



## wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 08:24 AM UTC

PDB ID : 4BED / pdb\_00004bed  
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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

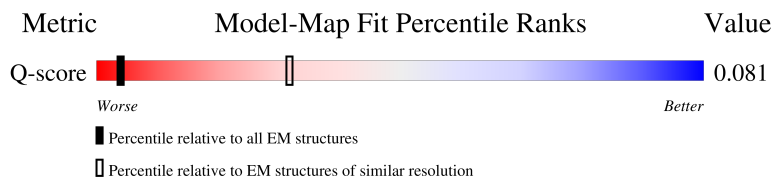
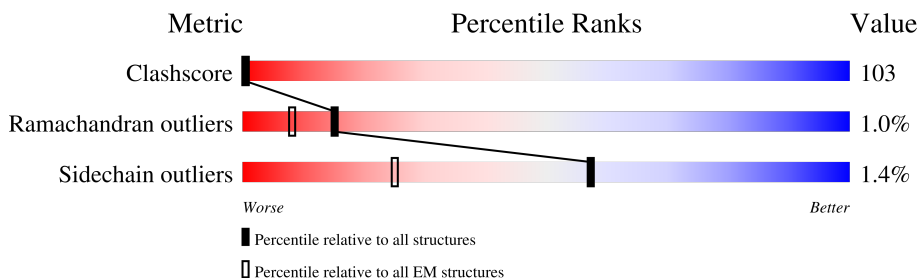
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	244 ( 8.60 - 9.60 )

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  $\geq 3$ , 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	A	1664	<p>28% (Upper red bar), 25% (Red), 66% (Yellow), 9% (Orange)</p>
1	C	1664	<p>27% (Upper red bar), 24% (Red), 66% (Yellow), 9% (Orange)</p>
2	B	1734	<p>33% (Upper red bar), 26% (Red), 64% (Yellow), 10% (Orange)</p>
2	D	1734	<p>29% (Upper red bar), 26% (Red), 64% (Yellow), 10% (Orange)</p>

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
3	CUO	B	9008	-	-	X	-
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
			Total	C	N	O	S		
1	A	1664	13530	8611	2347	2515	57	0	0
1	C	1664	13530	8611	2347	2515	57	0	0

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.

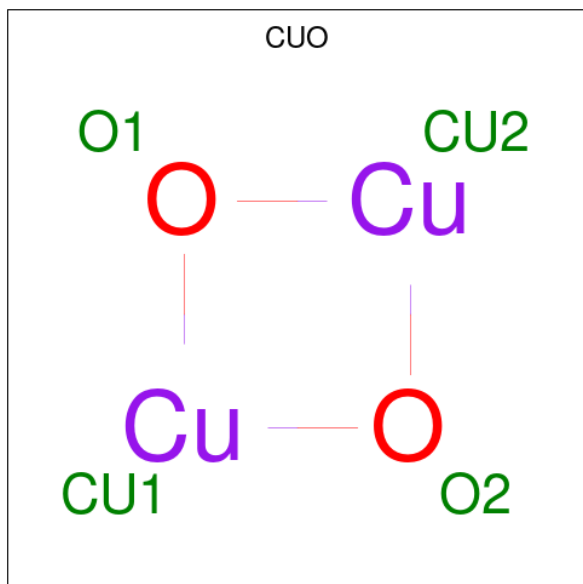
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1734	14084	8985	2438	2594	67	0	0

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

- Molecule 3 is CU2-O2 CLUSTER (CCD ID: CUO) (formula:  $\text{Cu}_2\text{O}_2$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	Cu	O	
3	A	1	4	2	2	0
3	A	1	4	2	2	0
3	A	1	4	2	2	0
3	A	1	4	2	2	0
3	B	1	4	2	2	0
3	B	1	4	2	2	0
3	B	1	4	2	2	0
3	B	1	4	2	2	0
3	C	1	4	2	2	0
3	C	1	4	2	2	0

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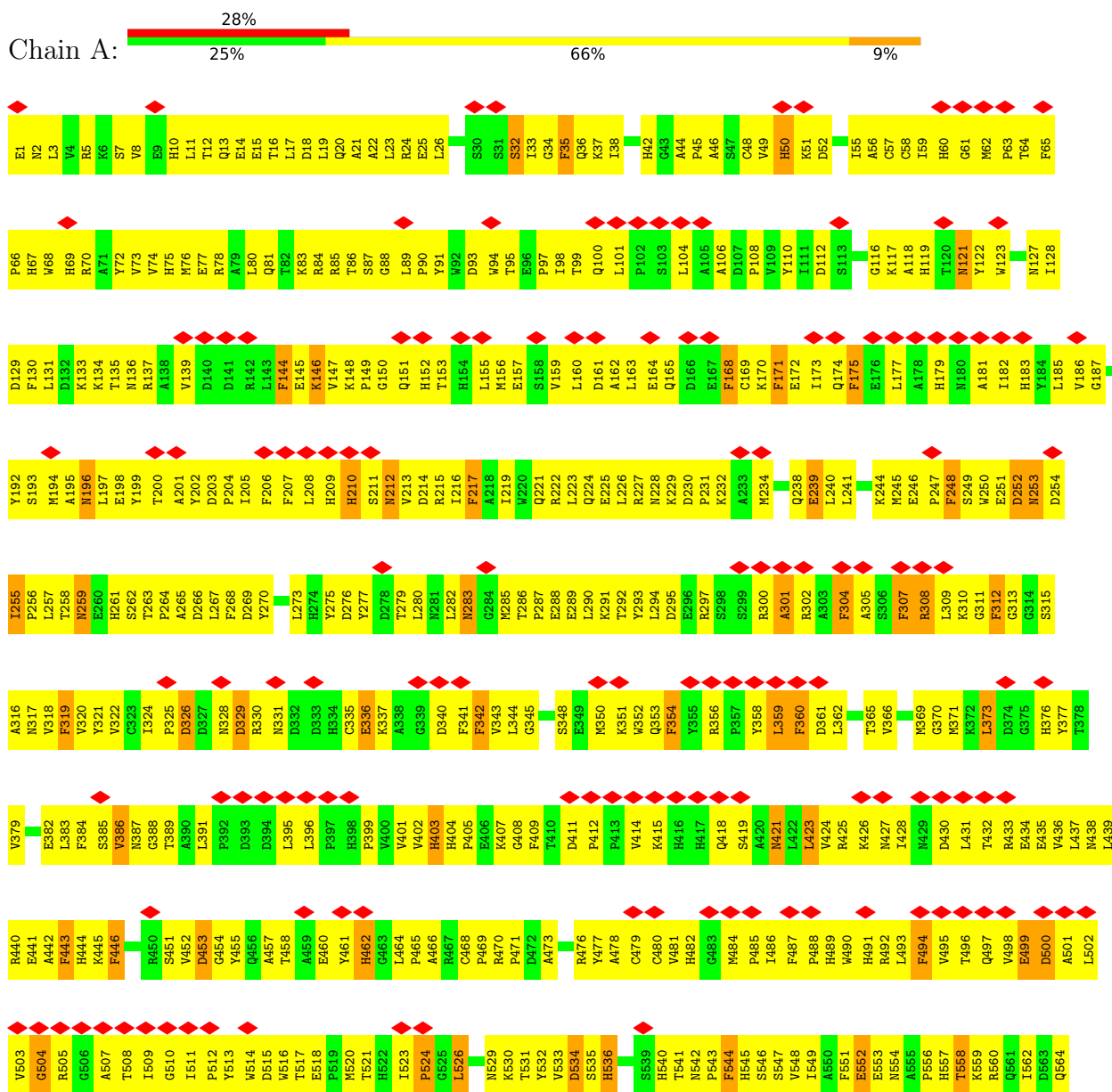
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>AltConf</b>
3	C	1	Total 4	Cu 2	O 2	0
3	C	1	Total 4	Cu 2	O 2	0
3	D	1	Total 4	Cu 2	O 2	0
3	D	1	Total 4	Cu 2	O 2	0
3	D	1	Total 4	Cu 2	O 2	0
3	D	1	Total 4	Cu 2	O 2	0

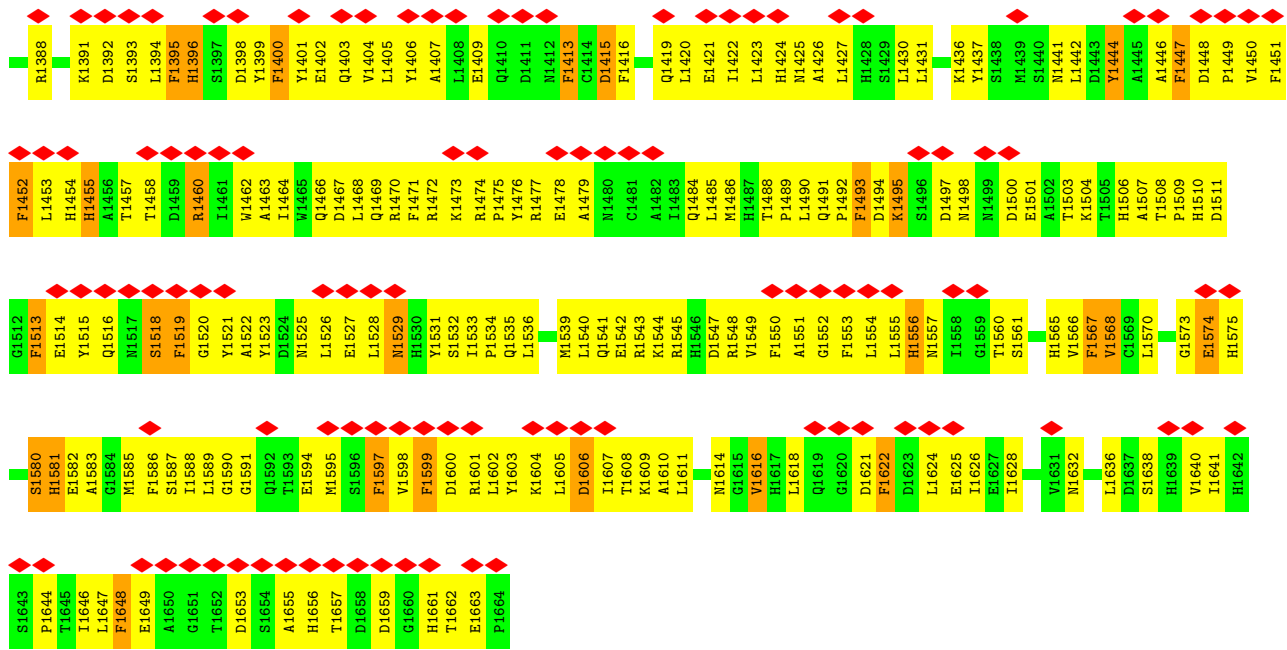
### 3 Residue-property plots

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.

