



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:39 AM UTC

PDB ID : 9EA7 / pdb_00009ea7
EMDB ID : EMD-47801
Title : The Structure of ApoB100 from Human Low-Density Lipoprotein
Authors : Berndsen, Z.T.; Cassidy, C.K.
Deposited on : 2024-11-10
Resolution : 9.00 Å (reported)
Based on initial model : .

This is a Full wwPDB EM Validation 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 ⓘ 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:

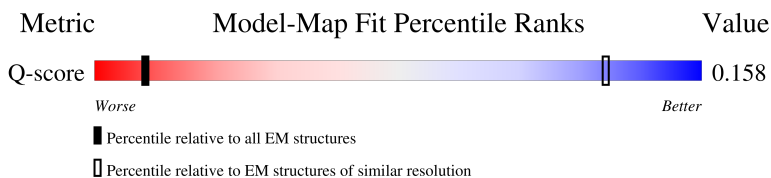
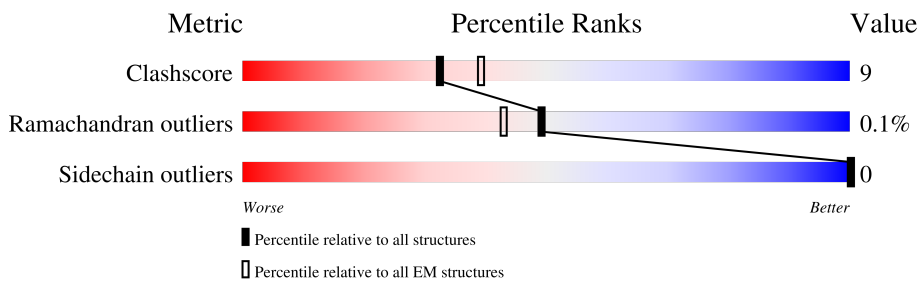
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	257 (8.50 - 9.50)

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	4563	<p>Quality of chain bar chart for Mol 1, Chain A. The bar is divided into segments: red (37%), orange (79%), yellow (20%), and grey (representing residues not modelled). A dot is shown at the end of the bar.</p>

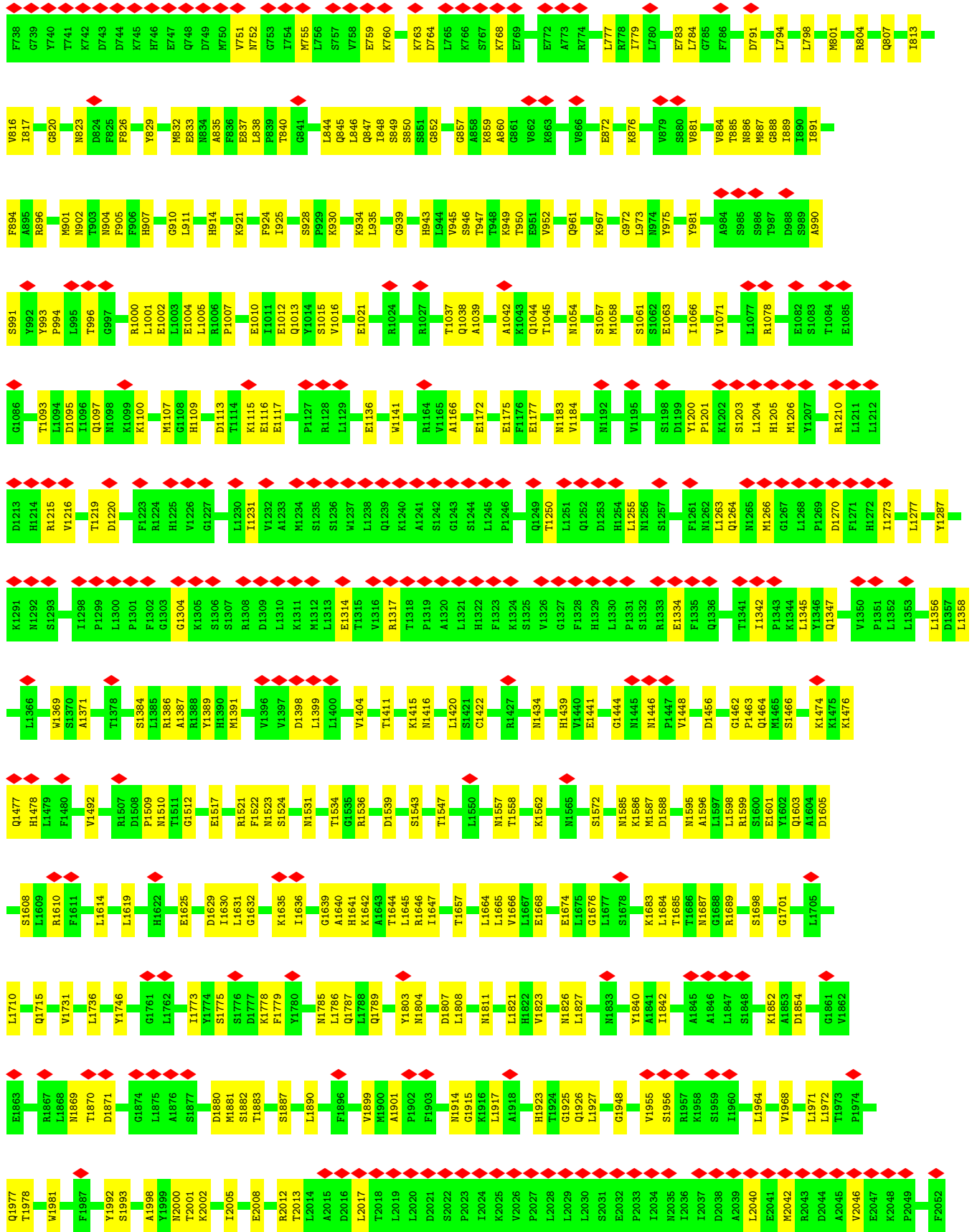
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 72328 atoms, of which 36245 are hydrogens and 0 are deuteriums.

