F829 D830 K831 V832 P833 R834 S835 R836 L837 I838 R839 K840 N841 V842 D843 R844 L845 S846 P847 E848 E849 M850 N851 E852 L853 R854 L857 L860 K861 K864 S865 A866 F869 Q870 Q871 L872 G873 A874 F875 H876 G877 E878 P879 K880 W881 C882 P883
S884 P885 E886 A887 S888 K889 K890 F891 A892 C893 C894 V895 H896 G897 M898 S899 V900 F901 P902 H903 W904 H905 R906 L907 L908 T909 V910 Q911 S912 E913 N914 A915 L916 R917 R918 H919 G920 Y921 D922 G923 A924 L925 P926 Y927 W928 D929 W930 T931 S932 P933 L934 N935 H936 L937 L940 H943 E944 K945
Y946 D951 G952 W953 E954 K955 H956 N957 P958 W959 F960 D961 G962 H963 I964 D965 T966 V967 D968 K969 T970 T971 T972 R973 S974 V975 Q976 N977 F980 E981 Q982 F983 E984 F985 G986 H987 Y988 T989 S990 I991 A992 K993 Q994 V995 L996 L997 A998 L999 E1000 Q1001 D1002 C1005 D1006 F1007 E1008 I1009 Q1010
Y1011 E1012 I1013 A1014 H1015 N1016 Y1017 I1018 H1019 A1020 L1021 V1022 G1023 Q1026 P1027 Y1028 G1029 M1030 A1031 S1032 L1033 R1034 Y1035 T1036 A1037 F1038 D1039 P1040 L1041 F1042 Y1043 L1044 H1045 H1046 S1047 N1048 T1049 D1050 R1051 I1052 W1053 A1054 I1055 W1056 Q1057 A1058 L1059 Q1060 K1061 Y1062 R1063 G1064 K1065 P1066 Y1067 N1068 V1069 A1070 M1071
C1072 A1073 V1074 T1075 S1076 M1077 R1078 E1079 P1080 L1081 Q1082 P1083 F1084 G1085 L1086 S1087 A1088 N1089 I1090 N1091 T1092 D1093 H1094 V1095 T1096 K1097 E1098 H1099 S1100 V1101 P1102 F1103 N1104 V1105 F1106 D1107 Y1108 K1109 T1110 N1111 F1112 N1113 Y1114 E1115 Y1116 D1117 T1118 L1119 E1120 F1121 N1122 G1123 L1124 S1125 I1126 S1127 Q1128 L1129 N1130 K1131
K1132 L1133 E1134 A1135 I1136 K1137 S1138 Q1139 D1140 R1141 F1142 F1143 A1144 G1145 F1146 L1147 L1148 S1149 G1150 F1151 K1152 K1153 S1154 S1155 L1156 V1157 K1158 F1159 N1160 I1161 C1162 T1163 D1164 N1167 C1168 H1169 P1170 A1171 G1172 E1173 F1174 Y1175 L1176 L1177 G1178 D1179 E1182 M1183 P1184 W1185 A1186 Y1187 D1188 R1189 V1190 F1191 K1192 Y1193
D1194 I1195 T1196 E1197 K1198 L1199 H1200 D1201 L1202 K1203 L1204 H1205 A1206 E1207 F1210 Y1211 I1212 D1213 Y1214 E1215 V1216 F1217 D1218 L1219 K1220 L1224 G1225 K1226 D1227 L1228 F1229 K1230 Q1231 P1232 S1233 V1234 I1235 H1236 E1237 P1238 R1239 I1240 G1241 H1242 H1243 E1244 G1245 E1246 V1247 Y1248 Q1249 A1250 E1251 V1252 T1253 S1254 A1255 N1256



• Molecule 2: HEMOCYANIN KLH1

Chain B:

