



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 04:44 PM EST

PDB ID : 3J32
EMDB ID : EMD-5586
Title : An asymmetric unit map from electron cryo-microscopy of Haliotis diversicolor molluscan hemocyanin isoform 1 (HdH1)
Authors : Zhang, Q.; Dai, X.; Cong, Y.; Zhang, J.; Chen, D.-H.; Dougherty, M.; Wang, J.; Ludtke, S.; Schmid, M.F.; Chiu, W.
Deposited on : 2013-02-20
Resolution : 4.50 Å(reported)

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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 ⓘ 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

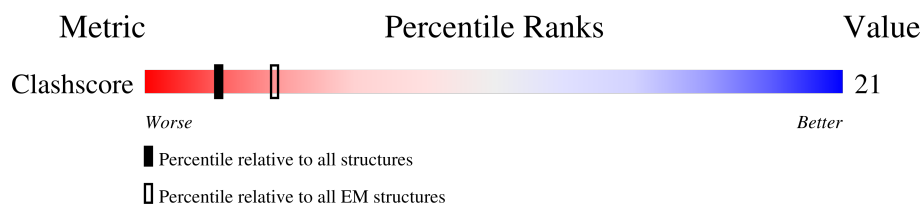
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

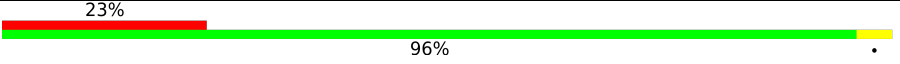
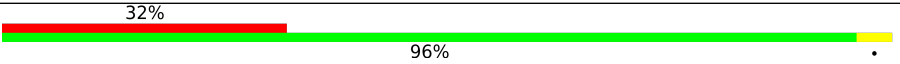
The reported resolution of this entry is 4.50 Å.

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

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	A	3303	
1	B	3303	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6606 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.

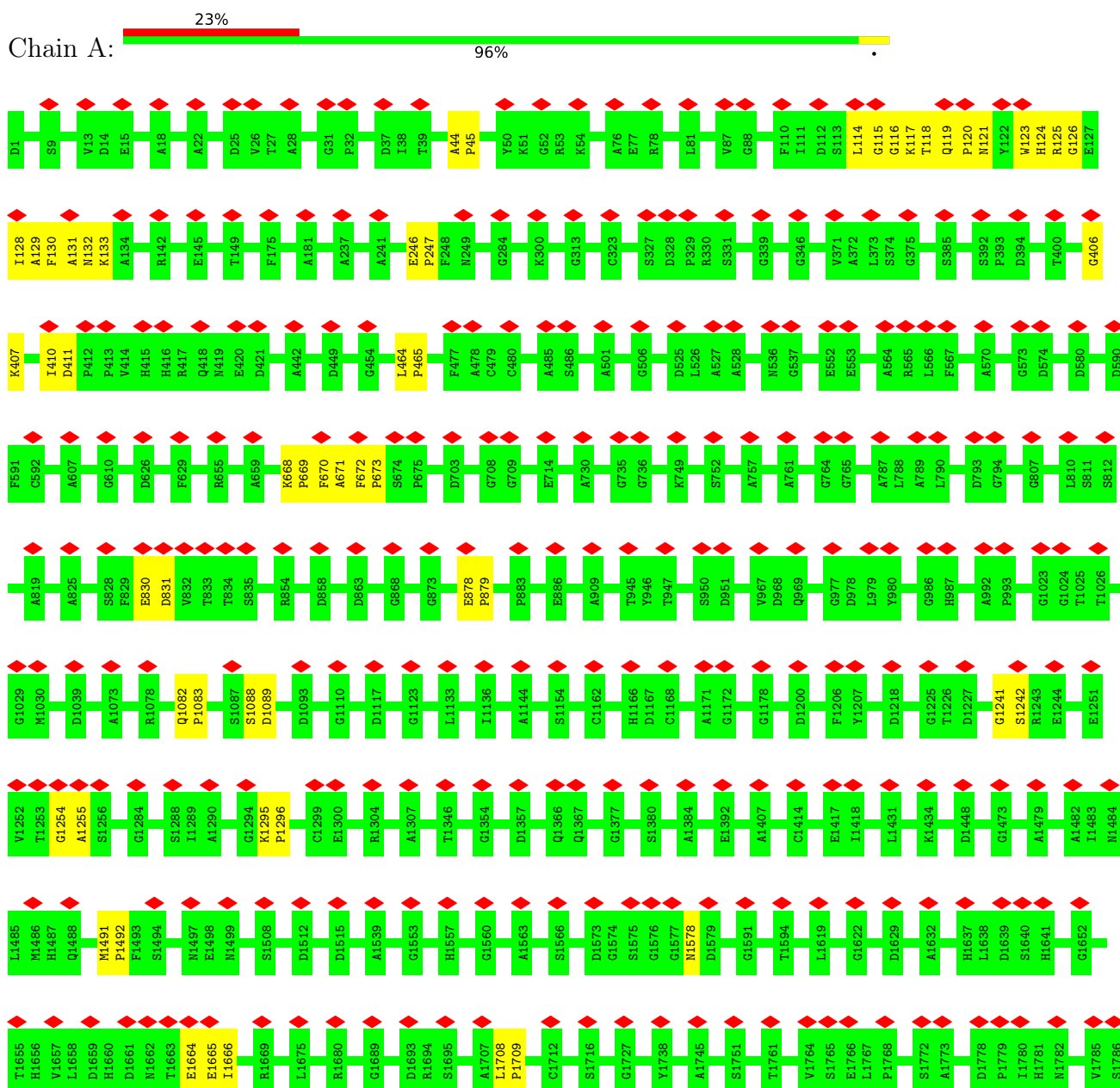
- Molecule 1 is a protein called Hemocyanin isoform 1.

Mol	Chain	Residues	Atoms		AltConf	Trace
1	A	3303	Total 3303	C 3303	0	3303
1	B	3303	Total 3303	C 3303	0	3303

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.