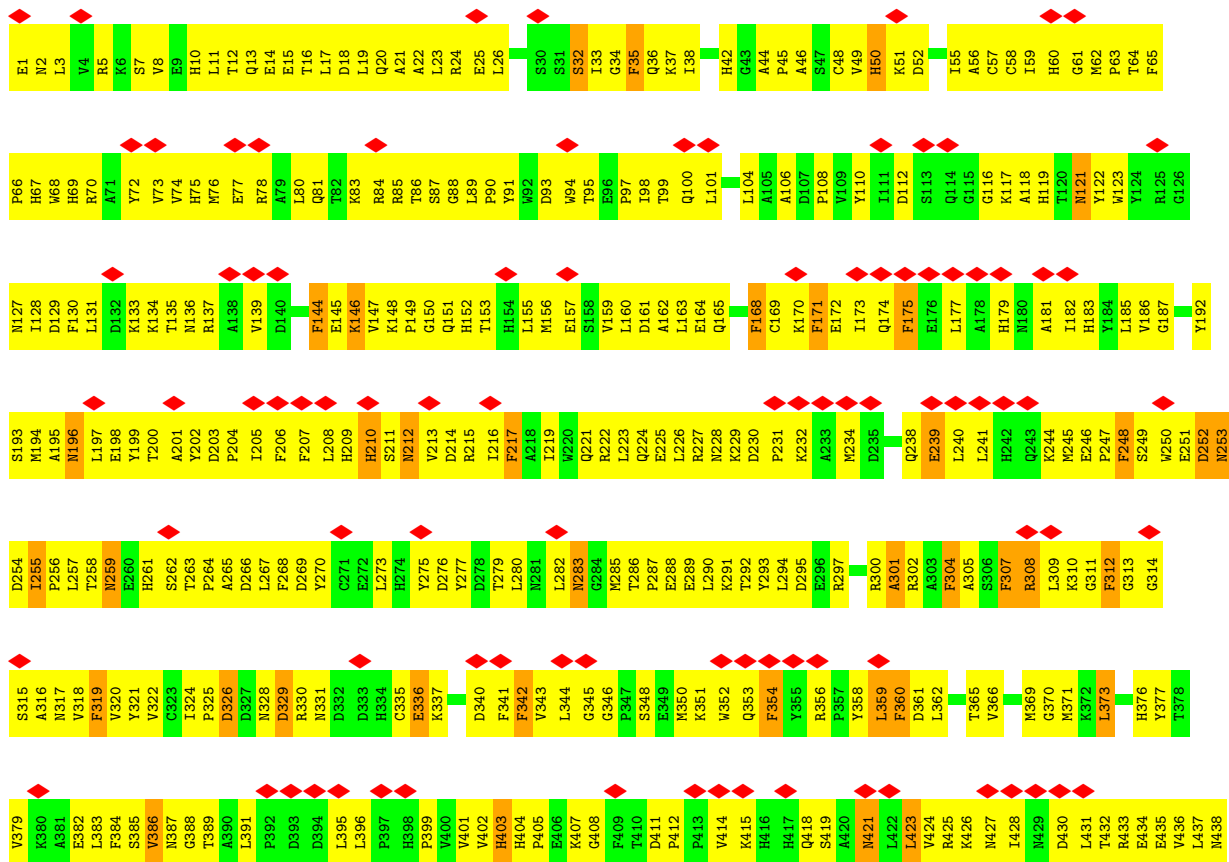
#### • Molecule 1: HEMOCYANIN KLH1

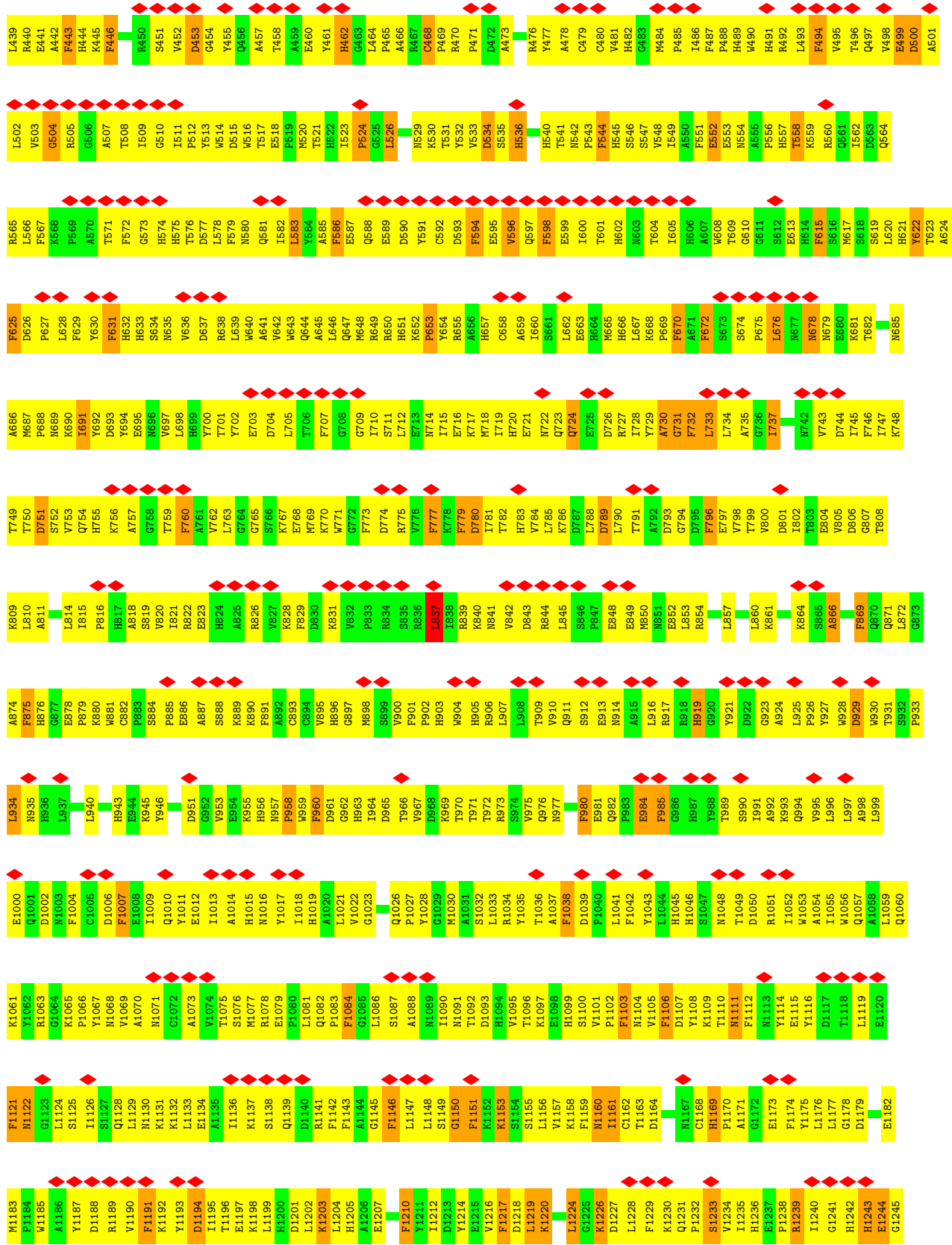


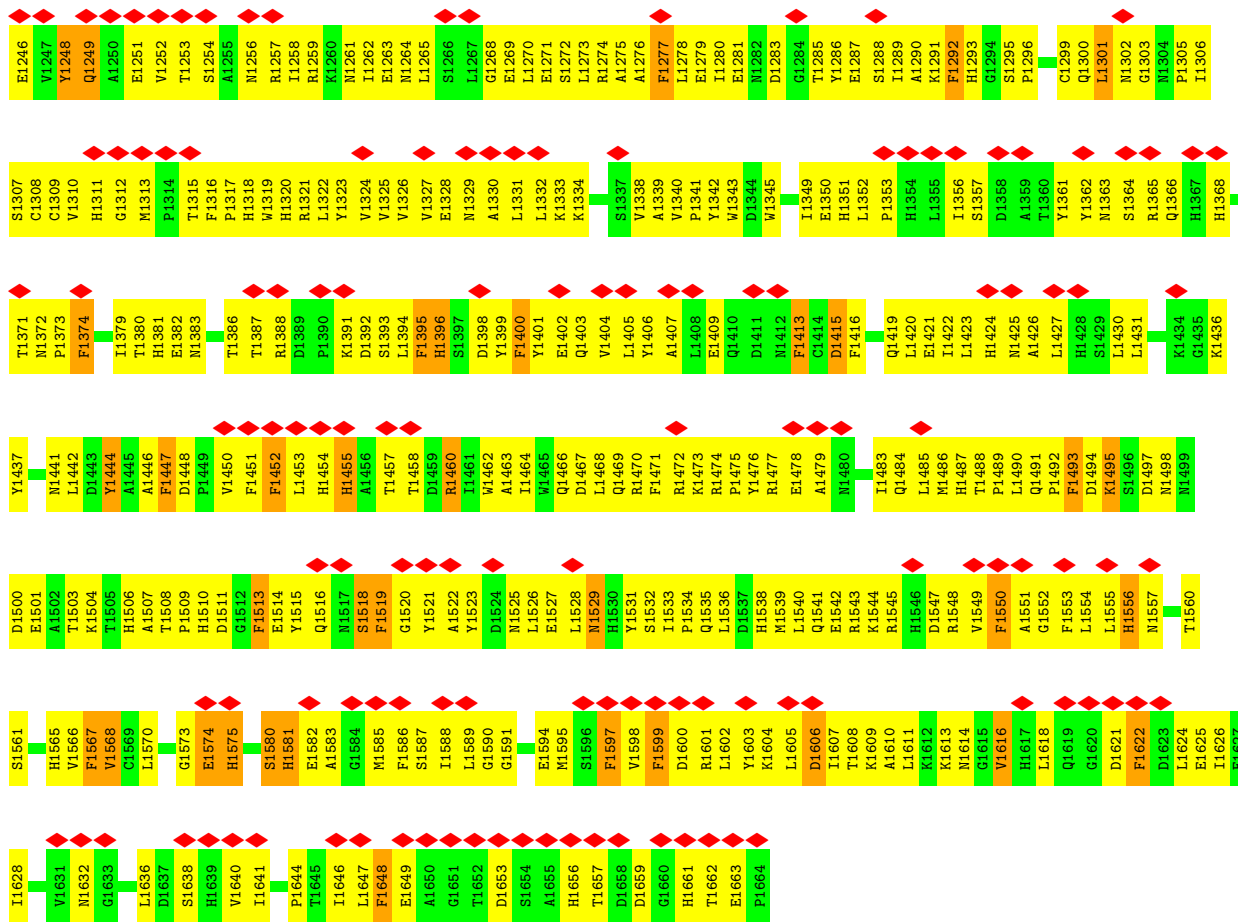
R665	R666	F567	T571	F572	G573	H574	H575	T576	D577	L578	F579	N580	Q581	I582	L583	Y584	A585	F586	E587	Q588	E589	D590	Y591	C592	D593	F594	E595	Q596	Q597	F598	E599	I600	T601	H602	M603	T604	I605	H606	A607	W608	T609	G610	E613	H614	F615	S616	M617	S618	S619	L620	H621	Y622	T623	A624	F625	D626	P627	L628	F629	Y630	F631	H632	H633	S634	M635	V636	D637	R638	L639	W640	A641	V642	W643	Q644	A645	L646	Q647	M648	R649	R650	H651	K652	P653	Y654	R655	E656	H657	C658	E659	I660	S661	L662	E663	H664	M665	H666	L667	K668	P669	F670	A671	F672	S673	S674	P675	L676	M677	N678	M679	E680	K681	T682	M685	A686	M687	P688	M689	K690	Y691	D692	A693	H694	E695	M696	H697	L698	Y700	T701	Y702	E703	D704	L705	T706	F707	G708	G709	I710	S711	L712	C713	N714	I715	E716	M717	M718	I719	H720	A721	E722	N723	Q724	E725	D726	R727	I728	Y729	A730	F731	F732	L733	L734	A735	G736	I737	N742	V743	D744	I745	F746	I747	K748	T749	D751	S752	V753	Q754	H755	K756	A757	G758	T759	F760	G765	K766	Y767	E768	M769	K770	W771	G772	F773	D774	G775	V776	F777	K778	F779	L780	I781	T782	H783	W784	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	P816	H817	A818	S819	V820	I821	R822	E823	R826	V827	K828	F829	D830	K831	Y832	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	C882	P883	S884	P885	E886	A887	S888	K889	K890	F891	A892	C893	C894	C895	V896	H896	G897	M898	S899	V900	F901	P902	H903	N904	H905	R906	R907	L908	T909	V910	Q911	S912	E913	N914	A915	L916	R917	H918	G919	G920	Y921	D922	A924	L925	P926	Y927	W928	D929	W930	T931	S932	R933	L934	N935	H936	L937	L940	H943	E944	Y946	D951	G952	Y953	K955	Y956	N957	A958	C959	P960	D961	H963	