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I2040 F2041 V2045 T2046 I2047 T2048 S2049 Y2050 D2051 G2052 T2053 G2058 L2059 I2060 P2061 T2062 P2063 S2064 I2065 I2066 Y2067 D2068 P2069 A2070 H2071 H2072 D2073 I2074 H2077 S2080 L2081 N2082 K2083 V2084 R2085 H2086 D2087 L2088 S2089 T2090 L2091 S2092 E2093 R2094 D2095 I2096 G2097 S2098 L2099 K2100 Y2101 A2102 L2103 S2104 S2105 L2106
D2109 T2110 S2111 A2112 F2115 A2116 A2117 I2118 F2121 H2122 G2123 L2124 P2125 A2126 K2127 C2128 N2129 D2130 S2131 H2132 N2133 N2134 E2135 V2136 A2137 C2138 C2139 I2140 H2141 G2142 M2143 P2144 T2145 F2146 P2147 H2148 W2149 H2150 R2151 L2152 Y2153 T2154 L2155 Q2156 F2157 E2158 Q2159 A2160 L2161 R2162 R2163 H2164 G2165 S2166 S2167 V2168 A2169
V2170 P2171 Y2172 W2173 D2174 W2175 T2176 K2177 P2178 I2179 H2180 W2181 I2182 P2183 H2184 L2185 F2186 T2187 D2188 K2189 E2190 Y2191 Y2192 D2193 V2194 W2195 R2196 N2197 K2198 V2199 M2200 P2201 N2202 P2203 F2204 A2205 R2206 G2207 Y2208 V2209 P2210 S2211 H2212 D2213 T2214 Y2215 T2216 V2217 R2218 D2219 V2220 Q2221 E2222 G2223 L2224 F2225 H2226 L2227 T2228 S2229
T2230 G2231 E2232 H2233 S2234 A2235 L2236 L2237 N2238 Q2239 A2240 L2241 L2242 A2243 L2244 E2245 Q2246 H2247 D2248 Y2249 C2250 D2251 F2252 A2253 V2254 Q2255 F2256 E2257 V2258 M2259 H2260 N2261 T2262 I2263 H2264 Y2265 L2266 V2267 G2268 G2269 P2270 Q2271 V2272 Y2273 S2274 L2275 S2276 S2277 L2278 H2279 Y2280 A2281 S2282 Y2283 D2284 P2285 I2286 F2287 F2288 I2289
H2290 H2291 S2292 F2293 V2294 D2295 K2296 V2297 W2298 A2299 V2300 W2301 Q2302 A2303 L2304 Q2305 E2306 K2307 R2308 D2313 R2314 A2318 V2319 S2320 L2321 M2322 T2323 Q2324 N2325 M2326 R2327 P2328 F2329 H2330 Y2331 E2332 I2333 N2334 H2335 N2336 Q2337 F2338 T2339 K2340 K2341 H2342 A2343 V2344 P2345 N2346 D2347 V2348 F2349 K2350 Y2351 E2352 L2353 L2354
G2355 Y2356 R2357 Y2358 E2362 I2363 G2364 G2365 M2366 N2367 L2368 H2369 E2370 I2371 E2372 K2373 E2374 I2375 K2376 D2377 H2380 H2381 V2382 R2383 V2384 F2385 A2386 G2387 F2388 L2389 L2390 H2391 G2392 I2393 R2394 T2395 S2396 A2397 D2398 V2399 Q2400 F2401 Q2402 I2403 C2404 K2405 T2406 S2407 E2408 D2409 C2410 H2411 H2412 G2413 G2414 Q2415 I2416 F2417