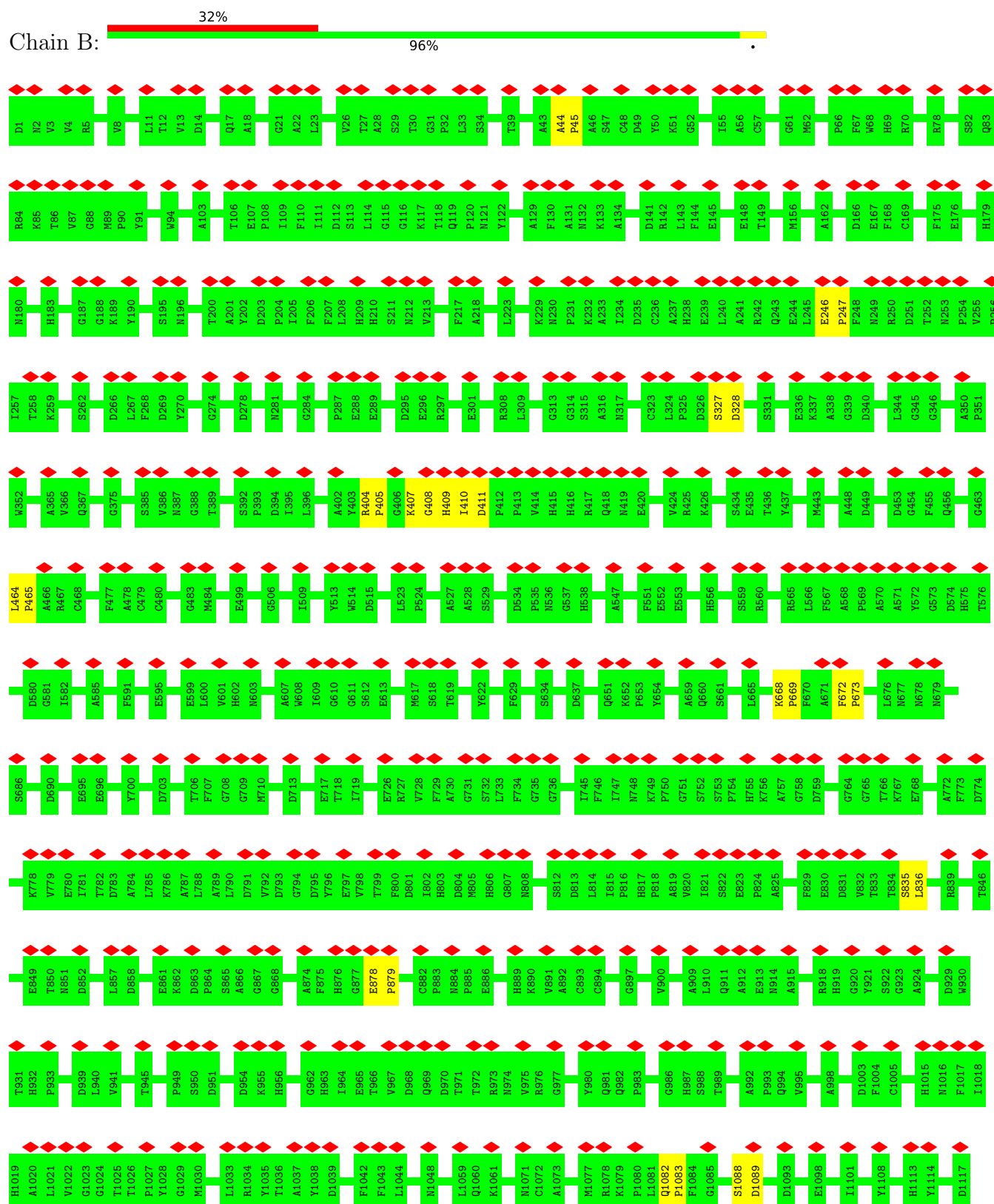
• Molecule 1: Hemocyanin isoform 1



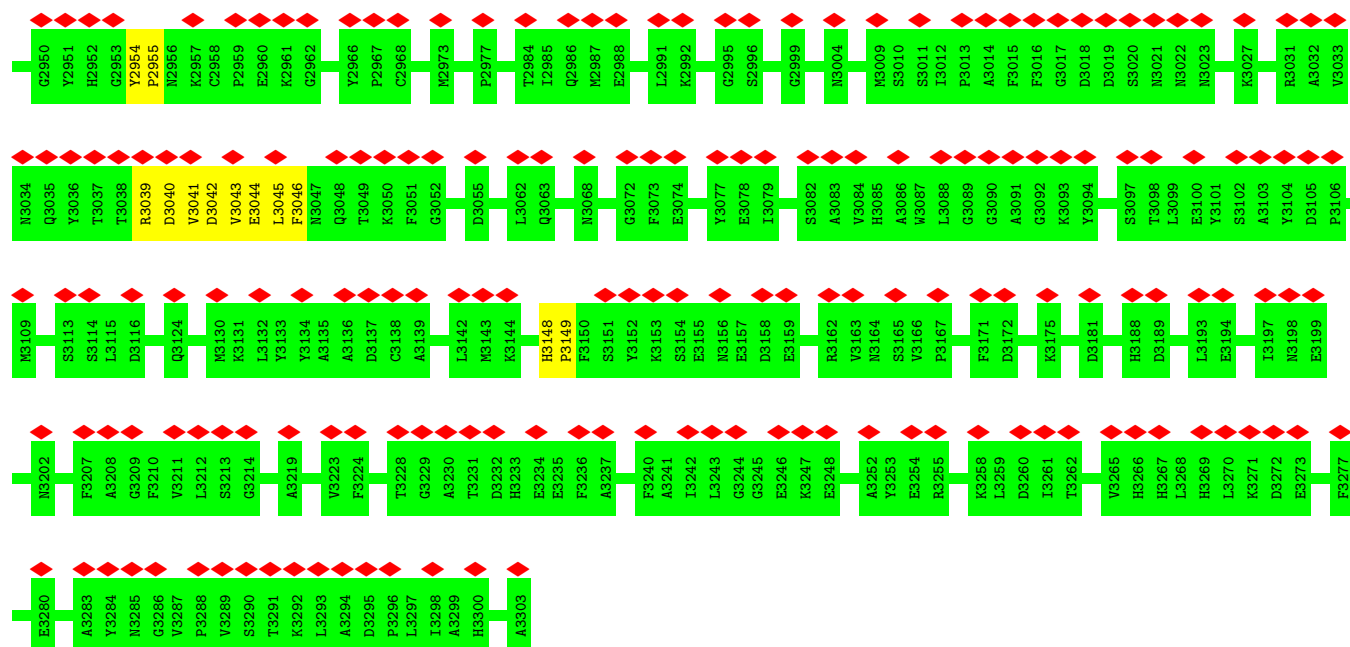
G3229	A3230	T3231	D3232	H3233	E3234	E3235	G3238	I3242	L3243	G3244	G3245	K3246	K3247	E3248	K3258	L3259	D3260	D3263	A3264	H3265	H3266	H3267	L3268	H3269	M3183	R3186	G3187	I3190	N3191	E3192	L3193	E3194	A3195	N3196	A3208	G3209	F3210	V3211	L3212	S3213	G3214	I3215	R3216	I3217	K3222	V3223	H3226	G3227	T3228	
D3116	A3136	T3037	T3038	R3039	D3040	V3041	D3042	H3148	H3149	F3150	S3151	S3152	K3153	E3157	D3158	S3165	V3166	F3167	D3172	H3173	N3177	D3181	N3182	M3183	R3186	G3187	T3190	N3191	E3192	L3193	E3194	A3195	N3196	A3208	G3209	F3210	V3211	L3212	S3213	G3214	I3215	R3216	I3217	K3222	V3223	H3226	G3227	T3228		
N3034	T3037	T3038	R3039	D3040	V3041	D3042	V3043	E3044	N3047	Q3048	T3049	K3050	F3051	G3052	E3053	Y3054	D3055	Y3056	S3060	V3064	E3067	N3068	S3069	F3070	C3071	G3072	V3075	I3079	L3080	H3081	S3082	H3085	G3089	G3090	A3091	G3092	K3093	Y3094	S3095	T3098	S3102	A3103	F3106	V3107	S3114	L3115				
G2950	G2953	Y2954	P2955	C2958	P2959	E2960	K2961	G2962	D2963	D2964	K2965	Y2966	P2967	G2972	M2973	P2974	I2975	H2983	M2987	L2991	G2995	S2996	Q2997	I2998	G2999	N3004	N3005	T3006	K3007	R3008	N3009	S3010	P3013	A3014	G3017	D3018	L3019	S3020	N3021	N3022	P3024	F3025	I3030	R3031	A3032	V3033				
S2862	F2866	D2874	D2875	L2876	E2877	P2880	G2881	I2882	L2883	K2884	A2893	L2894	G2895	D2896	G2897	L2898	K2899	H2900	E2901	D2902	E2903	G2904	H2905	D2906	D2907	R2908	L2909	S2910	H2911	V2912	L2913	L2914	R2915	V2918	D2919	S2922	L2923	K2924	E2925	A2926	N2927	A2928	I2929	K2935	L2936	Q2937	H2940	S2941	K2942	E2946
M2687	L2690	D2691	F2692	T2693	P2697	W2700	T2706	D2707	G2721	G2729	M2734	K2735	T2736	R2739	P2740	N2746	P2749	V2750	T2751	Y2763	D2784	H2785	A2798	S2803	G2804	I2805	P2810	V2811	V2812	E2817	H2820	E2821	C2822	A2825	A2829	L2830	L2831	G2832	G2833	P2884	Y2885	G2686								