I964	D965	V966	Y967	D968	K969	T970	T971	T972	S973	H974	Q976	N977	F980	E981	Q982	P983	F984	F985	T989	S990	I991	A992	K993	Q994	V995	L996	L997	A998	L999	E1000	D1001	D1002	N1003	F1004	C1005	N935	D1006	F1007	E1008	I1009	Q1010	E1011	I1012	A1014	H1015	N1016	I1017	I1018	H1019	A1020	C1021	V1022	G1023	Q1026	P1027	Y1028	H1029	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	G1063	G1064	K1065	P1066	S1067	N1068	V1069	A1070	N1071	C1072	A1073	V1074	T1075	S1076	M1077	R1078	E1079	A1080	L1081	Q1082	P1083	F1084	G1085	L1086	S1087	A1088	N1089	I1090	N1091	T1092	D1093	H1094	V1095	T1096	K1097	E1098	H1099	S1100	V1101	P1102	F1103	N1104	W1105	F1106	D1107	Y1108	K1109	T1110	N1111	F1112	M1113	Y1114	E1115	Y1116	D1117	T1118	L1119	E1120	F1121	N1122	G1123	G1124	S1125	L1126	Q1127	S1128	L1129	M1130	K1131	L1132	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	M1160	I1161	C1162	T1163	D1164	C1168	H1169	P1170	A1171	G1172	E1173	F1174	Y1175	L1176	L1177	G1178	D1179	E1180	M1181	E1182	M1183	P1184	W1185	A1186	Y1187	L1188	Q1189	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	I1232	S1233	V1234	I1235	H1236	E1237	P1238	R1239	I1240	G1241	H1242	H1243	E1244	G1245	E1246	V1247	Y1248	Q1249	V1310	H1311	G1312	L1313	G1314	T1315	F1316	P1317	H1318	H1319	H1320	R1321	L1322	Y1323	V1324	V1325	V1326	V1327	E1328	N1329	A1330	L1331	L1332	K1333	K1334	V1338	A1339	V1340	P1341	Y1342	H1343	L1344	W1345	I1349	E1350	H1351	L1352	P1353	H1354	S1288	L1355	I1356	S1357	D1358	A1359	H1360	Y1361	Y1362	M1363	S1364	R1365	Q1366	H1367	H1368	T1371	M1372	P1373	F1374	T1379	L1380	L1381	E1382	M1383	S1254
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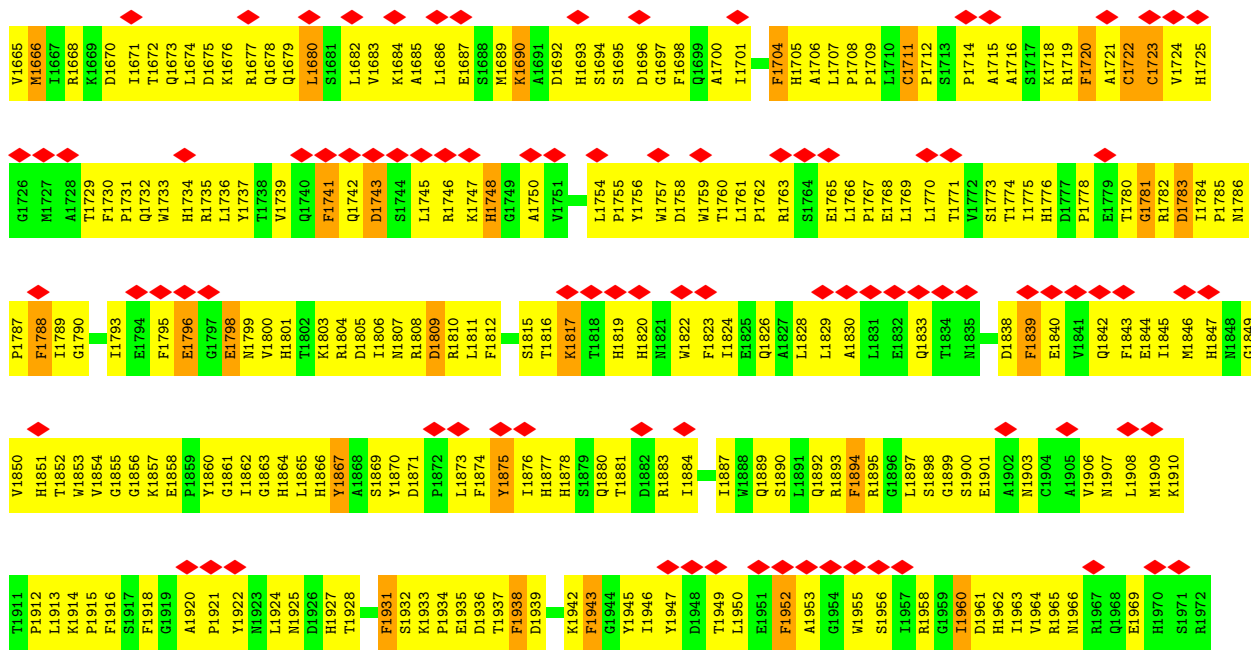
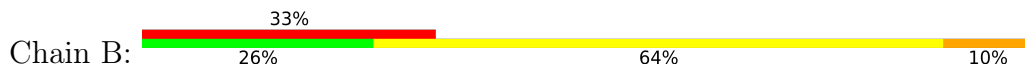
● Molecule 1: HEMOCYANIN KLH1