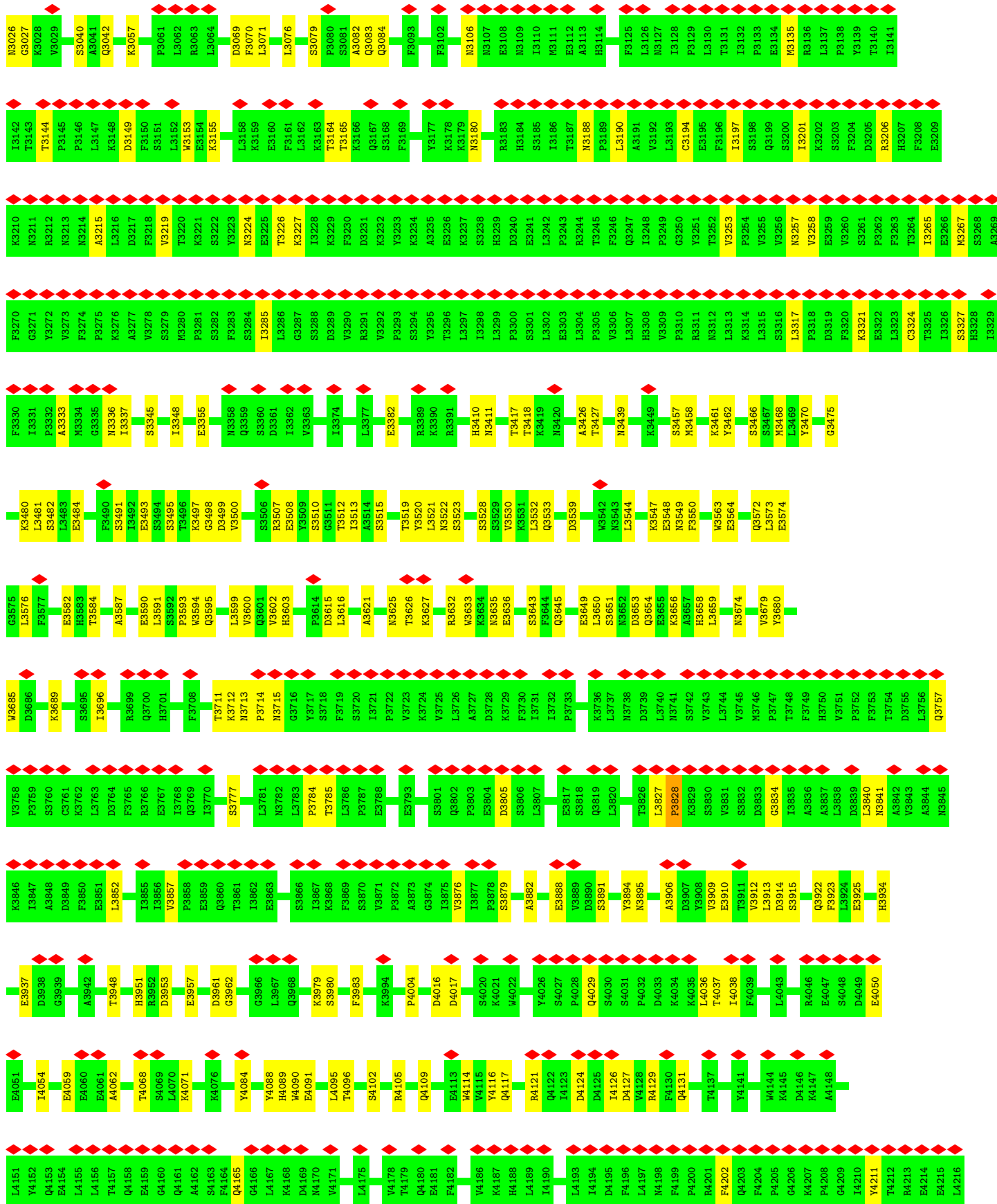
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

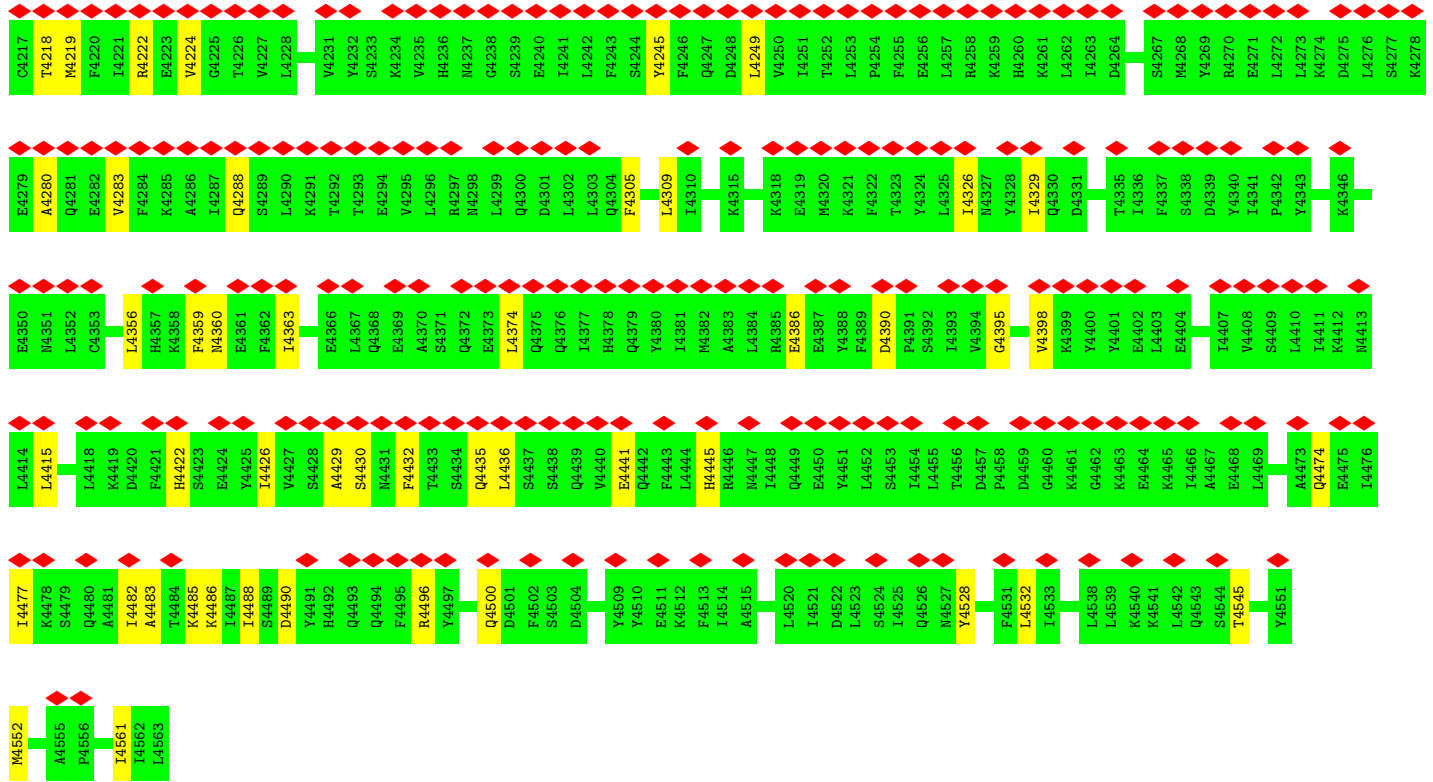
- Molecule 1 is a protein called Apolipoprotein B 100.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	4526	72328	23018	36245	6066	6897	102	0	0



V2065	L2126	K2186	W2248	E2308	Y2368	R2444	A2506	Q2583	T2655	E2715	V2803	D2899
K2059	N2127	D2187	L2249	R2309	K2369	Q2448	H2507	G2584	F2656	L2716	L2804	F2900
Y2060	S2128	D2190	Q2250	I2310	L2370	R2449	M2508	F2585	H2657	A2717	N2805	D2905
N2063	F2129	L2191	N2251	N2311	K2371	L2450	K2509	P2588	I2658	L2718	F2808	L2906
Q2064	N2130	H2192	D2252	D2312	E2372	G2451	A2450	E2589	P2659	P2719	Q2609	L2907
Q2065	W2131	D2193	V2253	L2313	T2373	G2452	K2510	E2590	S2660	E2720	A2810	K2907
V2066	N2133	L2196	D2254	L2314	I2374	E2453	F2512	T2592	F2661	F2721	L2814	T2912
H2067	R2133	A2197	K2255	E2315	Q2375	Q2454	R2513	L2594	T2662	L2722	S2815	L2916
S2068	Q2134	A2198	Y2256	H2316	K2376	A2456	R2514	L2594	T2663	L2723	N2816	L2917
I2069	S2136	I2198	Q2257	K2318	L2377	L2457	E2517	G2595	L2664	P2724	N2817	W2921
N2070	H2137	A2199	I2258	H2319	S2378	L2457	L2516	L2595	F2665	T2725	K2818	G2925
L2071	H2137	N2200	R2259	H2319	N2379	L2459	E2518	D2518	V2666	L2726	I2819	P2934
F2072	A2138	I2201	I2260	H2319	N2379	L2459	L2519	D2518	E2667	M2727	N2820	N2935
F2073	K2139	I2202	Q2261	H2320	P2460	Q2461	R2520	D2527	K2668	L2728	P2821	F2936
F2074	K2141	I2203	Q2262	V2321	L2381	Q2462	R2521	D2527	K2669	M2729	L2822	F2936
E2075	E2140	D2203	I2262	I2322	V2384	A2463	R2522	D2527	V2670	D2730	L2822	T2941
F2076	K2141	E2204	Q2263	N2323	K2385	A2463	R2522	D2527	K2671	F2731	K2833	T2941
L2077	L2142	I2205	E2264	I2324	I2386	E2464	M2523	Q2524	L2672	Q2732	R2836	S2944
F2081	T2143	E2207	E2265	L2325	K2387	A2465	Y2524	Q2525	L2673	V2733	T2837	E2951
N2084	A2144	E2208	L2266	G2326	D2388	E2466	Q2525	Q2526	I2674	P2734	E2838	L2954
Q2085	L2145	K2208	Q2267	L2266	Y2389	L2466	R2526	D2527	T2675	D2735	E2842	L2955
Q2086	T2146	K2209	Q2268	F2328	F2390	F2469	D2527	D2527	L2676	L2736	M2843	L2955
E2093	T2146	K2210	Q2269	E2329	E2391	F2469	D2528	D2528	L2677	H2737	F2845	L2955
Q2096	K2148	L2212	K2270	V2330	E2391	F2469	Q2529	Q2529	Q2678	L2738	F2846	N2964
R2097	R2149	D2213	R2271	E2332	L2393	E2472	Q2530	L2530	M2679	P2739	G2847	H2967
N2098	R2150	E2214	R2272	E2333	V2394	E2473	E2531	L2531	N2680	E2740	N2848	L2968
L2099	I2151	H2215	I2273	I2334	Q2395	K2474	L2532	L2532	S2682	F2741	E2851	N2971
K2100	I2151	H2216	Q2274	I2335	L2396	A2475	L2533	L2533	E2683	H2745	Q2851	Q2972
H2101	T2152	Y2217	Q2275	I2336	I2397	A2476	R2534	R2534	E2684	L2746	N2855	N2973