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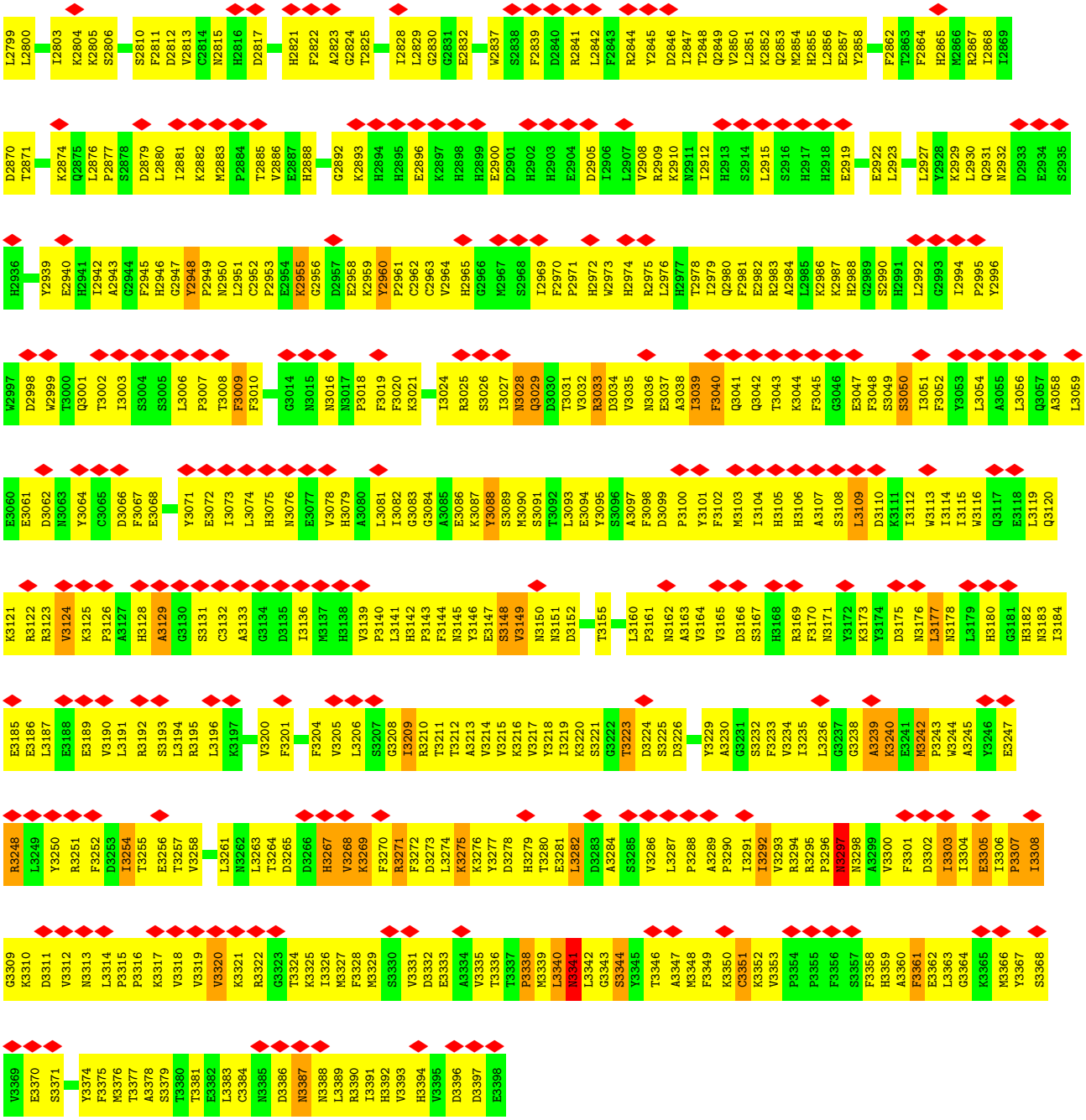
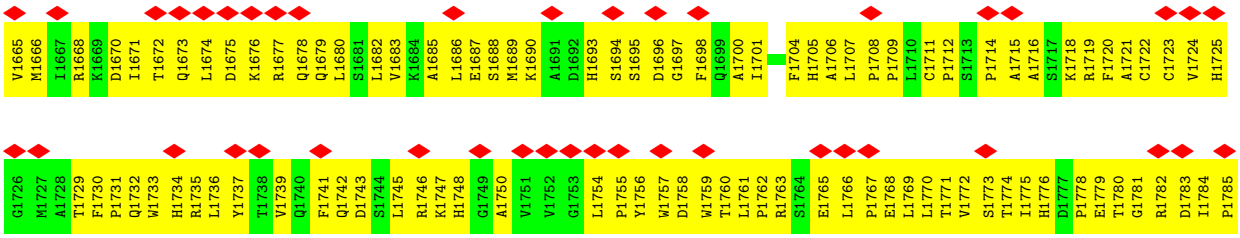
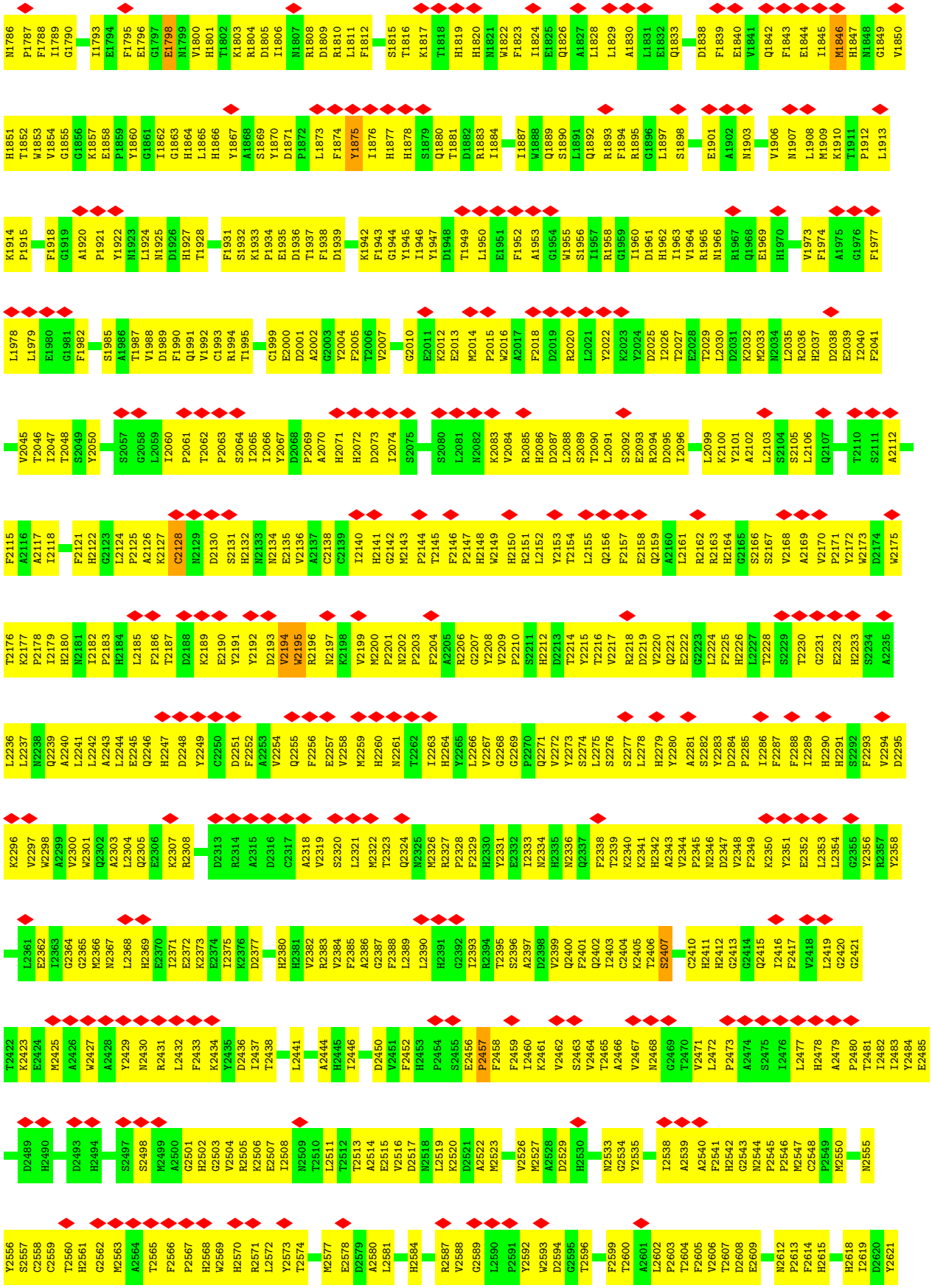
P2480 T2481 I2482 I2483 Y2484 M2547 C2548 P2549 M2550 P2486 G2487 L2488 D2489 H2490 H2491 E2492 D2493 H2494 H2495 S2496 S2497 S2498 M2499 A2500 G2501 H2502 G2503 K2506 E2507 I2508 N2509 T2510 L2511 T2512 T2513 A2514 E2515 V2516 D2517 N2518 L2519 K2520 D2521 A2522 M2523 V2526 M2527 A2528 D2529 H2530 G2531 P2532 N2533 G2534 Y2535 I2538 A2539 A2540 F2541 H2542
G2543 N2544 P2545 P2546 M2547 C2548 P2549 M2550 N2555 Y2556 S2557 C2558 C2559 T2560 H2561 G2562 M2563 A2564 T2565 F2566 P2567 H2568 W2569 H2570 R2571 L2572 Y2573 T2574 K2575 Q2576 M2577 E2578 D2579 A2580 L2581 T2582 A2583 H2584 R2587 V2588 G2589 L2590 P2591 Y2592 W2593 D2594 G2595 T2596 T2597 A2598 F2599 T2600 A2601 L2602 P2603 T2604 F2605 V2606
T2607 D2608 E2609 E2610 D2611 N2612 P2613 F2614 H2615 H2618 I2619 D2620 Y2621 L2622 G2623 V2624 D2625 T2626 T2627 R2628 R2631 D2632 K2633 L2634 F2635 N2636 D2637 P2638 E2639 R2640 G2641 S2642 E2643 S2644 F2645 F2646 Y2647 R2648 Q2649 V2650 L2651 L2652 A2653 L2654 E2655 Q2656 T2657 D2658 F2659 C2660 Q2661 F2662 E2663 V2664 Q2665 F2666 E2667 I2668
T2669 H2670 N2671 A2672 I2673 W2676 T2677 G2678 G2679 L2680 T2681 P2682 Y2683 G2684 M2685 S2686 T2687 L2688 E2689 Y2690 T2691 T2692 Y2693 D2694 P2695 L2696 F2697 W2698 L2699 H2700 H2701 A2702 N2703 T2704 D2705 R2706 I2707 W2708 W2711 Q2712 A2713 L2714 Q2715 E2716 Y2717 R2718 G2719 L2720 P2721 Y2722 D2723 H2724 C2727 E2728 I2729 M2732
K2733 R2734 P2735 L2736 R2737 P2738 D2741 P2742 I2743 N2744 H2745 N2752 A2753 K2754 P2755 T2756 D2757 V2758 F2759 E2760 Y2761 S2762 R2763 F2764 N2765 F2766 Q2767 Y2768 D2769 W2770 L2771 R2772 F2773 H2774 G2775 M2776 T2777 I2778 K2779 K2780 L2781 E2782 H2783 E2784 L2785 E2786 K2787 Q2788 K2789 E2790 E2791 D2792 R2793 T2794 F2795 A2796 A2797 F2798