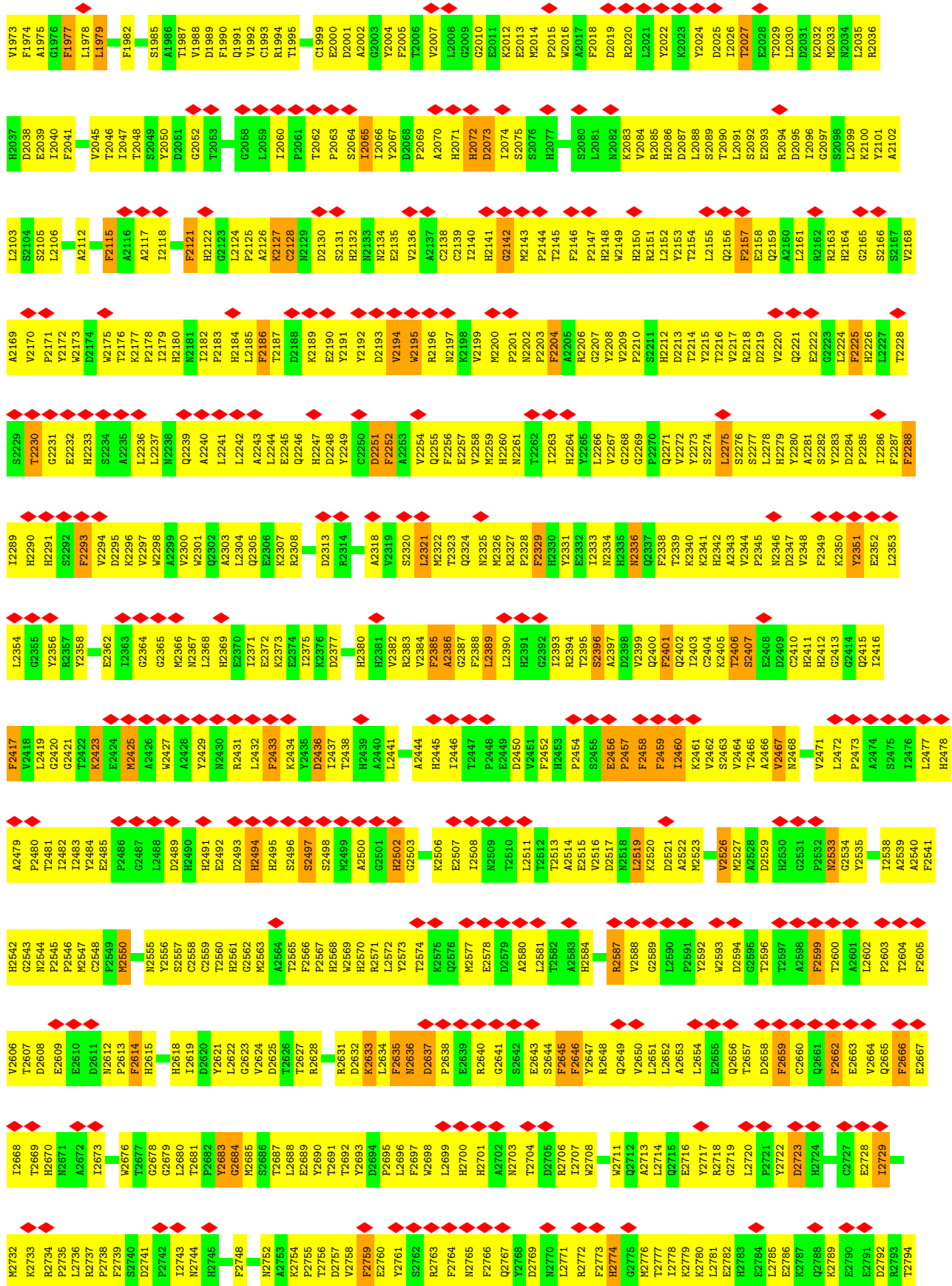


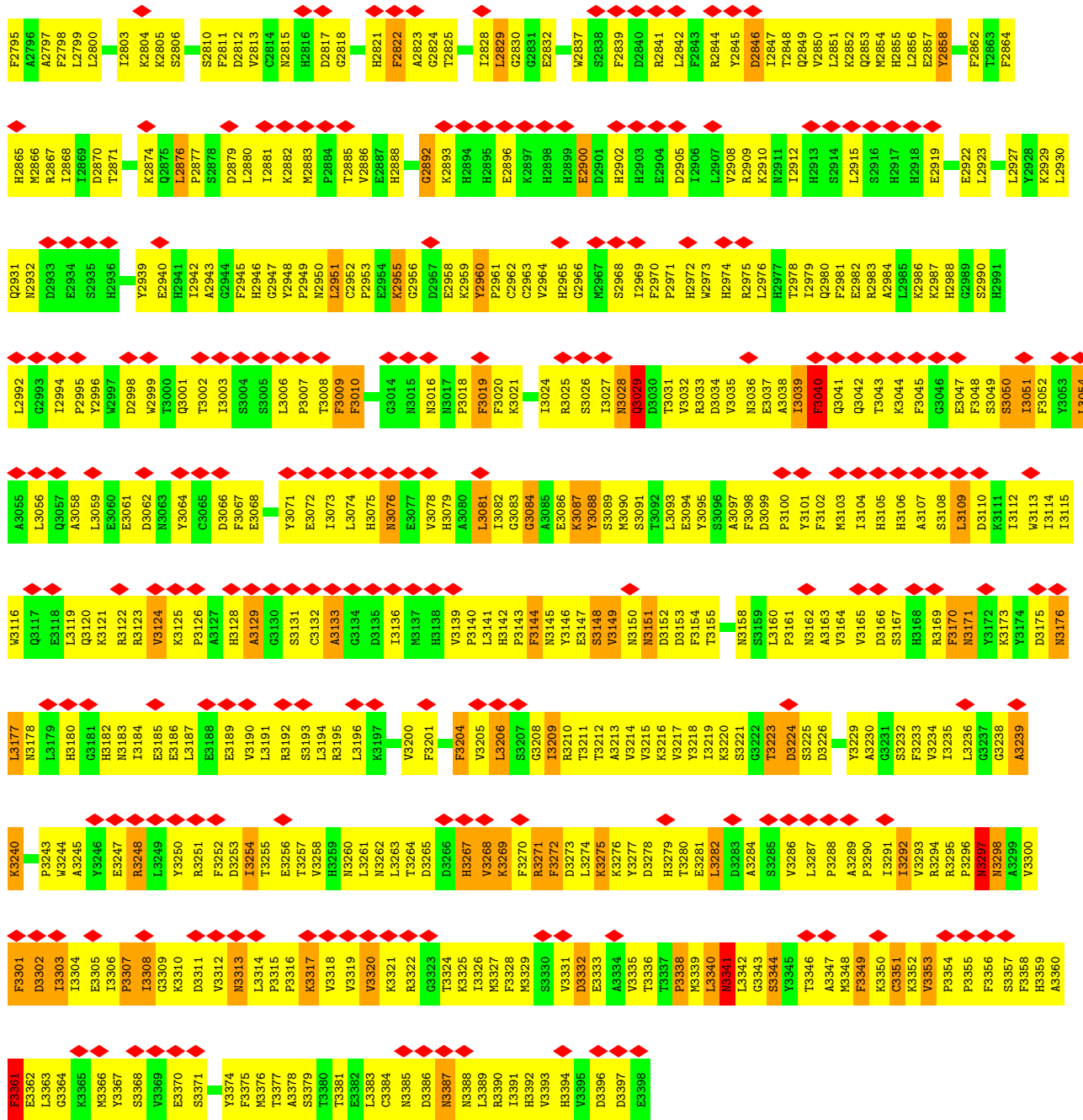




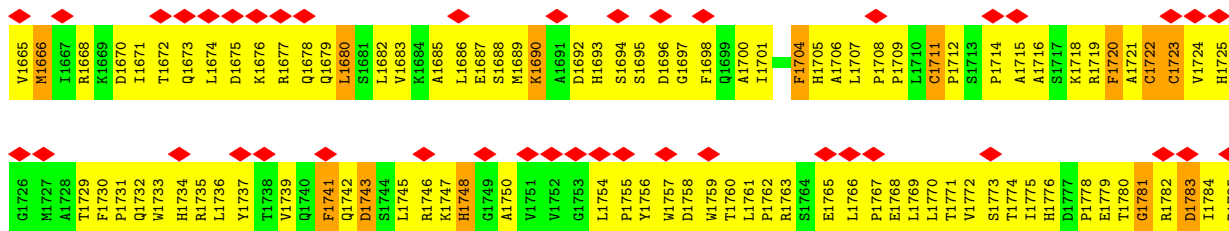
• Molecule 2: HEMOCYANIN KLH1







● Molecule 2: HEMOCYANIN KLH1



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M2550	M2555	Y2556	S2557	C2558	C2559	T2560	H2561	G2562	M2563	A2564	T2565	F2566	P2567	H2568	W2569	H2570	R2571	L2572	Y2573	T2574	M2577	E2578	S2579	A2580	L2581	H2584	R2587	V2588	G2589	L2590	P2591	Y2592	W2593	D2594	W2595	T2596	F2599	T2600	A2601	P2603	T2604	F2605	V2606	T2607	D2608	E2609	N2612	P2613	F2614	H2615	H2618							