H2102	E2153	H2218	N2276	I2337	D2398	T2476	Y2535	Y2535	E2685	E2751	N2855	L2974
N2103	E2154	I2218	D2277	I2338	A2400	V2477	R2536	R2536	Q2686	E2759	N2855	L2974
I2104	N2155	F2218	I2278	R2338	V2401	V2477	L2537	L2537	W2687	K2763	N2855	K2985
D2105	I2156	R2219	L2278	A2339	K2403	Y2479	S2537	S2537	W2688	L2764	N2855	L2986
Q2106	D2161	Y2220	G2283	K2340	K2403	Y2480	L2538	L2538	V2689	L2768	Q2872	E2987
F2107	A2163	Q2224	E2284	E2343	E2406	L2481	L2539	L2539	P2690	L2768	G2872	L2988
V2108	K2164	I2226	K2286	E2344	E2406	E2482	V2542	V2542	D2690	L2771	N2876	D2993
R2109	E2165	I2227	Q2287	L2344	L2407	S2483	Y2544	Y2544	I2691	D2772	Q2876	V2997
K2110	N2166	D2228	H2288	L2345	L2407	Q2485	T2545	T2545	I2692	L2772	N2876	H2999
Y2111	F2167	L2229	H2288	E2346	L2407	D2486	V2546	V2546	I2693	L2772	Q2880	S3000
R2112	N2168	H2230	I2289	E2347	F2412	T2487	L2547	L2547	L2694	N2779	N2880	V3001
R2113	E2169	L2231	I2290	R2348	K2418	K2488	W2553	W2553	D2695	G2760	N2886	K3004
A2114	K2170	F2232	A2291	E2349	T2424	L2489	K2559	K2559	L2696	L2781	T2887	A3004
L2115	L2171	E2234	E2292	V2350	K2426	T2490	L2562	L2562	K2697	T2782	K2888	K3005
G2116	S2172	N2235	D2293	D2351	L2427	L2491	D2563	D2563	I2698	S2783	Y2889	G3006
K2117	Q2173	I2236	V2294	I2354	K2428	N2494	F2564	F2564	E2699	A2784	H2891	F3017
L2118	Q2175	I2237	W2296	I2354	S2429	N2495	E2566	E2566	D2700	N2785	N2894	L2895
F2119	K2177	F2238	V2297	V2356	F2430	L2496	S2567	S2567	L2701	E2786	N2894	P2896
Q2120	Y2177	N2239	L2298	L2357	D2431	Q2497	Y2568	Y2568	A2704	G2788	K2897	L2898
Q2121	K2240	K2240	L2299	M2358	H2433	E2498	S2569	S2569	R2705	K2796	L2898	
A2122	S2241	S2241	D2299	D2359	Q2434	A2499	L2570	L2570	E2648	S2799	N2898	
N2123	G2242	G2242	Q2300	K2360	Q2434	L2500	Q2571	Q2571	E2649	K2800	N2898	
D2124	S2243	S2243	G2302	L2361	F2436	L2500	D2572	D2572	T2650	L2801	N2898	
Y2125	S2244	S2244	G2303	E2363	Y2436	S2502	W2573	W2573	T2651	E2802	N2898	
	A2246	A2246	T2304	L2364	L2436	S2503	E2582	E2582	L2652		N2898	
	S2247	S2247	I2306	H2366	T2439	L2504			L2654		N2898	
			S2306	Q2367		L2505					N2898	
			F2307								N2898	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52843	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.148	Depositor
Minimum map value	-0.560	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.182	Depositor
Map size (Å)	490.5, 490.5, 490.5	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.12	0/36813	0.30	0/49814

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2820	ASN	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	36083	36245	36243	617	0
All	All	36083	36245	36243	617	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 9.