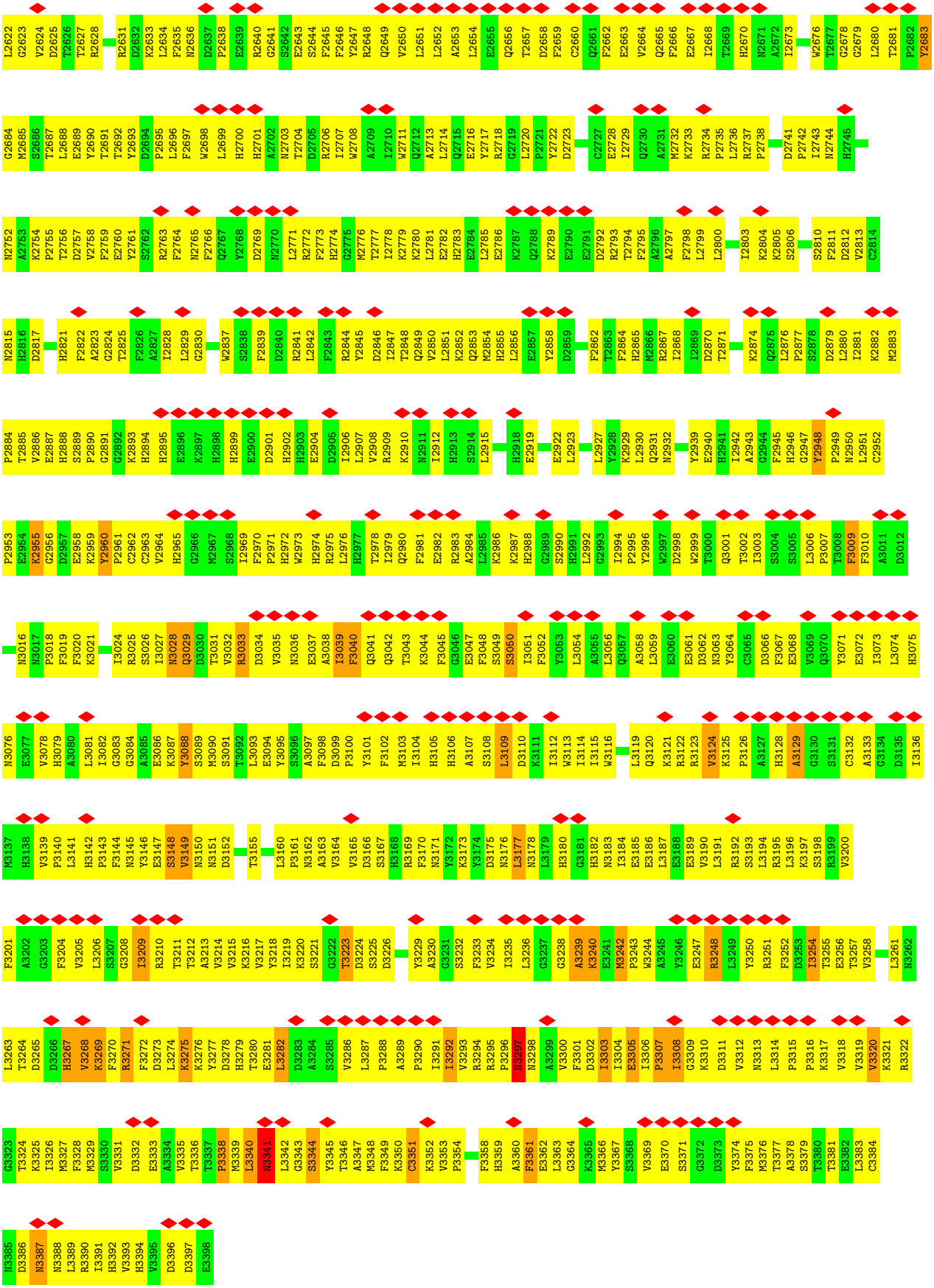


• Molecule 2: HEMOCYANIN KLH1

Chain D:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	4762	Depositor
Resolution determination method	Not provided	
CTF correction method	PER MICROGRAPH	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.037	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	558, 558, 558	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CUO

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	0.95	2/13940 (0.0%)	1.19	15/18926 (0.1%)
1	C	0.95	2/13940 (0.0%)	1.19	15/18926 (0.1%)
2	B	0.93	2/14526 (0.0%)	1.10	8/19734 (0.0%)
2	D	0.93	2/14526 (0.0%)	1.10	9/19734 (0.0%)
All	All	0.94	8/56932 (0.0%)	1.14	47/77320 (0.1%)

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	1
1	C	0	1
2	B	0	2
2	D	0	2
All	All	0	6

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	524	PRO	N-CD	16.06	1.70	1.47
1	A	524	PRO	N-CD	16.04	1.70	1.47
2	B	2457	PRO	N-CD	13.70	1.67	1.47
2	D	2457	PRO	N-CD	13.65	1.67	1.47
1	C	653	PRO	N-CD	8.88	1.60	1.47

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1632	ASN	CB-CG-OD1	-38.50	44.60	121.60
1	A	1632	ASN	CB-CG-OD1	-38.48	44.65	121.60
1	A	212	ASN	CB-CG-OD1	-38.25	45.10	121.60
1	C	212	ASN	CB-CG-OD1	-38.23	45.13	121.60
1	A	212	ASN	CB-CG-ND2	-9.73	93.35	116.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1150	GLY	Mainchain
2	B	2951	LEU	Peptide
2	B	3248	ARG	Sidechain
1	C	1150	GLY	Mainchain
2	D	2951	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	A	13530	0	12792	2867	0
1	C	13530	0	12792	2896	0
2	B	14084	0	13309	2799	0
2	D	14084	0	13311	2767	0
3	A	16	0	0	1	0
3	B	16	0	0	3	0
3	C	16	0	0	1	0
3	D	16	0	0	3	0
All	All	55292	0	52204	10910	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 102.

The worst 5 of 10910 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)
2:D:2279:HIS:HE1	2:D:2280:TYR:CZ	1.08	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2279:HIS:CE1	2:D:2280:TYR:CE2	1.80	1.65
1:C:724:GLN:HE22	1:C:828:LYS:CE	1.10	1.63
2:B:2279:HIS:CE1	2:B:2280:TYR:CE2	1.80	1.63
2:B:2279:HIS:HE1	2:B:2280:TYR:CZ	1.08	1.63

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	1662/1664 (100%)	1601 (96%)	56 (3%)	5 (0%)	41 77
1	C	1662/1664 (100%)	1599 (96%)	58 (4%)	5 (0%)	41 77
2	B	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	9 42
2	D	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	9 42
All	All	6788/6796 (100%)	6416 (94%)	302 (4%)	70 (1%)	20 55

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2960	TYR
2	B	3028	ASN
2	B	3050	SER
2	B	3148	SER
2	B	3225	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	1457/1457 (100%)	1456 (100%)	1 (0%)	93 97
1	C	1457/1457 (100%)	1456 (100%)	1 (0%)	93 97
2	B	1522/1522 (100%)	1502 (99%)	20 (1%)	69 81
2	D	1522/1522 (100%)	1502 (99%)	20 (1%)	69 81
All	All	5958/5958 (100%)	5916 (99%)	42 (1%)	84 90