S2559	C2560	C2561	M2579	E2580	G2581	A2582	A2585	H2586	G2587	S2588	H2589	V2590	G2591	H2603	T2606	L2607	V2608	D2610	N2611	D2612	G2619	T2620	I2621	E2622	T2629	R2630	S2631	P2632	R2633	N2638	D2639	P2640	E2641	H2642	G2643	S2644	E2645	S2646	F2647	F2648	K2663	W2678	T2679	G2680	G2681	P2684	Y2685	G2686		
S2465	A2468	V2469	D2470	G2471	T2472	S2477	L2478	H2480	T2483	P2488	D2489	V2490	G2491	H2492	H2493	E2494	D2495	H2496	E2497	S2498	G2499	S2500	L2501	A2502	G2503	S2504	G2505	V2506	L2513	A2516	E2519	E2520	G2536	A2539	A2542	G2545	K2546	P2547	A2548	W2549	C2550	F2551	D2554	L2558						
L2356	G2357	G2367	S2382	A2388	G2389	F2390	T2397	D2400	L2403	D2404	I2405	K2407	T2408	S2409	D2410	G2411	G2412	G2416	V2417	L2418	G2423	L2434	D2438	E2441	A2442	L2443	H2444	E2445	F2446	G2447	I2448	N2449	P2450	E2451	D2452	V2453	F2454	H2455	A2456	E2458	A2459	F2460	F2461	L2462	K2463	V2464				
G2233	K2234	H2235	F2239	L2244	E2247	D2253	F2258	E2259	T2264	I2265	G2270	G2271	R2272	Q2273	T2274	S2279	A2283	F2289	S2294	A2317	D2318	C2319	A2320	V2321	S2322	L2323	M2324	S2325	K2326	R2329	P2330	K2333	N2336	T2341	K2342	K2343	N2348	F2351	D2352	L2229	S2230	P2231	L2232							
D1998	Y1999	T2000	C2001	E2002	N2003	A2004	G2005	G2011	G2012	S2013	A2014	Y2026	N2036	G2047	T2048	V2049	T2050	P2058	G2059	D2060	L2061	A2065	H2074	N2075	L2076	N2077	S2078	R2079	K2080	H2081	N2084	K2085	S2095	S2100	L2101	K2102	A2103	A2104	S2107	D2112	G2116	A2121	A2122	L2126						
P2127	A2128	Q2129	S2134	Q2135	A2139	C2140	G2144	M2145	A2146	Y2155	G2167	A2171	D2176	P2185	H2186	I2187	L2188	T2189	D2190	E2191	E2192	Y2193	D2194	L2195	F2196	W2197	Q2198	D2199	A2200	V2201	M2202	P2203	S2207	R2208	G2209	H2210	V2211	E2214	N2215	V2222	R2223	K2224	A2225	L2229	S2230	P2231	L2232			
A1792	E1797	D1806	I1807	L1812	F1813	G1816	D1817	H1818	E1819	G1820	Y1821	H1822	D1837	G1857	G1858	S1859	A1860	Y1869	G1898	L1899	S1900	G1901	E1909	K1916	P1917	G1921	A1922	P1923	H1927	G1946	D1950	G1956	D1963	D1973	G1978	G1985	T1991													

• Molecule 1: Hemocyanin isoform 1

Chain B:



S2865	P2866	K2867	D2874	P2880	G2881	I2882	L2883	T2887	L2894	G2895	D2896	G2897	L2898	K2899	H2900	E2901	D2902	E2903	G2904	H2905	D2906	D2907	L2908	L2909	S2910	H2911	V2912	L2913	I2914	E2917	V2918	S2922	E2925	A2926	I2929	K2930	T2931	A2932	L2933	L2936	Q2937	N2938	D2939	K2942	G2943	G2944	F2945	E2946
Y2719	R2720	G2721	A2727	N2728	C2729	T2736	R2739	P2740	D2743	N2744	V2750	A2753	D2759	R2767	D2794	A2799	F2800	L2801	L2802	S2803	G2804	S2808	V2811	I2815	C2816	N2819	C2822	A2825	G2826	T2827	F2828	A2829	G2832	G2833	S2840	D2848	Q2854											
S2602	T2609	D2610	N2611	D2612	N2613	N2614	P2615	D2618	N2625	V2626	T2627	T2628	S2631	P2632	R2633	F2637	N2638	D2639	P2640	E2641	H2642	G2643	S2644	E2645	S2646	V2652	E2657	E2665	E2669	N2673	V2678	T2679	G2680	G2681	G2686	N2687	A2694	P2697	L2698	F2699	N2700	N2705	A2711					
D2495	H2496	E2497	S2498	G2499	S2500	L2501	A2502	G2503	S2504	V2505	R2507	L2513	T2514	T2515	A2524	G2527	H2532	G2536	A2542	G2545	K2546	P2547	D2548	M2549	C2550	P2551	M2552	A2553	D2554	L2558	S2559	C2560	G2564	M2565	A2566	M2579	E2580	G2581	G2587	G2591	L2592	P2593	A2599					
C2252	G2271	A2317	A2320	R2329	P2330	A2345	D2352	N2369	E2374	A2378	S2382	G2389	D2400	K2407	T2408	S2409	D2410	G2411	H2414	A2415	G2416	G2423	D2438	D2452	A2456	D2457	E2458	A2459	F2460	F2461	L2462	A2468	L2474	S2477	T2483	G2489												
G2125	L2126	P2127	A2128	Q2129	D2132	T2133	S2134	G2135	A2139	G2144	Y2155	A2162	G2167	A2171	G2191	E2192	Y2193	Y2194	D2195	F2196	W2197	Q2198	D2199	A2200	V2201	N2202	P2203	S2207	R2208	N2221	V2222	K2224	A2225	L2226	P2231	I2232	G2233	K2234	H2235	D2240	Q2241	A2242	E2247					
A1977	G1983	A1988	D1997	C2001	G2011	G2012	S2013	A2014	A2019	H2039	E2040	D2041	T2048	V2049	T2050	A2051	Y2052	D2053	G2054	T2055	D2060	A2065	H2074	N2075	L2076	N2077	S2078	R2079	N2084	K2085	L2090	T2091	S2092	A2099	S2100	A2104	G2116	A2119	I2120	A2121	A2122							
G1816	D1817	H1818	E1819	G1820	Y1821	H1822	C1839	E1846	G1851	I1856	G1857	G1858	S1859	A1860	D1884	A1888	G1898	L1899	S1900	G1901	N1905	C1906	E1909	K1916	P1917	F1918	S1919	F1920	G1921	A1922	P1923	Y1924	S1928	S1934	K1935	D1938	G1946	D1950	L1954	E1955	G1956	D1973						
L1675	R1680	D1693	R1694	D1697	A1701	S1704	L1708	P1709	P1710	P1713	S1716	A1717	A1718	N1719	R1720	F1721	V1725	A1745	S1751	L1752	V1753	G1621	G1622	L1623	F1624	E1627	A1632	S1636	S1640	G1652	I1653	D1654	D1659	H1660	D1661	N1662	T1663	E1664	E1665	I1666	L1667							
K1509	G1521	D1525	S1533	I1534	P1535	S1536	K1542	A1543	G1553	G1560	C1570	G1574	D1579	C1580	S1581	H1582	I1583	A1584	G1591	G1592	E1593	G1621	G1622	L1623	F1624	E1627	A1632	S1636	S1640	G1652	I1653	D1654	D1659	H1660	D1661	N1662	T1663	E1664	E1665	I1666	L1667							
G1521	S1223	L1224	G1225	Y1369	D1227	I1228	F1229	A1232	N1233	D1237	G1241	S1242	R1243	E1244	H1245	D1246	R1247	Y1248	E1251	V1252	T1253	G1254	A1255	S1256	D1264	E1269	D1283	A1290	G1294	K1295	P1296	G1297	E1300	L1301	N1302	Q1318	A1325	L1332	A1339	D1350	D1358	A1359	T1360					
Q1366	Q1367	R1368	Y1369	D1370	P1371	N1372	R1376	G1377	S1380	F1381	D1389	E1392	F1395	A1407	G1414	G1432	G1433	K1434	G1435	Q1436	Y1437	D1443	Y1444	S1445	F1451	H1454	N1457	E1478	I1483	M1486	H1487	Q1488	M1491	P1492	E1498	N1499	H1500	G1501	N1502	V1503								
T1118	L1119	G1123	Q1128	L1133	F1143	A1144	G1145	F1146	L1147	L1148	K1153	S1154	V1155	V1161	C1162	A1163	P1164	P1165	H1166	D1167	A1171	G1172	E1173	L1177	G1178	D1179	E1180	N1181	E1182	M1183	A1184	Y1187	D1188	R1189	V1190	F1191	D1194	T1195	T1196	N1197	V1198	E1201	Y1207	F1217	G1221			



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D5	Depositor
Number of particles used	28641	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	60000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.359	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.111	Depositor
Recommended contour level	1.5	Depositor
Map size (\AA)	612.0, 612.0, 612.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.02, 1.02, 1.02	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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3303	0	0	77	0
1	B	3303	0	0	67	0
All	All	6606	0	0	139	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 21.

The worst 5 of 139 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2641:GLU:CA	1:B:1536:SER:CA	2.39	0.99
1:A:2642:HIS:CA	1:B:1533:SER:CA	2.47	0.92
1:B:2075:ASN:CA	1:B:2076:LEU:CA	2.68	0.72
1:A:2641:GLU:CA	1:B:1535:PRO:CA	2.69	0.71
1:A:116:GLY:CA	1:A:117:LYS:CA	2.70	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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](#)

There are no chain breaks in this entry.

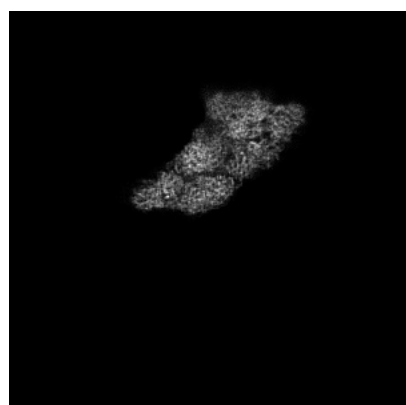
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5586. These allow visual inspection of the internal detail of the map and identification of artifacts.