All (617) 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:500:GLU:OE2	1:A:537:LYS:NZ	1.96	0.98
1:A:325:VAL:HG13	1:A:351:LEU:HD11	1.46	0.95
1:A:323:GLU:OE1	1:A:327:LYS:NZ	2.03	0.92
1:A:3632:ARG:NH1	1:A:3633:TRP:O	2.03	0.92
1:A:3482:SER:OG	1:A:3484:GLU:OE2	1.90	0.89
1:A:243:GLN:NE2	1:A:245:CYS:SG	2.48	0.86
1:A:3491:SER:OG	1:A:3493:GLU:OE2	1.93	0.84
1:A:3135:MET:SD	1:A:3144:THR:OG1	2.35	0.84
1:A:332:LEU:O	1:A:344:ARG:NH2	2.11	0.84
1:A:3649:GLU:OE2	1:A:3651:SER:OG	1.95	0.83
1:A:1038:GLN:NE2	1:A:1044:GLN:OE1	2.12	0.83
1:A:1684:LEU:O	1:A:1698:SER:OG	1.97	0.82
1:A:1608:SER:O	1:A:1610:ARG:NH1	2.13	0.81
1:A:57:GLU:N	1:A:57:GLU:OE1	2.14	0.80
1:A:2833:LYS:O	1:A:2836:ARG:NH1	2.15	0.80
1:A:907:HIS:ND1	1:A:935:LEU:O	2.14	0.80
1:A:2802:GLU:N	1:A:2802:GLU:OE1	2.15	0.80
1:A:1521:ARG:NH1	1:A:1522:PHE:O	2.15	0.80
1:A:336:THR:O	1:A:859:LYS:NZ	2.15	0.79
1:A:847:GLN:N	1:A:888:GLY:O	2.15	0.79
1:A:54:TYR:OH	1:A:256:VAL:O	2.00	0.79
1:A:79:LYS:NZ	1:A:81:GLU:OE2	2.15	0.79
1:A:4109:GLN:O	1:A:4496:ARG:NH2	2.17	0.78
1:A:1386:ARG:O	1:A:1386:ARG:NH1	2.17	0.77
1:A:143:LEU:N	1:A:306:MET:O	2.16	0.77
1:A:1881:MET:SD	1:A:1883:THR:OG1	2.42	0.76
1:A:3636:GLU:N	1:A:3636:GLU:OE1	2.18	0.76
1:A:1603:GLN:OE1	1:A:1605:ASP:N	2.19	0.76
1:A:271:SER:OG	1:A:276:TYR:N	2.20	0.75
1:A:1012:GLU:N	1:A:1012:GLU:OE1	2.20	0.75
1:A:4552:MET:HE1	1:A:4561:ILE:HG23	1.68	0.74
1:A:1668:GLU:OE2	1:A:1687:ASN:N	2.20	0.74
1:A:460:THR:OG1	1:A:462:GLU:OE1	2.04	0.74
1:A:1978:THR:OG1	1:A:1998:ALA:O	2.04	0.74
1:A:122:PHE:CD2	1:A:126:MET:HE1	2.23	0.73
1:A:1789:GLN:OE1	1:A:1789:GLN:N	2.20	0.73
1:A:3888:GLU:OE2	1:A:3895:ASN:ND2	2.21	0.73
1:A:1531:ASN:ND2	1:A:1547:THR:O	2.22	0.72
1:A:2183:GLN:NE2	1:A:2187:ASP:OD2	2.22	0.72
1:A:949:LYS:NZ	1:A:950:THR:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLU:N	1:A:120:GLU:OE1	2.23	0.72
1:A:3953:ASP:OD2	1:A:4088:TYR:OH	2.08	0.71
1:A:180:ASP:OD1	1:A:181:THR:N	2.23	0.71
1:A:3784:PRO:O	1:A:3785:THR:OG1	2.06	0.71
1:A:352:VAL:HG23	1:A:356:ARG:HH22	1.56	0.71
1:A:429:ILE:HG22	1:A:445:LEU:HD13	1.73	0.71
1:A:1977:GLN:OE1	1:A:2000:ASN:ND2	2.24	0.71
1:A:158:ARG:NH2	1:A:311:GLU:OE1	2.23	0.70
1:A:2855:ASN:ND2	1:A:2871:ASN:O	2.25	0.70
1:A:1955:VAL:O	1:A:1956:SER:OG	2.07	0.70
1:A:896:ARG:NH2	1:A:946:SER:O	2.23	0.70
1:A:4102:SER:OG	1:A:4105:ARG:NH2	2.24	0.70
1:A:991:SER:N	1:A:996:THR:OG1	2.24	0.69
1:A:389:GLN:NE2	1:A:390:CYS:SG	2.66	0.69
1:A:1039:ALA:N	1:A:1045:THR:OG1	2.26	0.69
1:A:3654:GLN:NE2	1:A:3805:ASP:O	2.25	0.69
1:A:1586:LYS:N	1:A:1601:GLU:OE2	2.26	0.69
1:A:186:CYS:SG	1:A:207:ARG:NH1	2.65	0.69
1:A:1715:GLN:OE1	1:A:1715:GLN:N	2.26	0.69
1:A:558:ARG:NH2	1:A:586:ASN:OD1	2.27	0.68
1:A:603:SER:HB3	1:A:608:ILE:HG21	1.75	0.68
1:A:1586:LYS:O	1:A:1599:ARG:NH1	2.25	0.68
1:A:1664:LEU:O	1:A:1689:ARG:NH1	2.26	0.68
1:A:4037:THR:N	1:A:4059:GLU:OE2	2.24	0.67
1:A:3480:LYS:NZ	1:A:3481:LEU:O	2.27	0.67
1:A:1915:GLY:N	1:A:1925:GLY:O	2.26	0.67
1:A:1869:ASN:ND2	1:A:1880:ASP:OD1	2.27	0.67
1:A:85:PRO:O	1:A:297:ARG:NH1	2.27	0.66
1:A:375:SER:O	1:A:378:THR:OG1	2.13	0.66
1:A:3180:ASN:ND2	1:A:3333:ALA:O	2.27	0.66
1:A:443:TYR:O	1:A:447:HIS:ND1	2.29	0.66
1:A:1314:GLU:N	1:A:1314:GLU:OE1	2.28	0.66
1:A:599:ASN:ND2	1:A:636:ASN:OD1	2.29	0.65
1:A:497:GLN:N	1:A:497:GLN:OE1	2.30	0.65
1:A:3355:GLU:N	1:A:3355:GLU:OE1	2.29	0.65
1:A:314:LYS:NZ	1:A:358:LEU:O	2.30	0.64
1:A:3548:GLU:N	1:A:3548:GLU:OE1	2.30	0.64