D3373	Y374	F375	K376	T377	A378	S379	R380	K381	F382	S383	K384	C385	D386	N387	K388	L389	R390	H391	V392	H393	L394	V395	N396	K397	E398	M399	L400	R401	L402	A403	G404	S405	Y406	F407	P408	S409	K410	L411	R412	L413	R414	L415	R416	L417	R418	L419	R420	L421	R422	L423	R424	L425	R426	L427	R428	L429	R430	L431	R432	L433	R434	L435	R436	L437	R438	L439	R440	L441	R442	L443	R444	L445	R446	L447	R448	L449	R450	L451	R452	L453	R454	L455	R456	L457	R458	L459	R460	L461	R462	L463	R464	L465	R466	L467	R468	L469	R470	L471	R472	L473	R474	L475	R476	L477	R478	L479	R480	L481	R482	L483	R484	L485	R486	L487	R488	L489	R490	L491	R492	L493	R494	L495	R496	L497	R498	L499	R500	L501	R502	L503	R504	L505	R506	L507	R508	L509	R510	L511	R512	L513	R514	L515	R516	L517	R518	L519	R520	L521	R522	L523	R524	L525	R526	L527	R528	L529	R530	L531	R532	L533	R534	L535	R536	L537	R538	L539	R540	L541	R542	L543	R544	L545	R546	L547	R548	L549	R550	L551	R552	L553	R554	L555	R556	L557	R558	L559	R560	L561	R562	L563	R564	L565	R566	L567	R568	L569	R570	L571	R572	L573	R574	L575	R576	L577	R578	L579	R580	L581	R582	L583	R584	L585	R586	L587	R588	L589	R590	L591	R592	L593	R594	L595	R596	L597	R598	L599	R600	L601	R602	L603	R604	L605	R606	L607	R608	L609	R610	L611	R612	L613	R614	L615	R616	L617	R618	L619	R620	L621	R622	L623	R624	L625	R626	L627	R628	L629	R630	L631	R632	L633	R634	L635	R636	L637	R638	L639	R640	L641	R642	L643	R644	L645	R646	L647	R648	L649	R650	L651	R652	L653	R654	L655	R656	L657	R658	L659	R660	L661	R662	L663	R664	L665	R666	L667	R668	L669	R670	L671	R672	L673	R674	L675	R676	L677	R678	L679	R680	L681	R682	L683	R684	L685	R686	L687	R688	L689	R690	L691	R692	L693	R694	L695	R696	L697	R698	L699	R700	L701	R702	L703	R704	L705	R706	L707	R708	L709	R710	L711	R712	L713	R714	L715	R716	L717	R718	L719	R720	L721	R722	L723	R724	L725	R726	L727	R728	L729	R730	L731	R732	L733	R734	L735	R736	L737	R738	L739	R740	L741	R742	L743	R744	L745	F748	M752	K753	L754	P755	T756	D757	V758	F759	D760	L761	P762	L763	L764	L765	F766	Q767	Y2768	D2769	F2839	M2770	L2771	R2772	F2773	R2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	S2810	F2811	D2812	G2813	C2814	N2815	H2816	D2817	G2818	H2821	F2822	A2823	G2824	T2825	F2826	A2827	L2828	L2829	G2830	W2837	S2838	F2839	D2840	L2842	F2843	R2844	L2845	D2846	L2847	L2848	Q2849	L2850	L2851	Q2852	L2853	L2785	E2786	Q2787	Q2788	K2789	E2790	E2791	R2792	R2793	F2795	A2796	L2797	F2798	L2799	L2800	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y2690	T2691	T2692	Y2693	D2694	P2695	L2696	W2698	L2699	H2700	H2701	A2702	N2703	T2704	D2705	D2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	S2810	F2811	D2812	G2813	C2814	N2815	H2816	D2817	G2818	H2821	F2822	A2823	G2824	T2825	F2826	A2827	L2828	L2829	G2830	W2837	S2838	F2839	D2840	L2842	F2843	R2844	L2845	D2846	L2847	L2848	Q2849	L2850	L2851	Q2852	L2853	L2785	E2786	Q2787	Q2788	K2789	E2790	E2791	R2792	R2793	F2795	A2796	L2797	F2798	L2799	L2800	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y2690	T2691	T2692	Y2693	D2694	P2695	L2696	W2698	L2699	H2700	H2701	A2702	N2703	T2704	D2705	D2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y2690	T2691	T2692	Y2693	D2694	P2695	L2696	W2698	L2699	H2700	H2701	A2702	N2703	T2704	D2705	D2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y2690	T2691	T2692	Y2693	D2694	P2695	L2696	W2698	L2699	H2700	H2701	A2702	N2703	T2704	D2705	D2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y2690	T2691	T2692	Y2693	D2694	P2695	L2696	W2698	L2699	H2700	H2701	A2702	N2703	T2704	D2705	D2706	L2707	L2708	A2709	L2710	W2711	Q2712	L2713	L2714	Q2715	E2716	Y2717	L2718	G2719	L2720	P2721	Y2722	F2723	C2727	E2728	I2729	Q2730	Q2665	A2731	M2732	K2733	R2734	P2735	L2736	R2737	P2738	F2739	S2740	L2803	K2804	L2805	S2806	K2874	Q2875	L2876	P2877	G2678	G2679	L2680	T2681	P2682	Y2683	G2684	M2685	S2686	T2687	L2688	E2689	Y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## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 ( $\text{\AA}$ )	558, 558, 558	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90, 90, 90	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.24, 1.24, 1.24	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	1.40	2/13940 (0.0%)	1.76	231/18926 (1.2%)
1	C	1.40	4/13940 (0.0%)	1.76	229/18926 (1.2%)
2	B	1.35	7/14526 (0.0%)	1.67	186/19734 (0.9%)
2	D	1.35	7/14526 (0.0%)	1.67	180/19734 (0.9%)
All	All	1.38	20/56932 (0.0%)	1.71	826/77320 (1.1%)

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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	524	PRO	N-CD	16.13	1.70	1.47
1	A	524	PRO	N-CD	16.11	1.70	1.47
2	B	2457	PRO	N-CD	13.77	1.67	1.47
2	D	2457	PRO	N-CD	13.72	1.67	1.47
1	C	468	CYS	CB-SG	-10.52	1.82	2.03

The worst 5 of 826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1632	ASN	CB-CG-OD1	-38.10	44.60	120.80
1	A	1632	ASN	CB-CG-OD1	-38.08	44.65	120.80
1	A	212	ASN	CB-CG-OD1	-37.85	45.10	120.80
1	C	212	ASN	CB-CG-OD1	-37.84	45.13	120.80
1	C	212	ASN	OD1-CG-ND2	15.90	138.50	122.60

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	2933	0
1	C	13530	0	12792	2963	0
2	B	14084	0	13309	2833	0
2	D	14084	0	13311	2814	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	11119	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 103.

The worst 5 of 11119 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%)	36	72
1	C	1662/1664 (100%)	1599 (96%)	58 (4%)	5 (0%)	36	72
2	B	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	7	36
2	D	1732/1734 (100%)	1608 (93%)	94 (5%)	30 (2%)	7	36
All	All	6788/6796 (100%)	6416 (94%)	302 (4%)	70 (1%)	15	49

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%)	1448 (99%)	9 (1%)	78	83
1	C	1457/1457 (100%)	1448 (99%)	9 (1%)	78	83
2	B	1522/1522 (100%)	1491 (98%)	31 (2%)	48	66
2	D	1522/1522 (100%)	1490 (98%)	32 (2%)	47	65
All	All	5958/5958 (100%)	5877 (99%)	81 (1%)	57	72

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	2460	ILE
2	D	3254	ILE
2	D	2829	LEU
2	D	3081	LEU
2	D	3275	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 240 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	3279	HIS
2	D	2932	ASN
1	C	903	HIS
2	D	2913	HIS
2	D	3178	ASN

### 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 oligosaccharides 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	B	9005	2	0,4,4	-	-	-		
3	CUO	B	9007	2	0,4,4	-	-	-		
3	CUO	A	9002	1	0,4,4	-	-	-		
3	CUO	B	9008	2	0,4,4	-	-	-		
3	CUO	C	9004	1	0,4,4	-	-	-		
3	CUO	A	9003	1	0,4,4	-	-	-		
3	CUO	D	9008	2	0,4,4	-	-	-		
3	CUO	C	9001	1	0,4,4	-	-	-		
3	CUO	D	9006	2	0,4,4	-	-	-		
3	CUO	B	9006	2	0,4,4	-	-	-		
3	CUO	C	9003	1	0,4,4	-	-	-		
3	CUO	A	9001	1	0,4,4	-	-	-		
3	CUO	C	9002	1	0,4,4	-	-	-		
3	CUO	D	9007	2	0,4,4	-	-	-		
3	CUO	A	9004	1	0,4,4	-	-	-		
3	CUO	D	9005	2	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	B	9005	2	-	-	0/1/1/1
3	CUO	B	9007	2	-	-	0/1/1/1
3	CUO	A	9002	1	-	-	0/1/1/1
3	CUO	B	9008	2	-	-	0/1/1/1
3	CUO	C	9004	1	-	-	0/1/1/1
3	CUO	A	9003	1	-	-	0/1/1/1
3	CUO	D	9008	2	-	-	0/1/1/1
3	CUO	C	9001	1	-	-	0/1/1/1
3	CUO	D	9006	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CUO	B	9006	2	-	-	0/1/1/1
3	CUO	C	9003	1	-	-	0/1/1/1
3	CUO	A	9001	1	-	-	0/1/1/1
3	CUO	C	9002	1	-	-	0/1/1/1
3	CUO	D	9007	2	-	-	0/1/1/1
3	CUO	A	9004	1	-	-	0/1/1/1
3	CUO	D	9005	2	-	-	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	B	9008	CUO	3	0
3	A	9003	CUO	1	0
3	D	9008	CUO	3	0
3	C	9003	CUO	1	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.