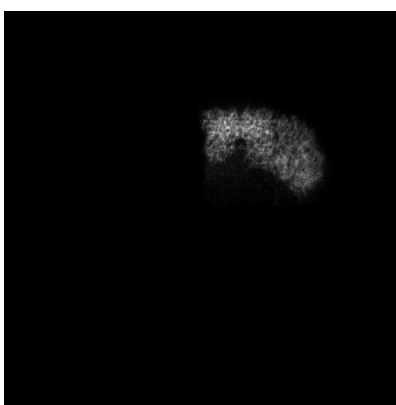
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

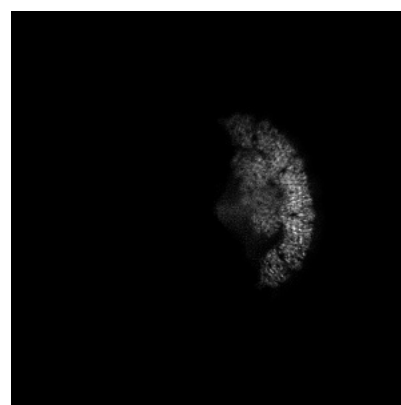
6.1.1 Primary map



X



Y

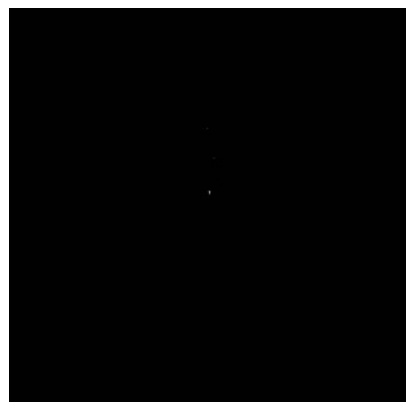


Z

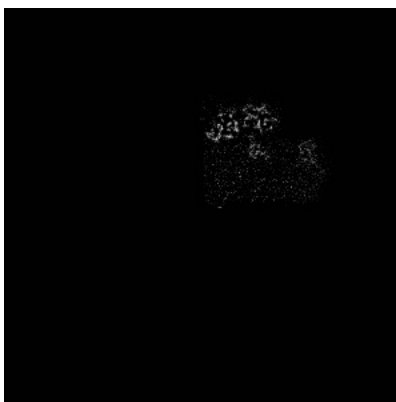
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300