1:A:4004:PRO:O	1:A:4029:GLN:NE2	2.30	0.64
1:A:1172:GLU:N	1:A:1172:GLU:OE1	2.30	0.64
1:A:431:ASN:OD1	1:A:434:ARG:NH2	2.30	0.64
1:A:586:ASN:O	1:A:589:VAL:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1632:GLY:O	1:A:1639:GLY:N	2.30	0.64
1:A:2925:GLY:N	1:A:2944:SER:O	2.29	0.64
1:A:3582:GLU:OE1	1:A:3582:GLU:N	2.30	0.64
1:A:764:ASP:O	1:A:768:LYS:NZ	2.30	0.64
1:A:1683:LYS:NZ	1:A:1698:SER:OG	2.31	0.63
1:A:4124:ASP:OD1	1:A:4485:LYS:NZ	2.27	0.63
1:A:967:LYS:O	1:A:975:TYR:N	2.31	0.63
1:A:3522:ASN:OD1	1:A:3523:SER:N	2.31	0.63
1:A:1585:ASN:ND2	1:A:1601:GLU:O	2.31	0.63
1:A:3079:SER:OG	1:A:3082:ALA:O	2.14	0.63
1:A:3602:VAL:HG23	1:A:3603:HIS:ND1	2.14	0.63
1:A:396:GLN:N	1:A:396:GLN:OE1	2.29	0.63
1:A:2512:PHE:CZ	1:A:2516:LEU:HD11	2.34	0.62
1:A:967:LYS:NZ	1:A:4050:GLU:OE2	2.33	0.62
1:A:2867:LEU:HD23	1:A:2868:GLU:N	2.13	0.62
1:A:1334:GLU:OE1	1:A:1334:GLU:N	2.33	0.62
1:A:2888:LYS:NZ	1:A:2889:TYR:O	2.33	0.61
1:A:1273:ILE:HD12	1:A:1277:LEU:HD11	1.82	0.61
1:A:777:LEU:O	1:A:784:LEU:N	2.31	0.61
1:A:2912:THR:HG1	1:A:2921:TRP:CD1	2.18	0.61
1:A:3004:ALA:HB1	1:A:3017:PHE:CZ	2.36	0.61
1:A:2017:LEU:N	1:A:2046:VAL:O	2.32	0.61
1:A:2889:TYR:OH	1:A:2891:HIS:ND1	2.30	0.61
1:A:3689:LYS:NZ	1:A:4091:GLU:OE2	2.32	0.61
1:A:181:THR:HG22	1:A:184:GLY:O	2.01	0.61
1:A:3001:VAL:O	1:A:3021:HIS:ND1	2.33	0.61
1:A:1061:SER:OG	1:A:1063:GLU:OE2	2.11	0.61
1:A:3040:SER:OG	1:A:3042:GLN:NE2	2.34	0.61
1:A:325:VAL:HG13	1:A:351:LEU:CD1	2.28	0.60
1:A:1595:ASN:ND2	1:A:1619:LEU:O	2.34	0.60
1:A:462:GLU:O	1:A:466:ILE:HD12	2.00	0.60
1:A:194:THR:OG1	1:A:202:GLU:OE1	2.18	0.60
1:A:961:GLN:N	1:A:981:TYR:O	2.34	0.60
1:A:1523:ASN:OD1	1:A:1524:SER:N	2.35	0.60
1:A:3417:THR:O	1:A:3418:THR:OG1	2.18	0.60
1:A:179:LEU:O	1:A:186:CYS:N	2.35	0.59
1:A:424:GLN:O	1:A:428:GLU:OE1	2.20	0.59
1:A:623:GLN:OE1	1:A:623:GLN:N	2.34	0.59
1:A:1701:GLY:HA2	1:A:1710:LEU:HD23	1.82	0.59
1:A:4038:ILE:HD13	1:A:4062:ALA:HB1	1.84	0.59
1:A:2339:ALA:O	1:A:2343:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LEU:HD22	1:A:891:ILE:HG13	1.84	0.59
1:A:2838:GLU:N	1:A:2838:GLU:OE1	2.36	0.59
1:A:505:GLU:OE1	1:A:505:GLU:N	2.32	0.59
1:A:1852:LYS:NZ	1:A:1854:ASP:OD2	2.34	0.59
1:A:2144:ALA:O	1:A:2148:LYS:N	2.36	0.59
1:A:3149:ASP:O	1:A:3155:LYS:NZ	2.34	0.59
1:A:3508:GLU:OE1	1:A:3510:SER:OG	2.14	0.59
1:A:2801:LEU:O	1:A:2804:LEU:N	2.30	0.59
1:A:2008:GLU:OE1	1:A:2008:GLU:N	2.35	0.59
1:A:2040:LEU:HD13	1:A:2042:MET:HE3	1.83	0.59
1:A:155:ASN:OD1	1:A:158:ARG:NH1	2.35	0.58
1:A:2005:ILE:HG22	1:A:2060:TYR:HD2	1.68	0.58
1:A:233:ARG:NH1	1:A:237:THR:OG1	2.36	0.58
1:A:3153:TRP:NE1	1:A:3164:THR:O	2.36	0.58
1:A:3411:ASN:ND2	1:A:3426:ALA:O	2.34	0.58
1:A:990:ALA:HB1	1:A:996:THR:HG21	1.84	0.58
1:A:1512:GLY:O	1:A:1539:ASP:N	2.31	0.58
1:A:135:ILE:O	1:A:135:ILE:HG23	2.04	0.58
1:A:1175:GLU:N	1:A:1175:GLU:OE1	2.36	0.58
1:A:445:LEU:O	1:A:449:VAL:HG23	2.03	0.58
1:A:901:MET:SD	1:A:901:MET:N	2.77	0.58
1:A:910:GLY:C	1:A:911:LEU:HD22	2.29	0.58
1:A:1948:GLY:O	1:A:1964:LEU:N	2.36	0.58
1:A:837:GLU:C	1:A:838:LEU:HD22	2.29	0.57
1:A:1314:GLU:OE2	1:A:1317:ARG:NH2	2.38	0.57
1:A:471:MET:HE1	1:A:509:SER:OG	2.04	0.57
1:A:891:ILE:HG22	1:A:894:PHE:HB2	1.87	0.57
1:A:4090:TRP:HE1	1:A:4096:THR:HG22	1.69	0.57
1:A:801:MET:HE3	1:A:801:MET:O	2.04	0.57
1:A:2451:ASN:OD1	1:A:2455:GLN:NE2	2.38	0.57
1:A:359:SER:O	1:A:363:VAL:HG23	2.05	0.56
1:A:4435:GLN:OE1	1:A:4436:LEU:HD22	2.05	0.56
1:A:515:GLN:NE2	1:A:546:GLN:OE1	2.36	0.56