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	3209	ILE
2	D	3275	LYS
2	D	3240	LYS
2	D	3267	HIS
2	D	3292	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 230 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3341	ASN
2	D	3145	ASN
1	C	936	HIS
2	D	3105	HIS
2	D	2700	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CUO	C	9003	1	0,4,4	-	-	-		
3	CUO	C	9001	1	0,4,4	-	-	-		
3	CUO	A	9003	1	0,4,4	-	-	-		
3	CUO	C	9004	1	0,4,4	-	-	-		
3	CUO	D	9008	2	0,4,4	-	-	-		
3	CUO	A	9002	1	0,4,4	-	-	-		
3	CUO	D	9005	2	0,4,4	-	-	-		
3	CUO	D	9006	2	0,4,4	-	-	-		
3	CUO	B	9005	2	0,4,4	-	-	-		
3	CUO	D	9007	2	0,4,4	-	-	-		
3	CUO	A	9004	1	0,4,4	-	-	-		
3	CUO	B	9007	2	0,4,4	-	-	-		
3	CUO	C	9002	1	0,4,4	-	-	-		
3	CUO	B	9008	2	0,4,4	-	-	-		
3	CUO	B	9006	2	0,4,4	-	-	-		
3	CUO	A	9001	1	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CUO	C	9003	1	-	-	0/1/1/1
3	CUO	C	9001	1	-	-	0/1/1/1
3	CUO	A	9003	1	-	-	0/1/1/1
3	CUO	C	9004	1	-	-	0/1/1/1
3	CUO	D	9008	2	-	-	0/1/1/1
3	CUO	A	9002	1	-	-	0/1/1/1
3	CUO	D	9005	2	-	-	0/1/1/1
3	CUO	D	9006	2	-	-	0/1/1/1
3	CUO	B	9005	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CUO	D	9007	2	-	-	0/1/1/1
3	CUO	A	9004	1	-	-	0/1/1/1
3	CUO	B	9007	2	-	-	0/1/1/1
3	CUO	C	9002	1	-	-	0/1/1/1
3	CUO	B	9008	2	-	-	0/1/1/1
3	CUO	B	9006	2	-	-	0/1/1/1
3	CUO	A	9001	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	9003	CUO	1	0
3	A	9003	CUO	1	0
3	D	9008	CUO	3	0
3	B	9008	CUO	3	0

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.

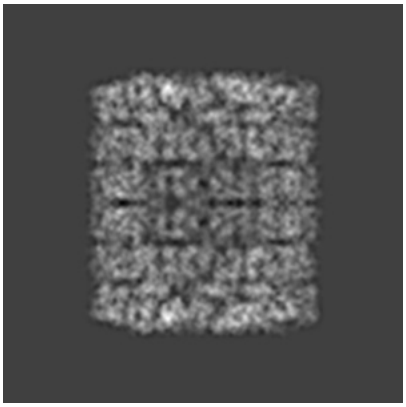
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1569. These allow visual inspection of the internal detail of the map and identification of artifacts.

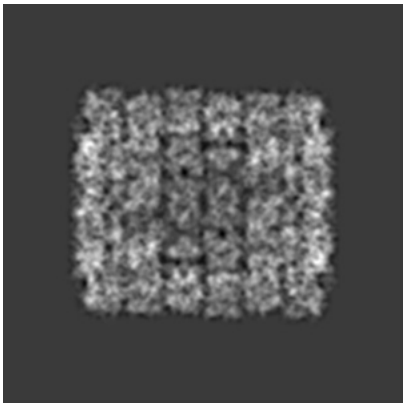
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 225

Y Index: 225

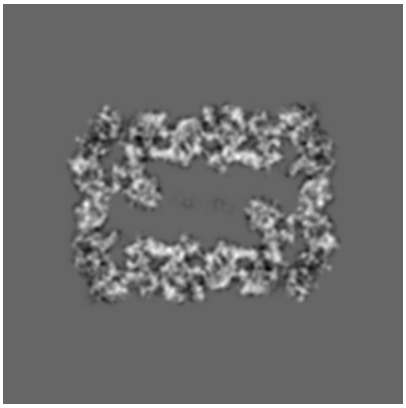
Z Index: 225

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

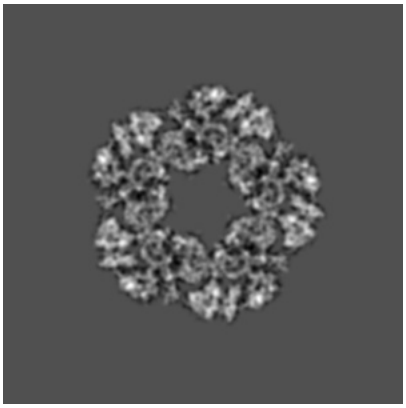
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 168



Y Index: 149

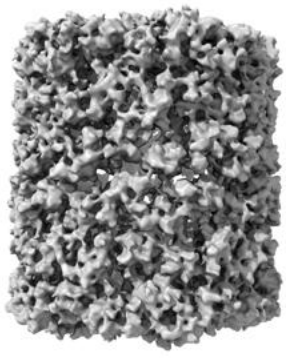


Z Index: 98

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

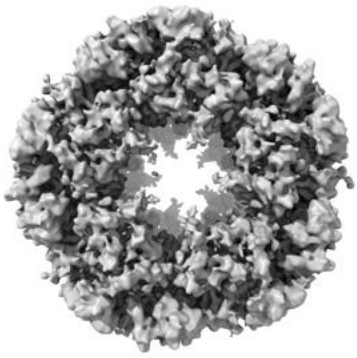
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

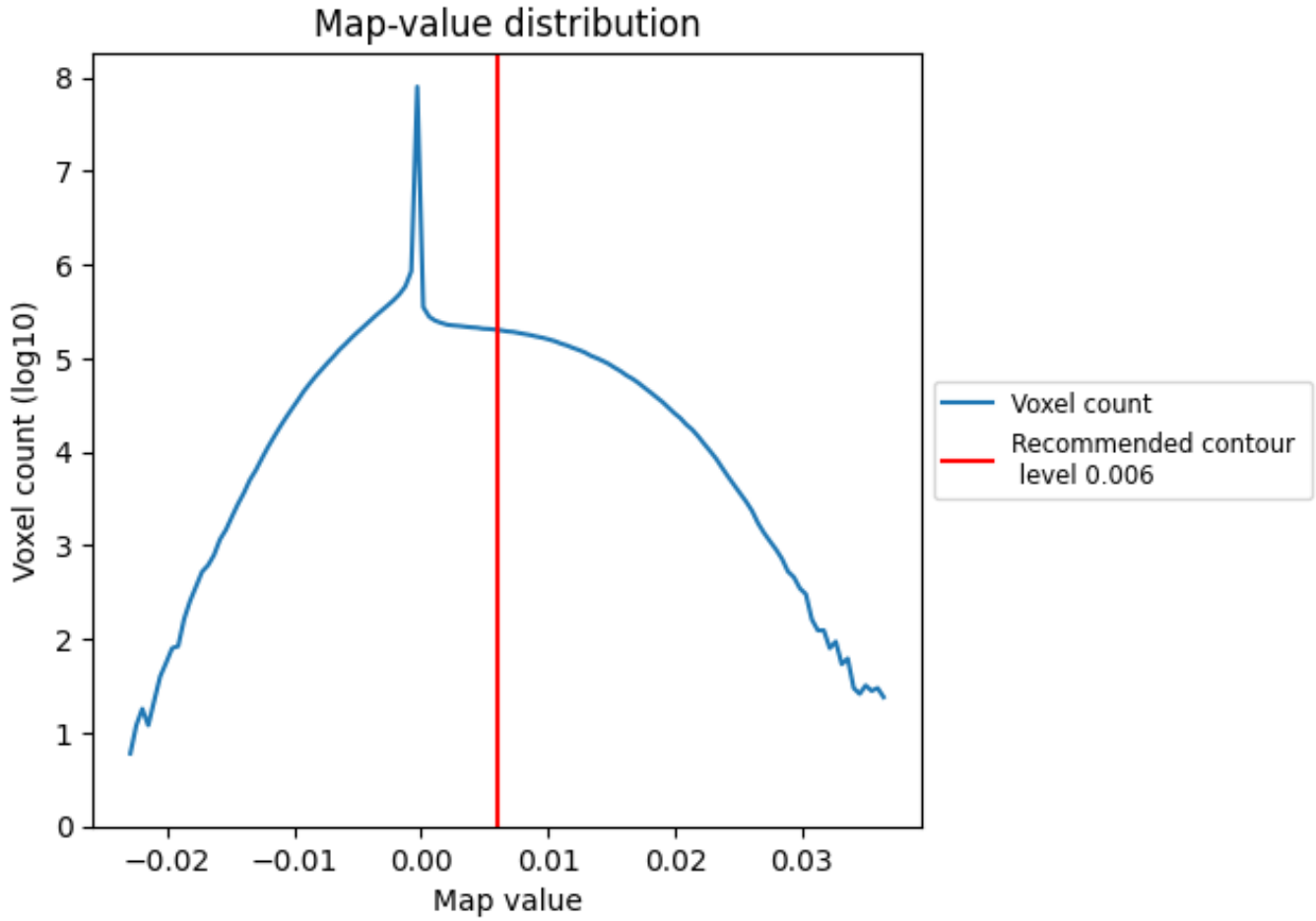
6.5 Mask visualisation (i)