Y Index: 300



Z Index: 300

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: 425



Y Index: 284



Z Index: 331

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

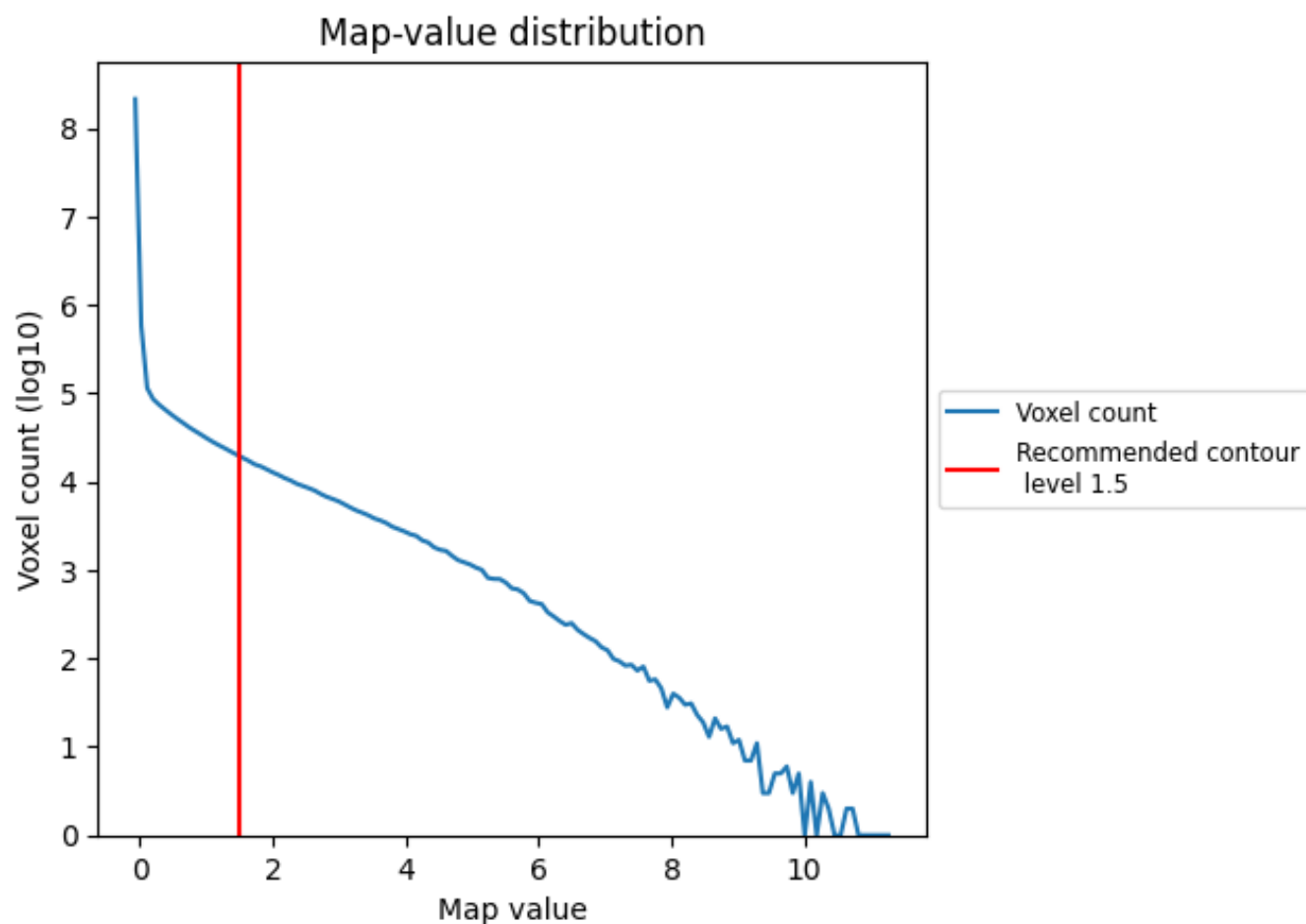
6.5 Mask visualisation

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

7 Map analysis [i](#)

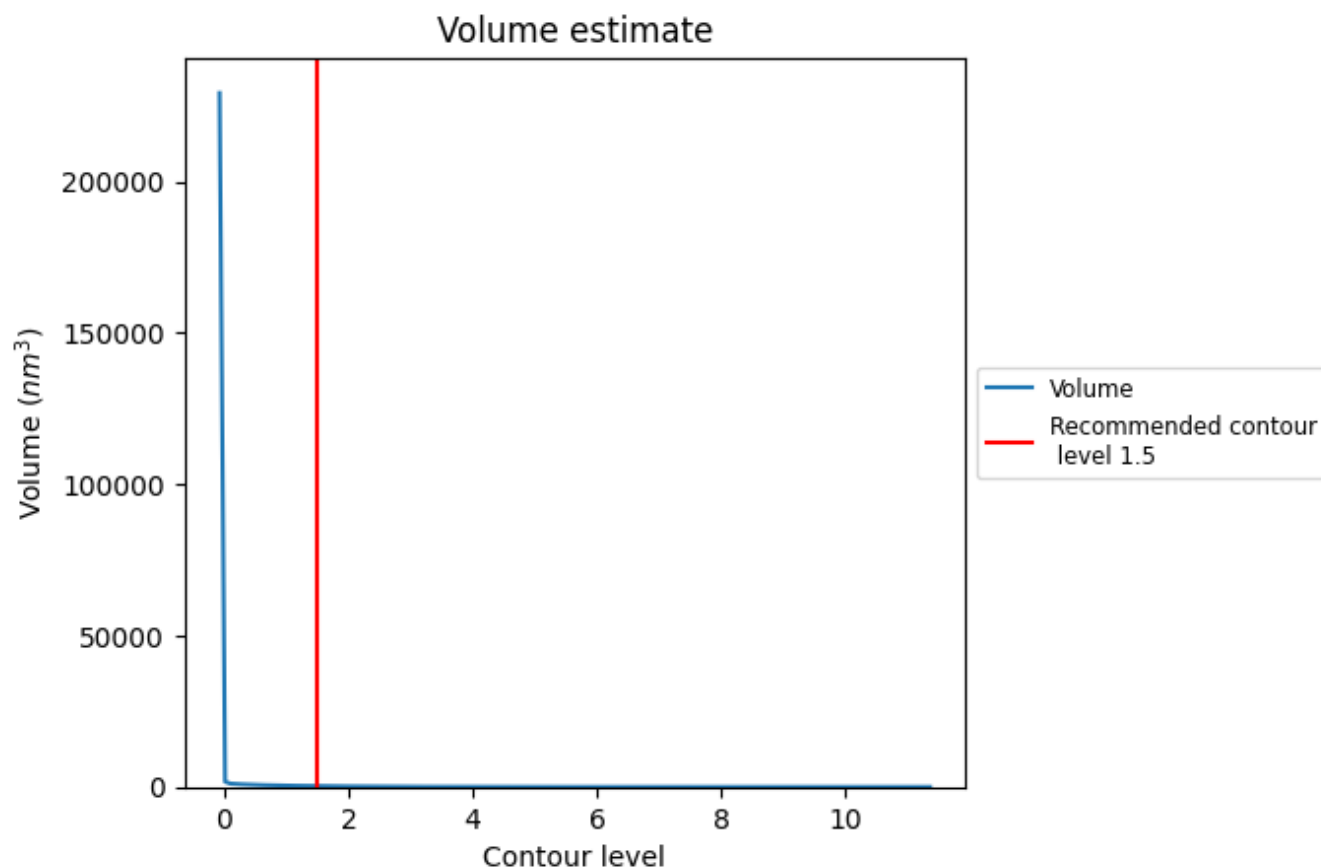
This section contains the results of statistical analysis of the map.

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.

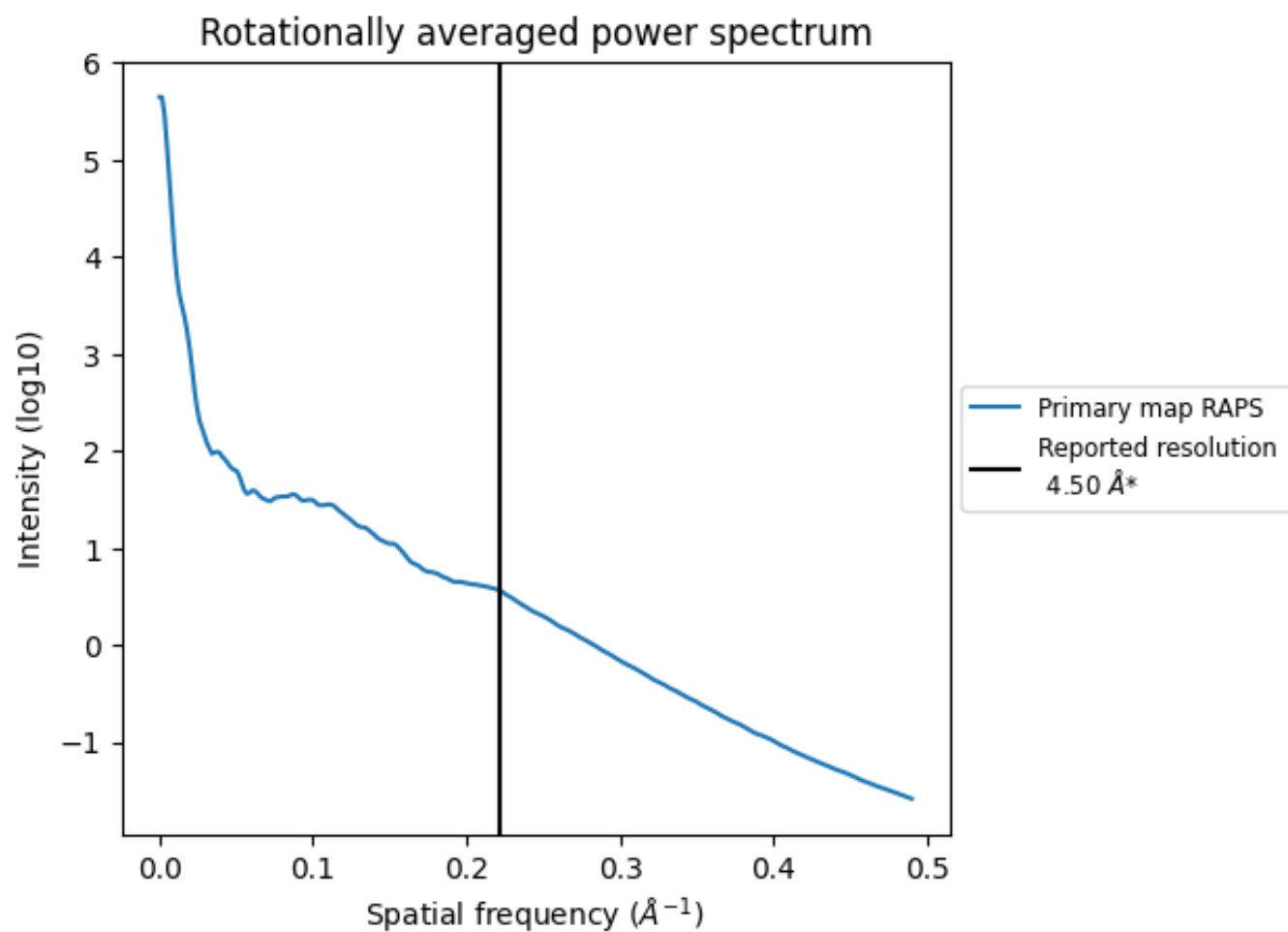
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290 nm^3 ; this corresponds to an approximate mass of 262 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