1:A:1666:VAL:HG23	1:A:1689:ARG:HH21	1.70	0.56
1:A:2986:LEU:O	1:A:3006:GLY:N	2.34	0.56
1:A:3532:LEU:N	1:A:3549:ASN:OD1	2.33	0.56
1:A:4114:TRP:O	1:A:4117:GLN:NE2	2.38	0.56
1:A:3643:SER:OG	1:A:3645:GLN:NE2	2.39	0.56
1:A:826:PHE:HA	1:A:857:GLY:HA3	1.88	0.56
1:A:329:LEU:HG	1:A:373:VAL:HG11	1.88	0.56
1:A:3711:THR:OG1	1:A:3882:ALA:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:MET:SD	1:A:4545:THR:HG23	2.46	0.56
1:A:914:HIS:O	1:A:925:ILE:N	2.30	0.55
1:A:626:THR:HG22	1:A:628:MET:HE3	1.89	0.55
1:A:2449:ARG:O	1:A:2453:GLU:OE1	2.24	0.55
1:A:2764:ILE:HD13	1:A:2771:LEU:HD23	1.88	0.55
1:A:75:ARG:CB	1:A:113:LEU:HD13	2.37	0.55
1:A:3253:VAL:O	1:A:3257:ASN:N	2.40	0.55
1:A:239:ILE:HD13	1:A:267:PHE:HD1	1.71	0.55
1:A:3439:ASN:OD1	1:A:3461:LYS:NZ	2.26	0.55
1:A:395:LEU:HD22	1:A:428:GLU:HB3	1.89	0.55
1:A:507:LYS:NZ	1:A:540:ASP:OD2	2.39	0.54
1:A:1016:VAL:HG23	1:A:1037:THR:HG22	1.90	0.54
1:A:1093:THR:OG1	1:A:1107:MET:SD	2.64	0.54
1:A:3057:LYS:NZ	1:A:3069:ASP:OD1	2.38	0.54
1:A:1881:MET:SD	1:A:1882:SER:N	2.80	0.54
1:A:1478:HIS:CE1	1:A:1509:PRO:HG2	2.42	0.54
1:A:3714:PRO:O	1:A:3876:VAL:HG11	2.07	0.54
1:A:476:ASP:OD1	1:A:509:SER:OG	2.18	0.54
1:A:973:LEU:HD13	1:A:1007:PRO:HA	1.88	0.54
1:A:2973:ASN:O	1:A:2974:LEU:HD22	2.07	0.54
1:A:3265:ILE:HG22	1:A:3267:MET:HE1	1.89	0.54
1:A:1746:TYR:OH	1:A:4390:ASP:OD1	2.22	0.54
1:A:2779:ASN:OD1	1:A:2780:GLY:N	2.41	0.54
1:A:4386:GLU:N	1:A:4386:GLU:OE1	2.41	0.54
1:A:3961:ASP:OD1	1:A:3962:GLY:N	2.41	0.54
1:A:1420:LEU:HD11	1:A:1422:CYS:SG	2.48	0.54
1:A:2040:LEU:HD21	1:A:2800:LYS:NZ	2.22	0.54
1:A:352:VAL:HG23	1:A:356:ARG:NH2	2.22	0.53
1:A:397:TRP:CZ2	1:A:401:VAL:HG11	2.43	0.53
1:A:881:VAL:N	1:A:905:PHE:O	2.41	0.53
1:A:837:GLU:O	1:A:838:LEU:HD22	2.08	0.53
1:A:1826:ASN:OD1	1:A:1827:LEU:N	2.42	0.53
1:A:4165:GLN:OE1	1:A:4165:GLN:N	2.36	0.53
1:A:2523:MET:HE1	1:A:2672:ILE:HG22	1.91	0.53
1:A:3206:ARG:NH2	1:A:3834:GLY:O	2.37	0.53
1:A:3914:ASP:OD1	1:A:3915:SER:N	2.42	0.53
1:A:225:LEU:O	1:A:829:TYR:OH	2.23	0.53
1:A:466:ILE:O	1:A:470:LEU:HD23	2.09	0.53
1:A:1078:ARG:NH1	1:A:1095:ASP:OD2	2.38	0.53
1:A:203:ILE:HD12	1:A:249:LEU:HD11	1.90	0.53
1:A:397:TRP:CE2	1:A:401:VAL:HG11	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ASP:O	1:A:577:ILE:HG13	2.09	0.53
1:A:519:PRO:O	1:A:524:GLN:NE2	2.39	0.53
1:A:1446:ASN:O	1:A:1448:VAL:N	2.42	0.53
1:A:2105:ASP:OD1	1:A:2106:GLN:N	2.42	0.53
1:A:3757:GLN:N	1:A:3777:SER:OG	2.36	0.53
1:A:2988:ILE:HD11	1:A:3004:ALA:HB3	1.91	0.53
1:A:3194:CYS:O	1:A:3321:LYS:NZ	2.41	0.53
1:A:3715:ASN:O	1:A:3876:VAL:HG13	2.08	0.53
1:A:713:ASP:OD2	1:A:760:LYS:NZ	2.33	0.52
1:A:3948:THR:HG23	1:A:3957:GLU:HG3	1.91	0.52
1:A:122:PHE:CE2	1:A:126:MET:HE1	2.44	0.52
1:A:1870:THR:HG22	1:A:1871:ASP:N	2.24	0.52
1:A:2941:THR:N	1:A:2964:ASN:OD1	2.39	0.52
1:A:327:LYS:O	1:A:331:GLU:HG2	2.10	0.52
1:A:595:SER:N	1:A:627:VAL:HG11	2.25	0.52
1:A:3495:SER:OG	1:A:3515:SER:O	2.25	0.52
1:A:3910:GLU:N	1:A:3910:GLU:OE1	2.42	0.52
1:A:4360:ASN:HB2	1:A:4426:ILE:HG21	1.92	0.52
1:A:813:ILE:HD12	1:A:2240:LYS:HE3	1.92	0.52
1:A:934:LYS:HA	1:A:1004:GLU:HG2	1.91	0.52
1:A:1386:ARG:O	1:A:1386:ARG:HG2	2.10	0.52
1:A:1463:PRO:O	1:A:1464:GLN:NE2	2.43	0.52
1:A:212:CYS:O	1:A:215:PHE:HD1	1.93	0.51
1:A:235:LEU:O	1:A:238:LEU:N	2.42	0.51
1:A:325:VAL:CG1	1:A:351:LEU:HD11	2.31	0.51
1:A:2799:SER:O	1:A:2805:ASN:ND2	2.41	0.51
1:A:921:LYS:NZ	1:A:1021:GLU:OE2	2.41	0.51