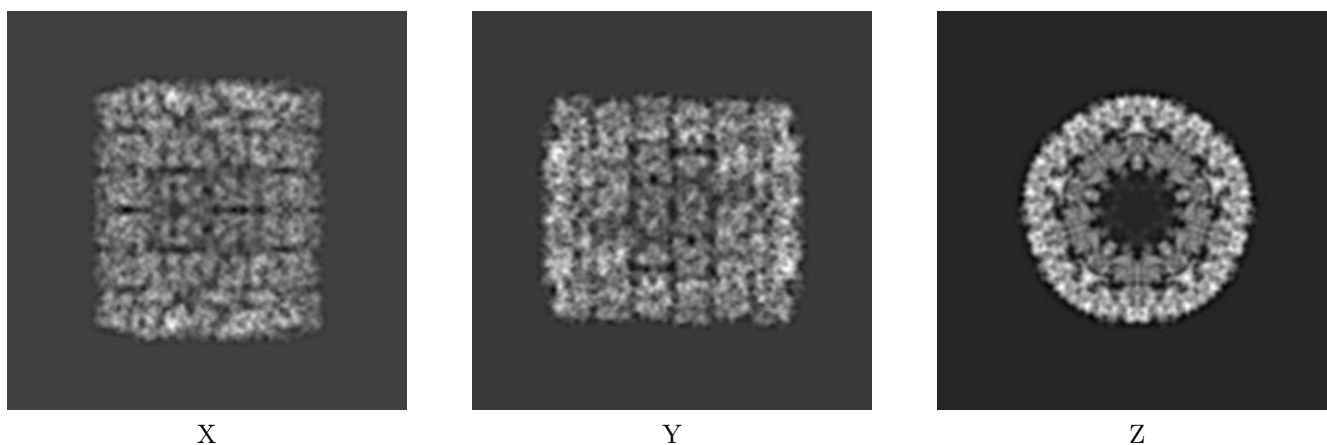
## 6 Map visualisation [i](#)

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 [i](#)

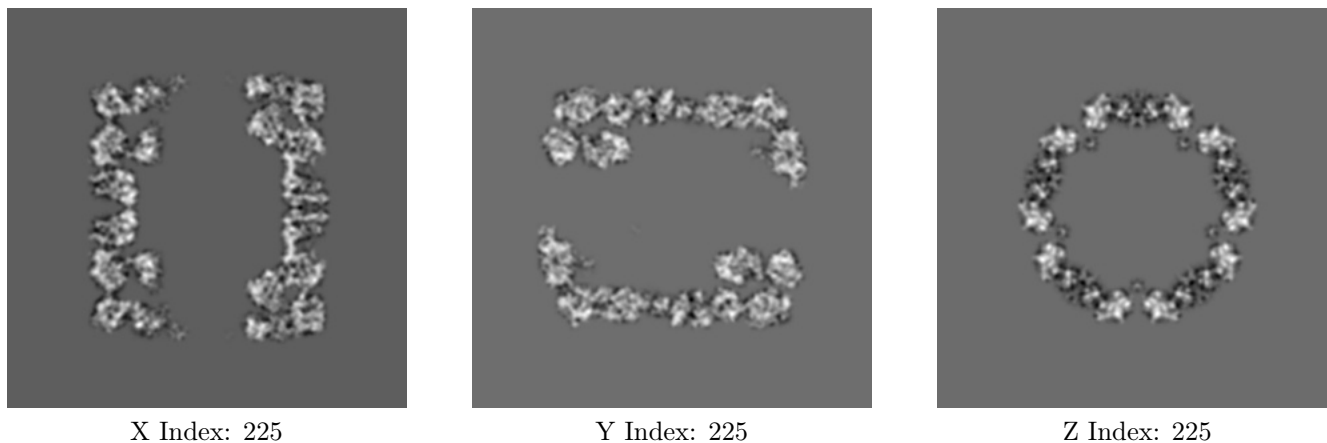
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



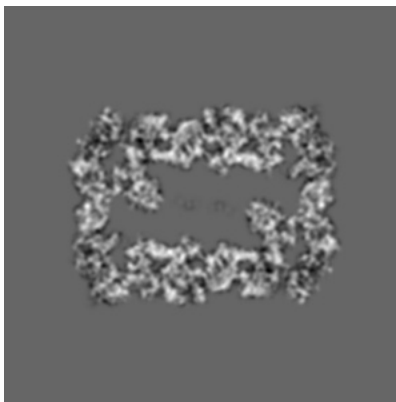
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

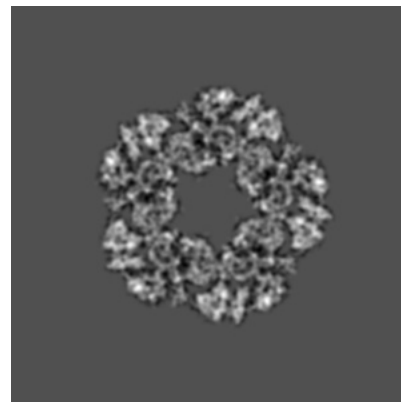
### 6.3.1 Primary map



X Index: 168



Y Index: 149

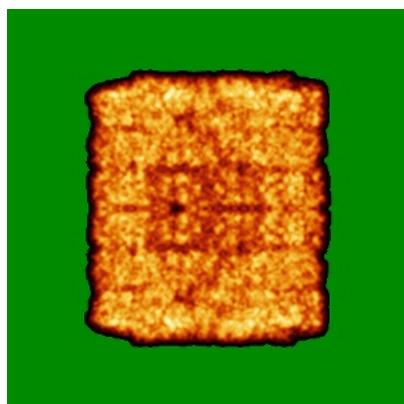


Z Index: 98

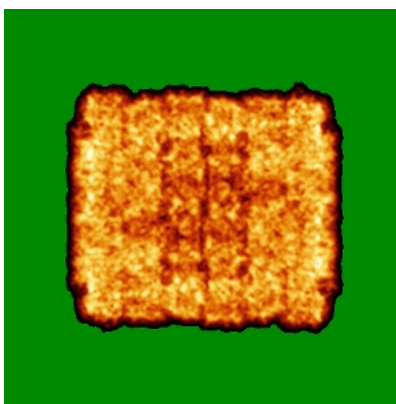
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

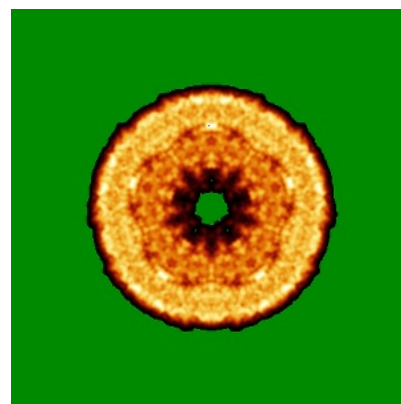
### 6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



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.

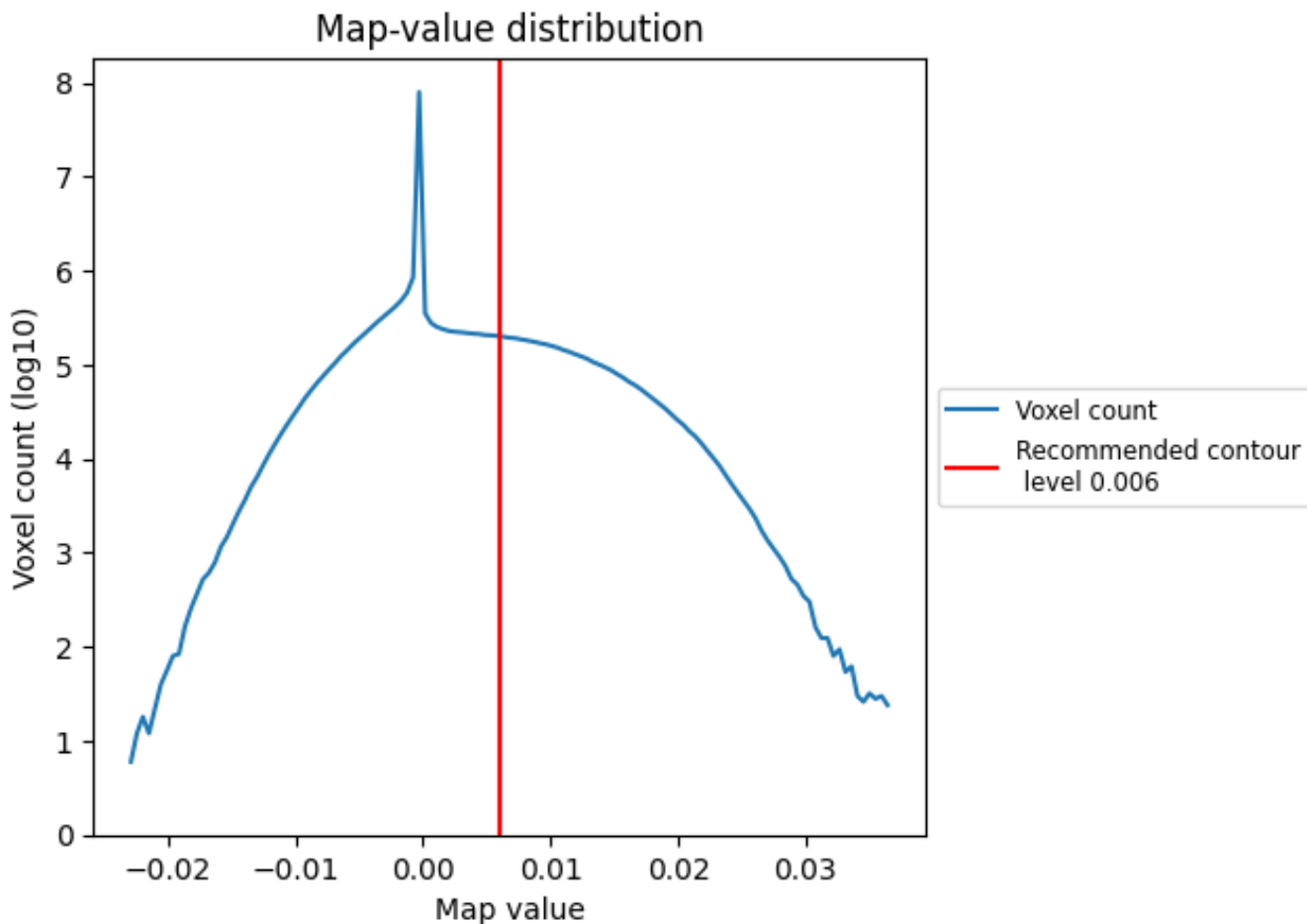
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