8 Fourier-Shell correlation ⓘ

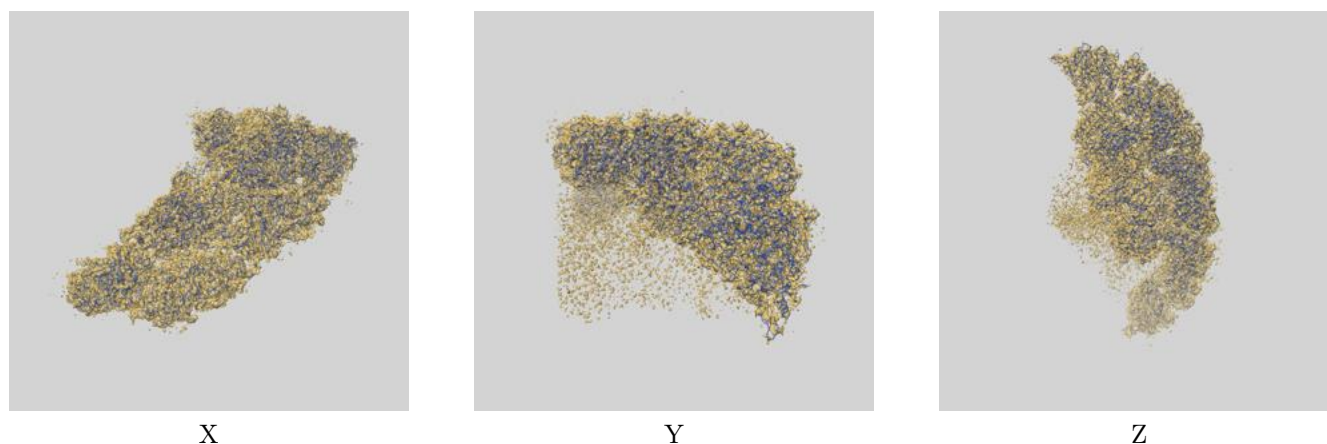
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

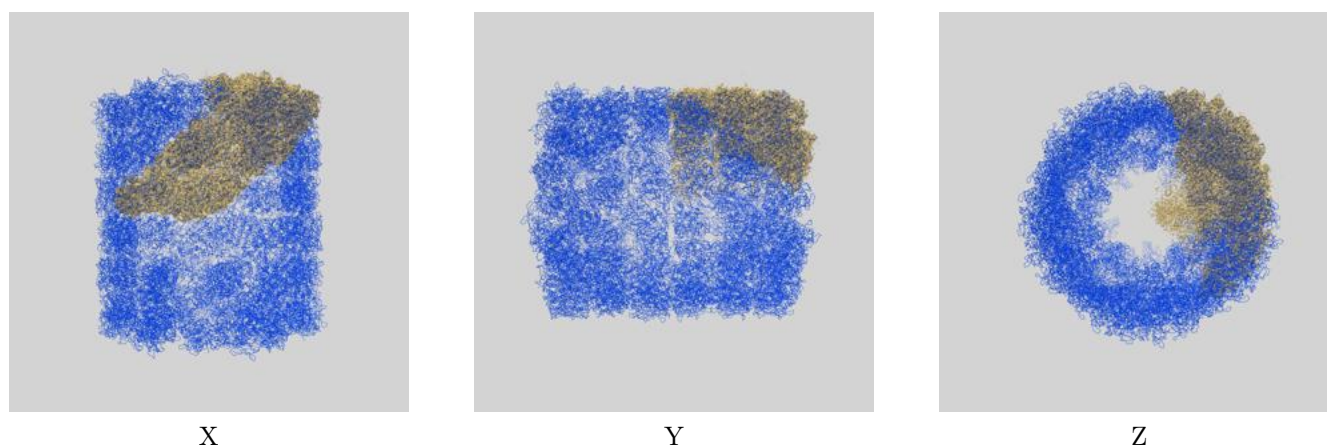
This section contains information regarding the fit between EMDB map EMD-5586 and PDB model 3J32. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlays

9.1.1 Map-model overlay ⓘ

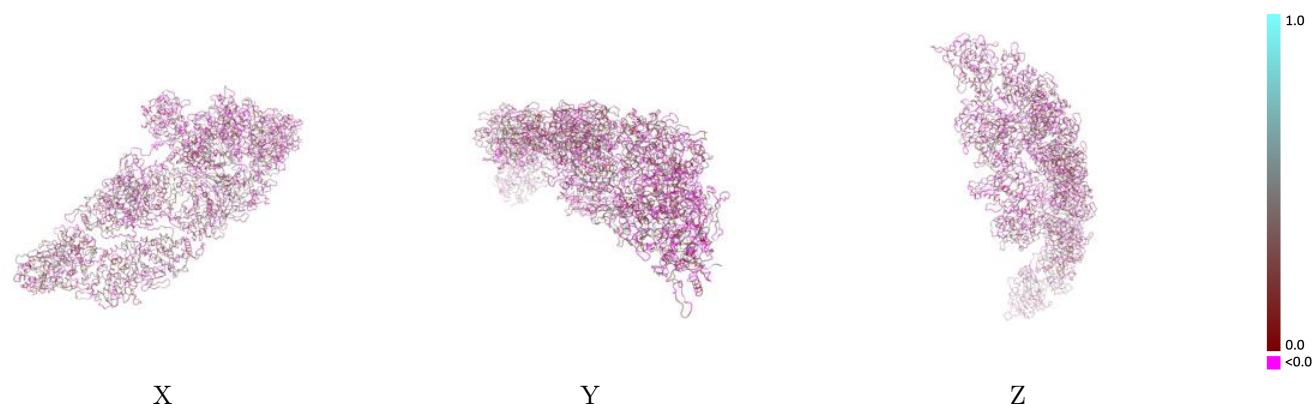


9.1.2 Map-model assembly overlay ⓘ



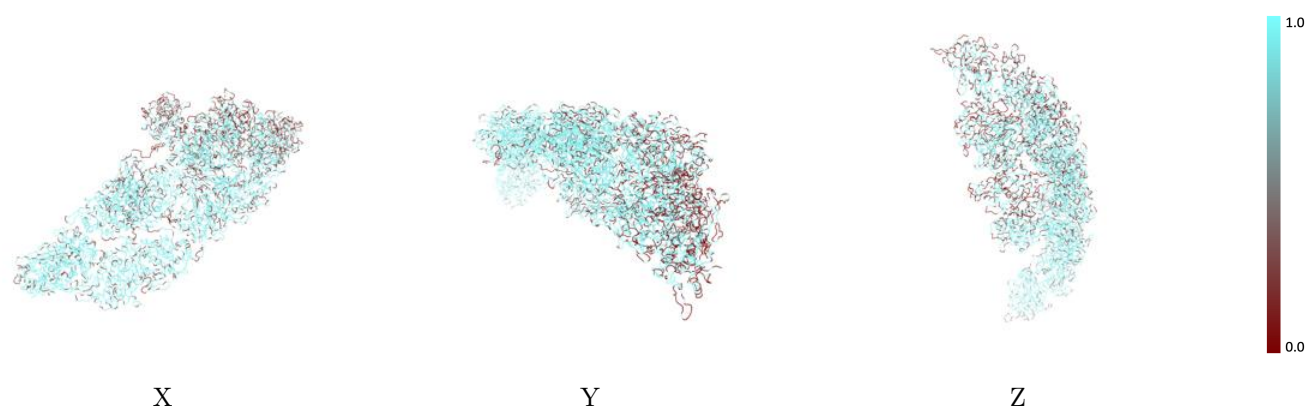
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



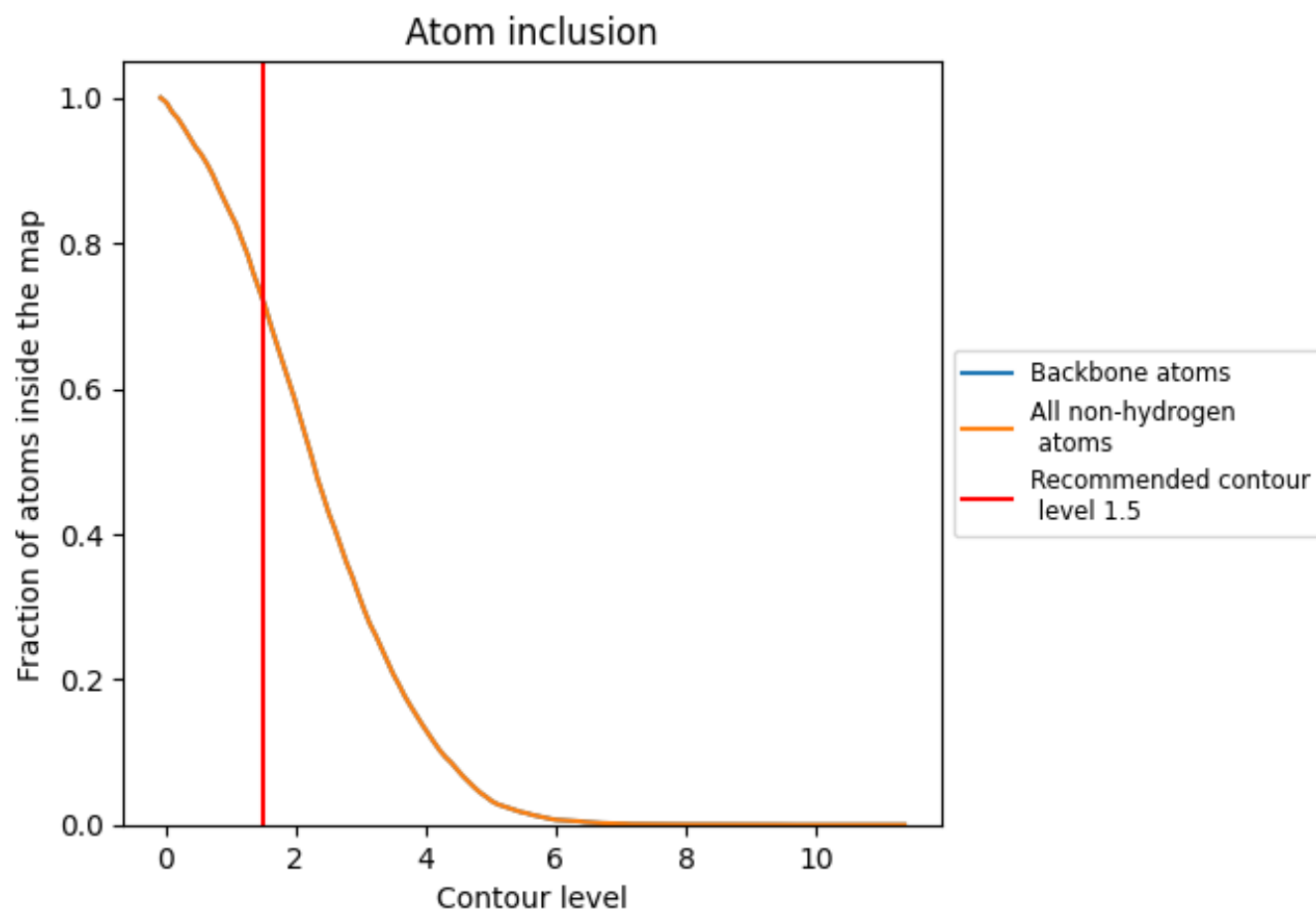
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7227	<div></div> 0.2030
A	<div></div> 0.7693	<div></div> 0.2160
B	<div></div> 0.6761	<div></div> 0.1890