1:A:1644:THR:C	1:A:1645:LEU:HD22	2.36	0.51
1:A:1968:VAL:HG13	1:A:1981:TRP:CD1	2.45	0.51
1:A:2592:THR:OG1	1:A:2595:GLY:O	2.17	0.51
1:A:3626:THR:OG1	1:A:3627:LYS:N	2.38	0.51
1:A:2585:PHE:O	1:A:2602:VAL:HG22	2.10	0.51
1:A:2997:VAL:O	1:A:3026:ASN:N	2.42	0.51
1:A:336:THR:HB	1:A:344:ARG:HH22	1.75	0.51
1:A:794:LEU:O	1:A:798:LEU:HG	2.11	0.51
1:A:101:GLU:N	1:A:101:GLU:OE1	2.44	0.51
1:A:3468:MET:SD	1:A:3468:MET:N	2.83	0.51
1:A:833:GLU:OE2	1:A:835:ALA:HB2	2.09	0.51
1:A:2547:VAL:HG11	1:A:2634:LYS:HD3	1.93	0.51
1:A:3564:GLU:OE1	1:A:3584:THR:HG21	2.11	0.51
1:A:3658:HIS:C	1:A:3659:LEU:HD22	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3674:ASN:ND2	1:A:3696:ILE:O	2.40	0.51
1:A:4305:PHE:CE2	1:A:4309:LEU:HD11	2.45	0.51
1:A:702:GLU:O	1:A:706:GLY:N	2.40	0.51
1:A:1625:GLU:OE1	1:A:1625:GLU:N	2.43	0.51
1:A:850:SER:HB2	1:A:885:THR:HG23	1.93	0.51
1:A:3507:ARG:NH2	1:A:3539:ASP:O	2.41	0.51
1:A:4202:PHE:N	1:A:4211:TYR:O	2.39	0.51
1:A:1304:GLY:N	1:A:1342:ILE:O	2.36	0.51
1:A:4117:GLN:OE1	1:A:4121:ARG:NH1	2.43	0.51
1:A:175:GLN:O	1:A:190:PHE:N	2.38	0.50
1:A:3925:GLU:O	1:A:3951:HIS:ND1	2.44	0.50
1:A:881:VAL:O	1:A:905:PHE:N	2.43	0.50
1:A:1993:SER:OG	1:A:2012:ARG:NH2	2.43	0.50
1:A:75:ARG:HB3	1:A:113:LEU:HD13	1.92	0.50
1:A:3544:LEU:HD23	1:A:3544:LEU:O	2.11	0.50
1:A:490:ARG:NH1	1:A:783:GLU:OE2	2.37	0.50
1:A:847:GLN:OE1	1:A:888:GLY:N	2.45	0.50
1:A:1369:TRP:CH2	1:A:1371:ALA:HB2	2.46	0.50
1:A:2008:GLU:OE2	1:A:2059:LYS:NZ	2.40	0.50
1:A:3190:LEU:N	1:A:3324:CYS:O	2.45	0.50
1:A:3345:SER:OG	1:A:3348:ILE:O	2.19	0.50
1:A:3615:ASP:C	1:A:3616:LEU:HD22	2.37	0.50
1:A:3083:GLN:OE1	1:A:3106:ASN:ND2	2.44	0.49
1:A:3533:GLN:OE1	1:A:3547:LYS:N	2.40	0.49
1:A:3595:GLN:OE1	1:A:3625:ASN:ND2	2.45	0.49
1:A:3653:ASP:OD1	1:A:3656:LYS:N	2.40	0.49
1:A:3498:GLY:N	1:A:3513:ILE:O	2.44	0.49
1:A:2894:ASN:ND2	1:A:2900:PHE:O	2.45	0.49
1:A:266:LEU:HD13	1:A:279:VAL:HA	1.93	0.49
1:A:816:VAL:O	1:A:820:GLY:N	2.40	0.49
1:A:1917:LEU:O	1:A:1923:HIS:N	2.42	0.49
1:A:3520:TYR:O	1:A:3521:LEU:HD22	2.13	0.49
1:A:4109:GLN:NE2	1:A:4500:GLN:OE1	2.45	0.49
1:A:1398:ASP:OD1	1:A:1399:LEU:N	2.44	0.49
1:A:1915:GLY:O	1:A:1925:GLY:N	2.41	0.49
1:A:3512:THR:HG23	1:A:3512:THR:O	2.11	0.49
1:A:943:HIS:ND1	1:A:952:VAL:HA	2.27	0.49
1:A:3564:GLU:CD	1:A:3564:GLU:O	2.56	0.49
1:A:817:ILE:HD13	1:A:2240:LYS:HB3	1.94	0.49
1:A:1646:ARG:NH1	1:A:1647:ILE:O	2.46	0.49
1:A:3572:GLN:OE1	1:A:3574:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3599:LEU:HD13	1:A:3621:ALA:HA	1.93	0.49
1:A:1266:MET:SD	1:A:1266:MET:N	2.86	0.48
1:A:4359:PHE:O	1:A:4363:ILE:HG23	2.13	0.48
1:A:209:LEU:HD11	1:A:263:GLU:OE1	2.13	0.48
1:A:333:LYS:O	1:A:336:THR:HG22	2.13	0.48
1:A:884:VAL:HG23	1:A:902:ASN:OD1	2.12	0.48
1:A:1887:SER:OG	1:A:1890:LEU:O	2.13	0.48
1:A:2483:SER:OG	1:A:2700:ASP:OD1	2.29	0.48
1:A:2609:LYS:O	1:A:2634:LYS:NZ	2.46	0.48
1:A:840:THR:HG21	1:A:889:ILE:HD13	1.94	0.48
1:A:1971:LEU:C	1:A:1972:LEU:HD22	2.38	0.48
1:A:3576:LEU:O	1:A:3576:LEU:HD12	2.13	0.48
1:A:2213:ASP:OD2	1:A:2219:ARG:HD3	2.14	0.48
1:A:2219:ARG:NH2	1:A:2277:ASP:OD2	2.46	0.48
1:A:1448:VAL:HG13	1:A:1474:LYS:HG2	1.96	0.48
1:A:1587:MET:HE1	1:A:1598:LEU:HD12	1.96	0.48
1:A:594:ALA:HB3	1:A:627:VAL:HG12	1.94	0.48
1:A:872:GLU:OE1	1:A:872:GLU:N	2.46	0.48
1:A:4068:THR:O	1:A:4071:LYS:HG3	2.13	0.48
1:A:4374:LEU:HD11	1:A:4415:LEU:HD12	1.95	0.48
1:A:331:GLU:O	1:A:335:LEU:HG	2.14	0.48
1:A:1345:LEU:O	1:A:1347:GLN:NE2	2.44	0.48