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

7 Map analysis

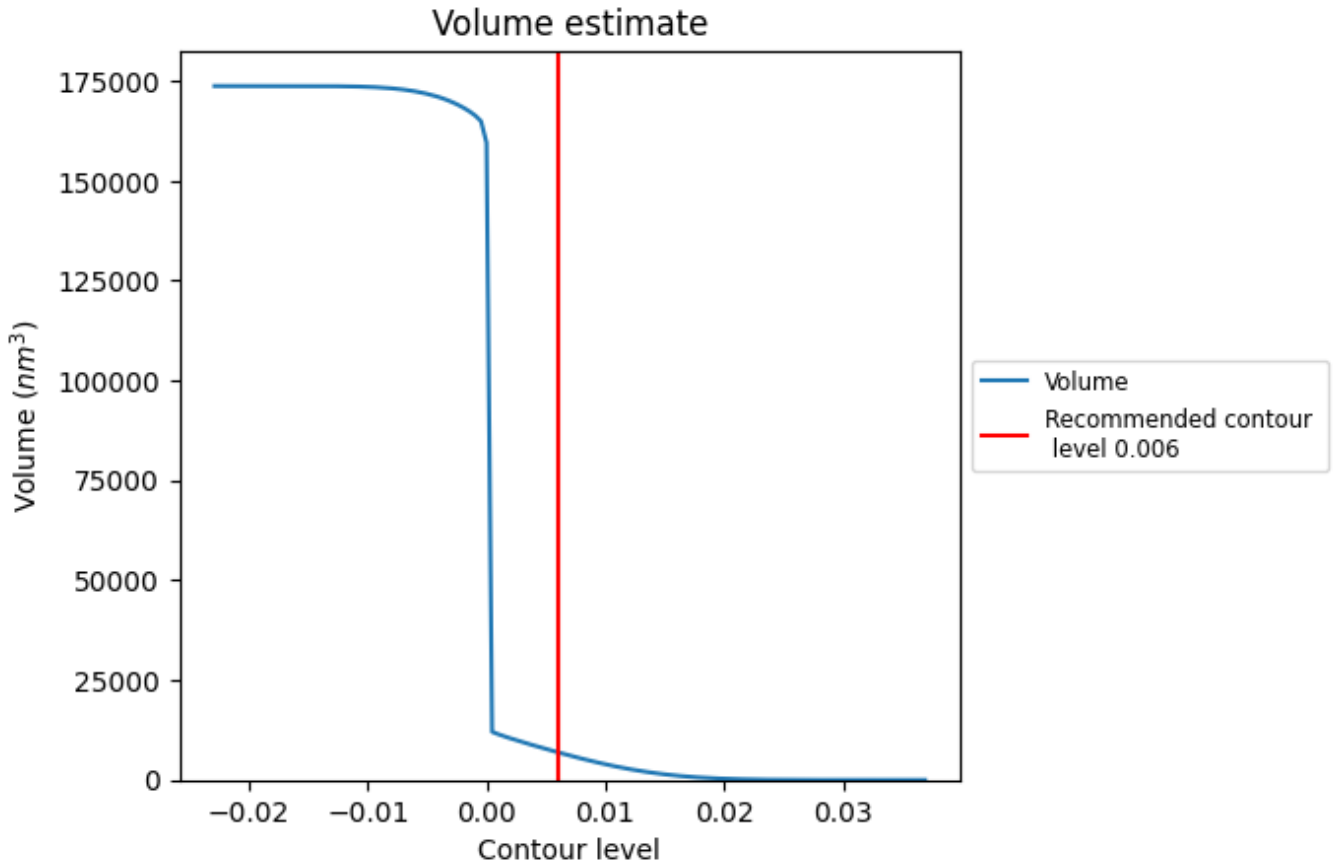
This section contains the results of statistical analysis of the map.

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.