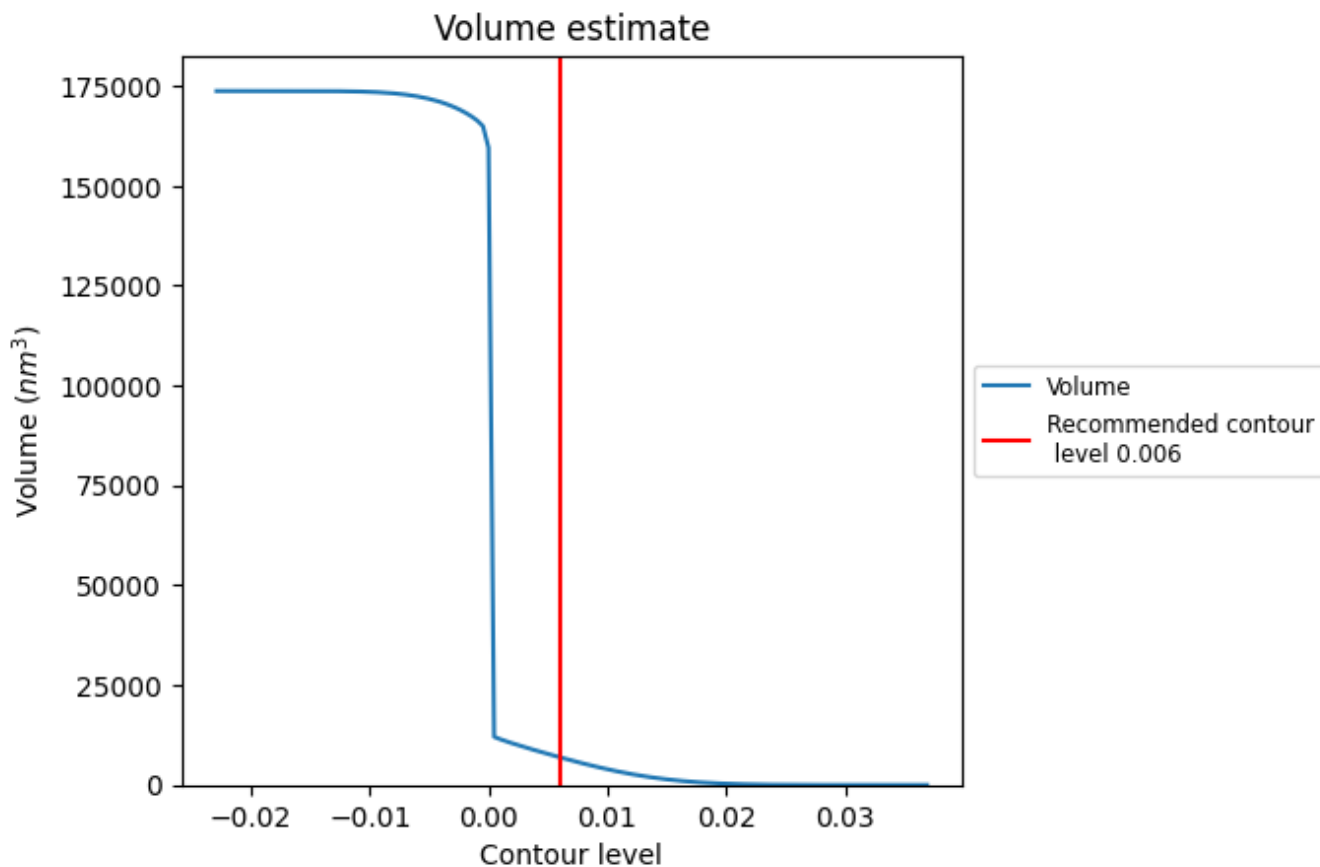
This section contains the results of statistical analysis of the map.

### 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.

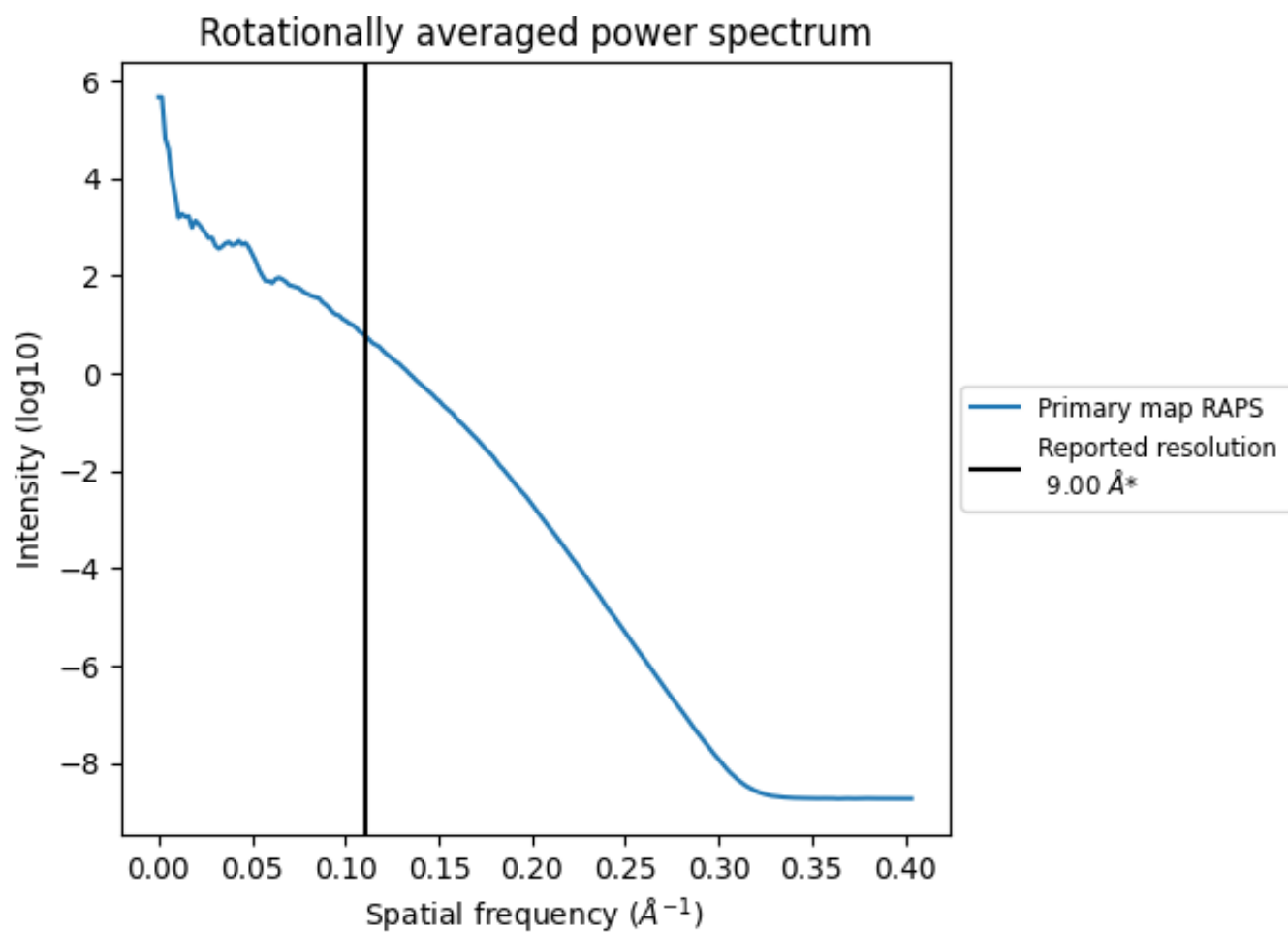
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 69260  $\text{nm}^3$ ; 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<sup>-1</sup>

## 8 Fourier-Shell correlation

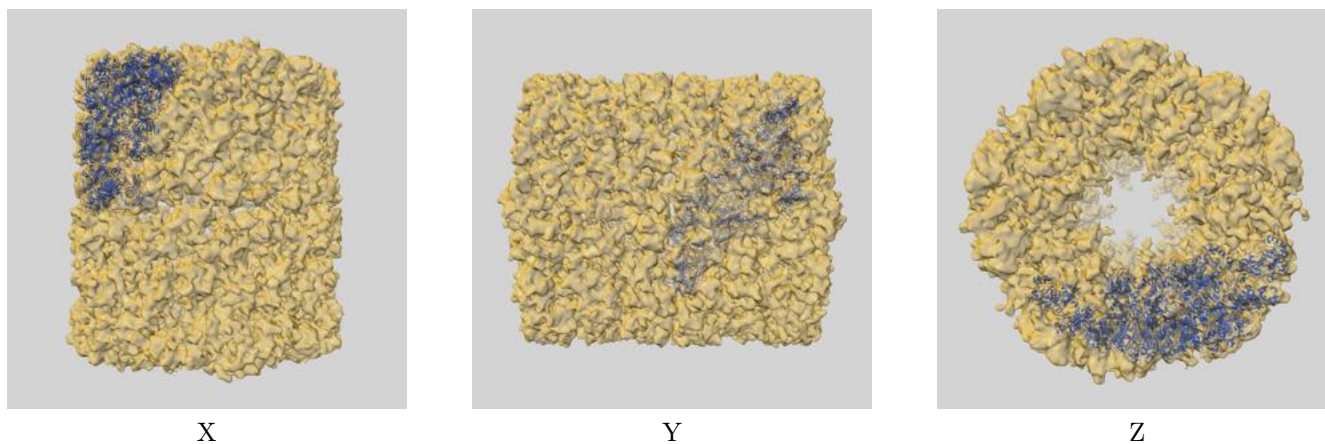
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