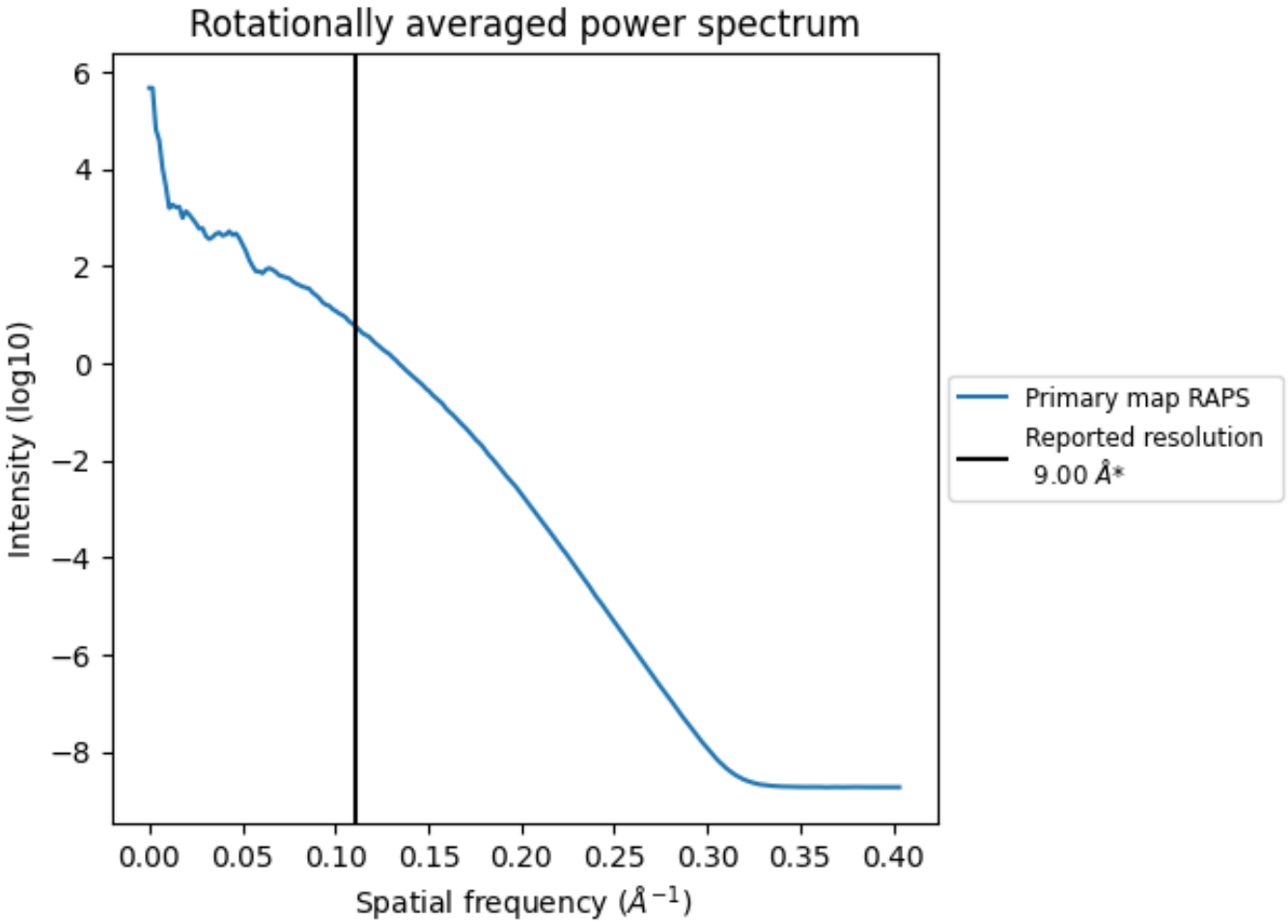
7.2 Volume estimate (i)



The volume at the recommended contour level is 6926 nm^3; this corresponds to an approximate mass of 6256 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 0.111 Å^{-1}

8 Fourier-Shell correlation (i)

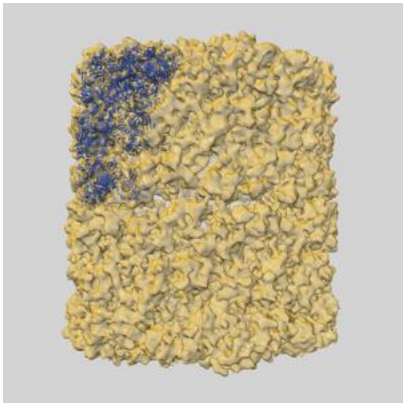
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

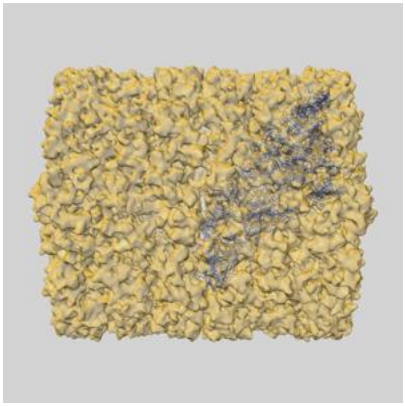
This section contains information regarding the fit between EMDB map EMD-1569 and PDB model 4BED. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlays

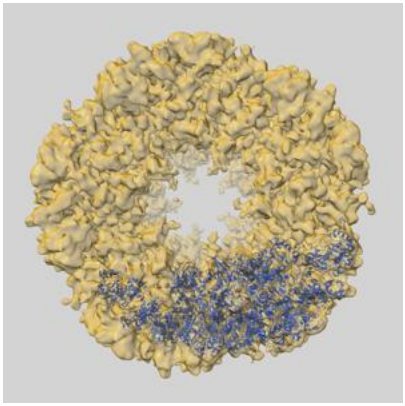
9.1.1 Map-model overlay



X

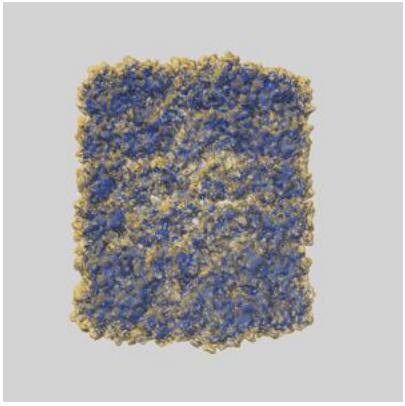


Y

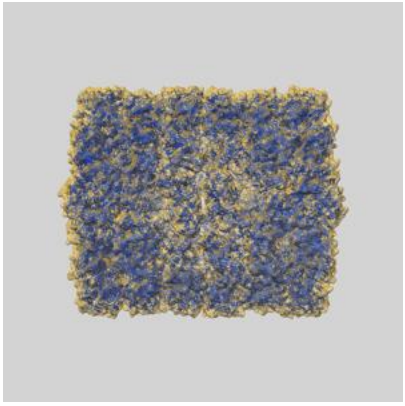


Z

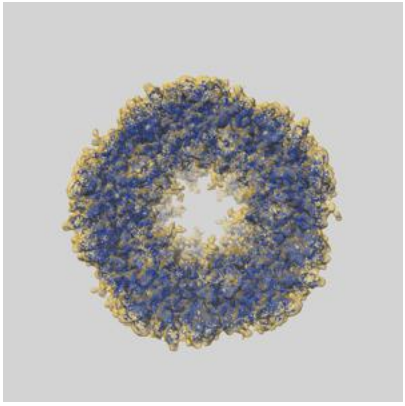
9.1.2 Map-model assembly overlay



X



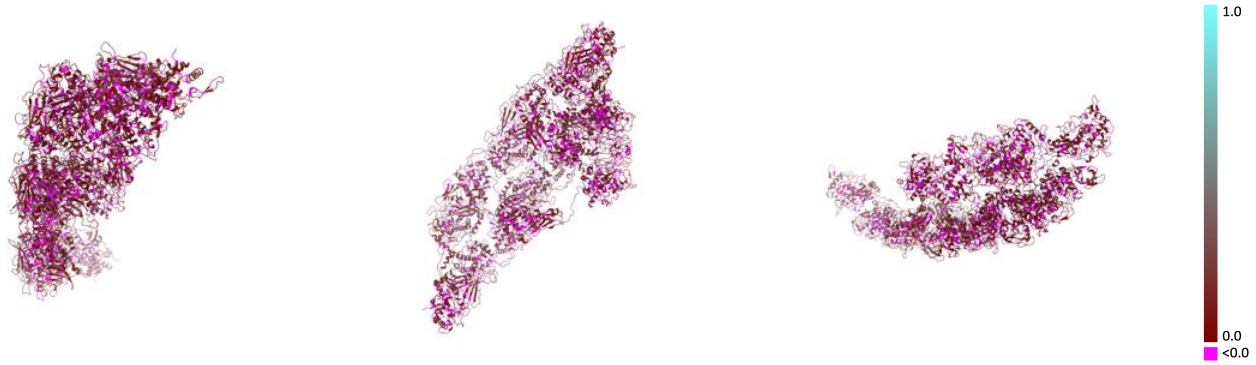
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

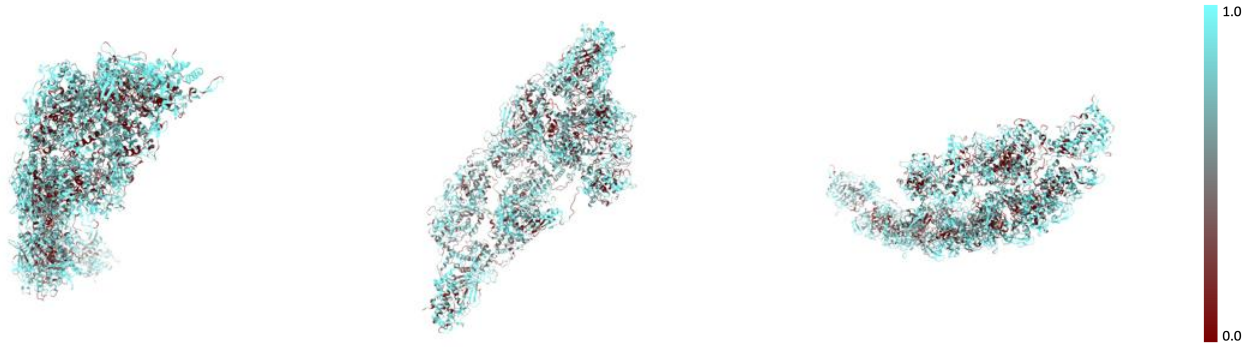
9.2 Q-score mapped to coordinate model (i)



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.

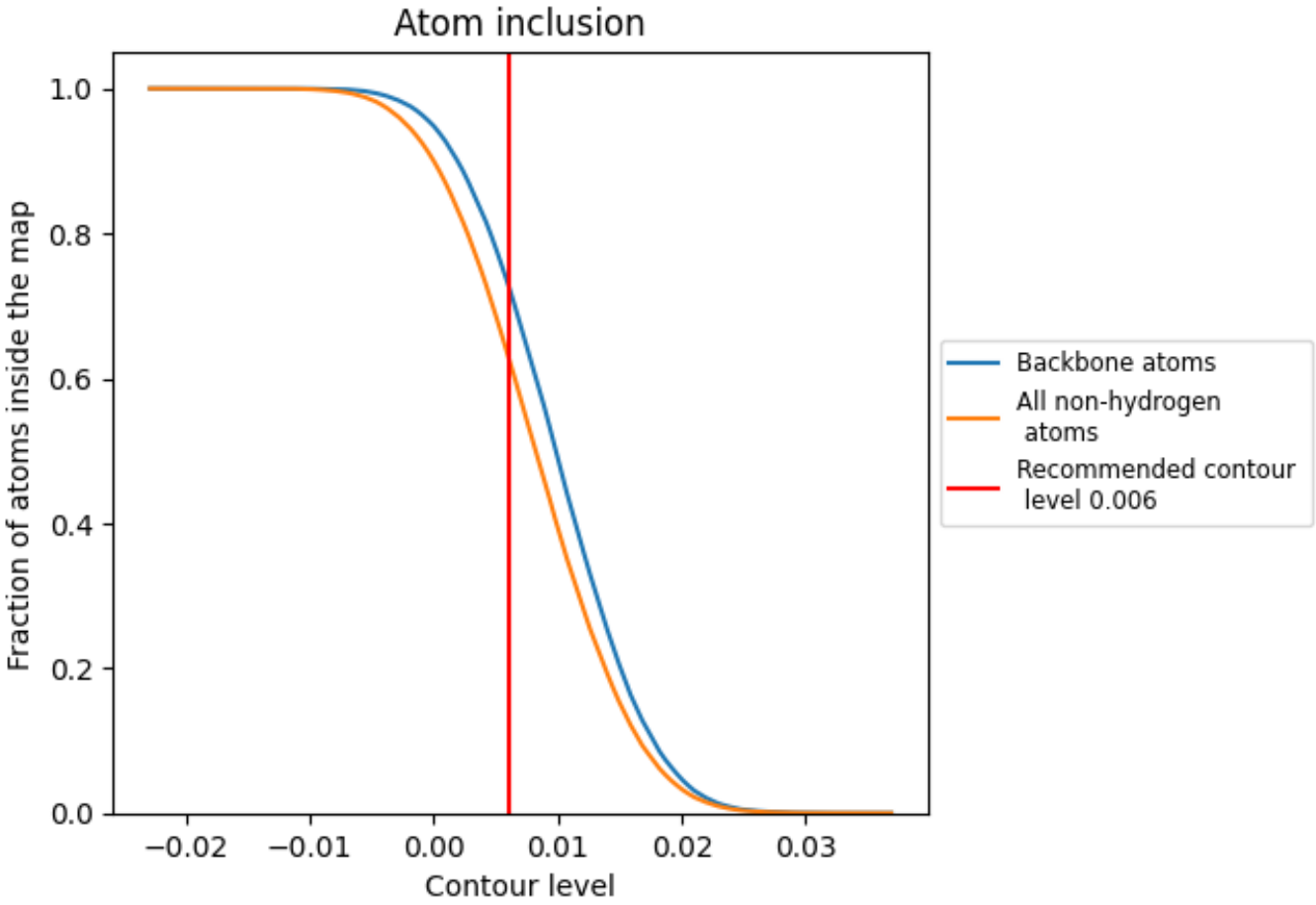
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 63% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6312	0.0810
A	0.6485	0.0860
B	0.5914	0.0730
C	0.6464	0.0900
D	0.6397	0.0770