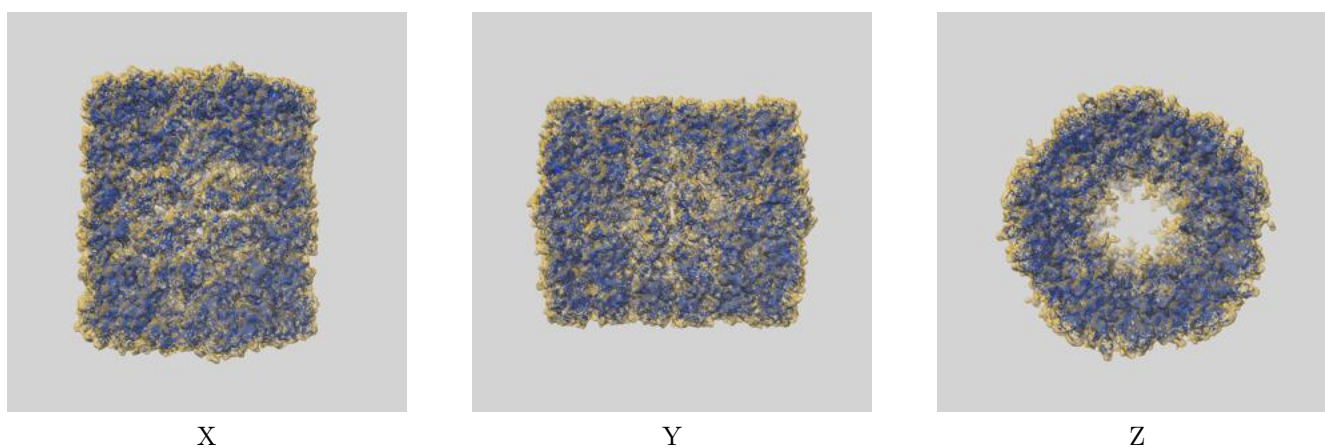
This section contains information regarding the fit between EMDB map EMD-1569 and PDB model 4BED. Per-residue inclusion information can be found in section 3 on page 8.

### 9.1 Map-model overlays

#### 9.1.1 Map-model overlay [i](#)

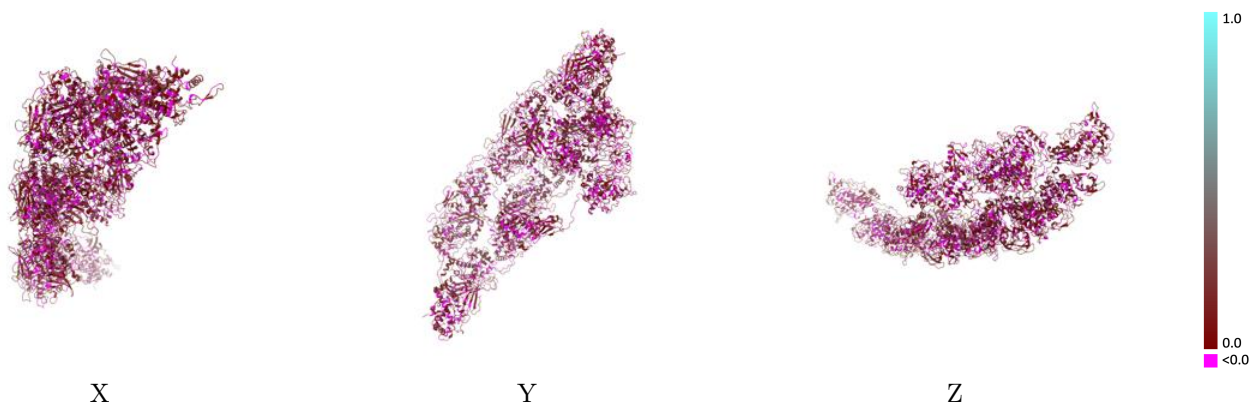


#### 9.1.2 Map-model assembly overlay [i](#)



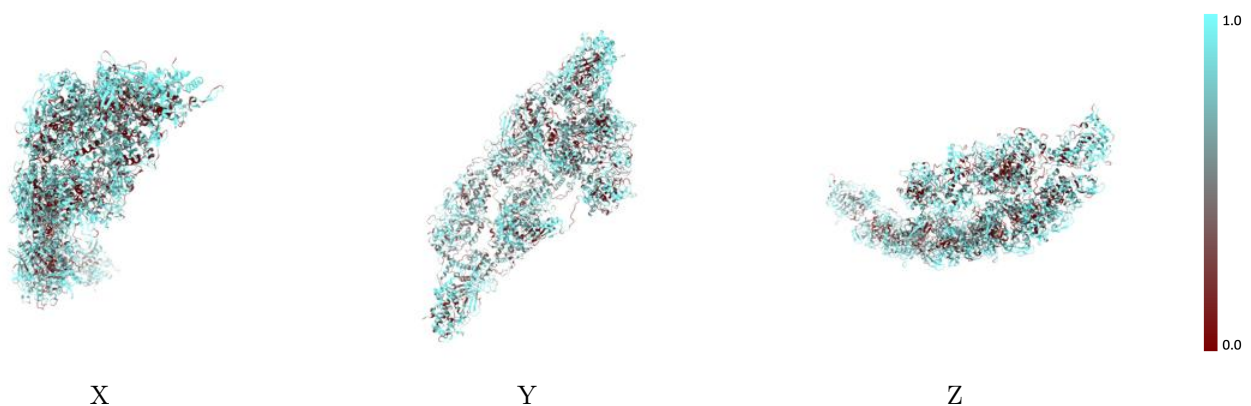
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



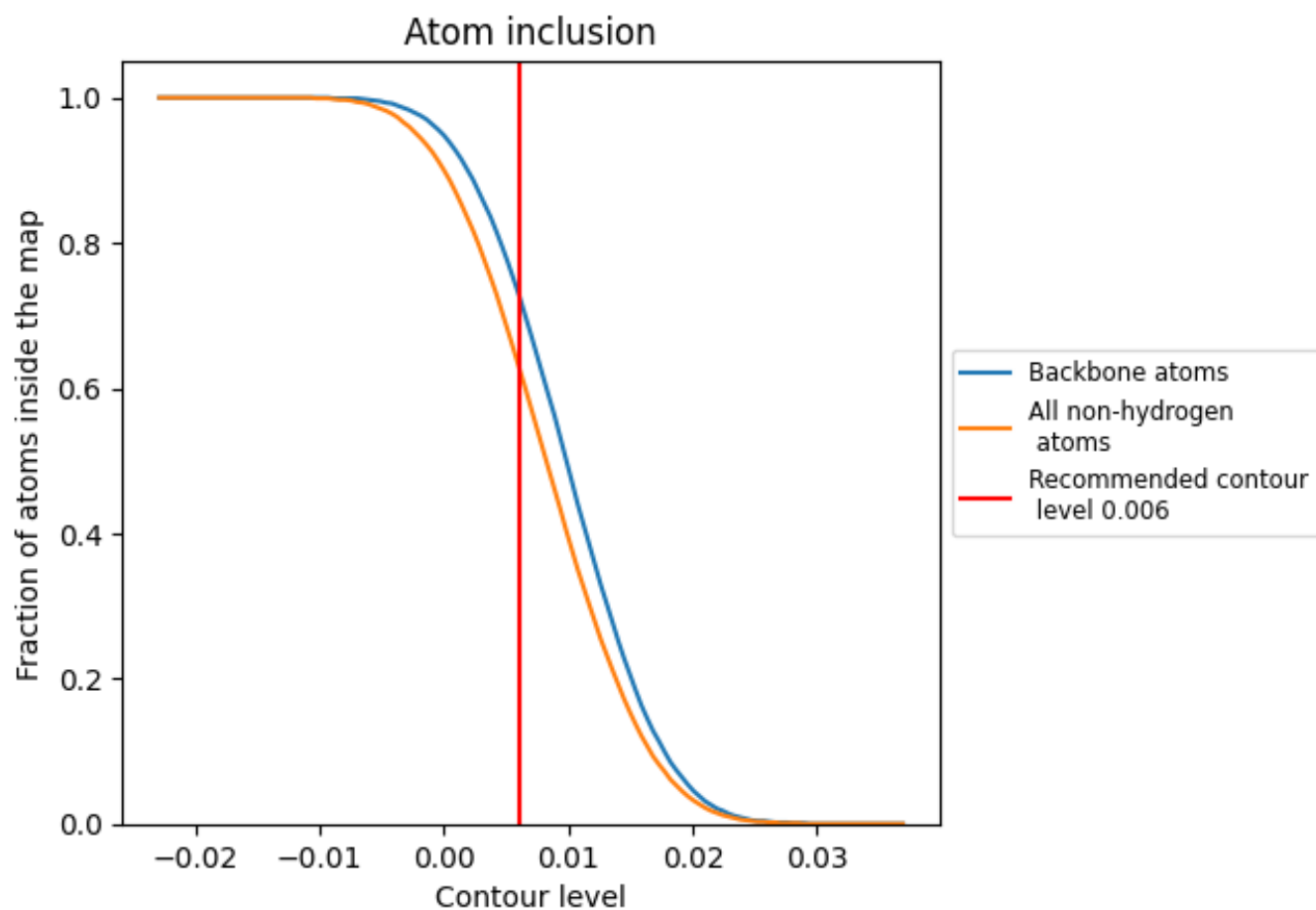
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).











## 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 [i](#)

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	 0.6310	 0.0810
A	 0.6480	 0.0860
B	 0.5910	 0.0730
C	 0.6460	 0.0900
D	 0.6400	 0.0770