1:A:1439:HIS:NE2	1:A:1441:GLU:OE2	2.47	0.48
1:A:1992:TYR:HD1	1:A:2013:THR:HG1	1.61	0.48
1:A:104:GLY:O	1:A:112:LEU:N	2.47	0.48
1:A:1811:ASN:O	1:A:1840:TYR:OH	2.28	0.48
1:A:914:HIS:N	1:A:925:ILE:O	2.42	0.48
1:A:1166:ALA:N	1:A:1177:GLU:OE2	2.46	0.48
1:A:945:VAL:HG22	1:A:950:THR:HG23	1.96	0.47
1:A:2066:VAL:HG21	1:A:2751:GLU:HB3	1.96	0.47
1:A:3827:LEU:HD12	1:A:3857:VAL:HG23	1.96	0.47
1:A:1731:VAL:HG22	1:A:1736:LEU:HD13	1.95	0.47
1:A:3550:PHE:HB3	1:A:3563:TRP:O	2.14	0.47
1:A:183:TYR:CE2	1:A:212:CYS:HB2	2.49	0.47
1:A:3713:ASN:ND2	1:A:3879:SER:OG	2.47	0.47
1:A:326:LEU:HD21	1:A:366:LEU:HD11	1.96	0.47
1:A:348:PHE:O	1:A:352:VAL:HG22	2.14	0.47
1:A:804:ARG:O	1:A:807:GLN:HG3	2.15	0.47
1:A:928:SER:O	1:A:930:LYS:NZ	2.45	0.47
1:A:2103:ASN:OD1	1:A:2104:ILE:N	2.48	0.47
1:A:2905:ASP:O	1:A:2907:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3572:GLN:OE1	1:A:3573:LEU:N	2.47	0.47
1:A:4245:TYR:CZ	1:A:4249:LEU:HD11	2.49	0.47
1:A:1899:VAL:HG12	1:A:1901:ALA:H	1.80	0.47
1:A:2384:VAL:HG23	1:A:2386:ILE:HG23	1.96	0.47
1:A:3563:TRP:CZ2	1:A:3587:ALA:HB3	2.49	0.47
1:A:1201:PRO:O	1:A:1205:HIS:ND1	2.43	0.47
1:A:2905:ASP:O	1:A:2905:ASP:OD1	2.32	0.47
1:A:505:GLU:HG2	1:A:506:LEU:HD12	1.97	0.47
1:A:1203:SER:HA	1:A:1206:MET:HE2	1.97	0.47
1:A:2973:ASN:C	1:A:2974:LEU:HD22	2.39	0.47
1:A:1415:LYS:O	1:A:1416:ASN:HB2	2.15	0.47
1:A:1572:SER:N	1:A:1587:MET:O	2.39	0.47
1:A:2523:MET:HE2	1:A:2673:ILE:HG13	1.96	0.47
1:A:3026:ASN:OD1	1:A:3027:GLY:N	2.48	0.47
1:A:3827:LEU:HB3	1:A:3828:PRO:HD2	1.97	0.47
1:A:848:ILE:C	1:A:849:SER:HG	2.22	0.47
1:A:1264:GLN:N	1:A:1264:GLN:OE1	2.47	0.47
1:A:1476:LYS:O	1:A:1478:HIS:N	2.49	0.47
1:A:2040:LEU:HG	1:A:2800:LYS:HE3	1.96	0.47
1:A:3462:TYR:OH	1:A:3499:ASP:O	2.30	0.47
1:A:239:ILE:HD13	1:A:267:PHE:CD1	2.51	0.46
1:A:1968:VAL:HG13	1:A:1981:TRP:NE1	2.30	0.46
1:A:102:VAL:HG22	1:A:111:ALA:HB1	1.96	0.46
1:A:1183:ASN:OD1	1:A:1184:VAL:N	2.49	0.46
1:A:2868:GLU:N	1:A:2868:GLU:OE1	2.48	0.46
1:A:934:LYS:O	1:A:934:LYS:HG3	2.14	0.46
1:A:1391:MET:N	1:A:1404:VAL:O	2.42	0.46
1:A:1478:HIS:CE1	1:A:1510:ASN:OD1	2.69	0.46
1:A:1775:SER:N	1:A:1778:LYS:O	2.43	0.46
1:A:2851:GLU:N	1:A:2851:GLU:OE1	2.48	0.46
1:A:367:LEU:HD23	1:A:371:ILE:HD13	1.97	0.46
1:A:1010:GLU:O	1:A:1042:ALA:N	2.49	0.46
1:A:2451:ASN:O	1:A:2455:GLN:OE1	2.33	0.46
1:A:2967:HIS:C	1:A:2968:LEU:HD22	2.41	0.46
1:A:442:LEU:HD12	1:A:487:LEU:HD21	1.97	0.46
1:A:813:ILE:O	1:A:817:ILE:HD12	2.15	0.46
1:A:2381:LEU:O	1:A:2384:VAL:HG22	2.16	0.46
1:A:2985:LYS:C	1:A:2986:LEU:HD22	2.41	0.46
1:A:3070:PHE:C	1:A:3071:LEU:HD22	2.41	0.46
1:A:846:LEU:HD11	1:A:887:MET:HE2	1.97	0.46
1:A:1356:LEU:HD21	1:A:1358:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3382:GLU:N	1:A:3382:GLU:OE1	2.49	0.46
1:A:4127:ASP:O	1:A:4131:GLN:HG2	2.16	0.46
1:A:4441:GLU:O	1:A:4445:HIS:ND1	2.49	0.46
1:A:178:PHE:HA	1:A:186:CYS:O	2.15	0.45
1:A:1536:ARG:HA	1:A:1536:ARG:NE	2.31	0.45
1:A:1557:ASN:OD1	1:A:1558:THR:N	2.48	0.45
1:A:2512:PHE:CE2	1:A:2516:LEU:HD11	2.51	0.45
1:A:2898:LEU:H	1:A:2898:LEU:HD23	1.81	0.45
1:A:2993:ASP:OD1	1:A:2999:HIS:NE2	2.50	0.45
1:A:886:ASN:OD1	1:A:887:MET:N	2.50	0.45
1:A:1210:ARG:NH2	1:A:4545:THR:OG1	2.46	0.45
1:A:2842:GLU:C	1:A:2843:MET:HE2	2.41	0.45
1:A:2880:GLN:OE1	1:A:2880:GLN:N	2.44	0.45
1:A:426:LEU:HD11	1:A:452:TYR:CG	2.50	0.45
1:A:2273:ILE:HD13	1:A:2276:ILE:HD12	1.98	0.45
1:A:3923:PHE:O	1:A:3951:HIS:NE2	2.49	0.45
1:A:3957:GLU:N	1:A:3957:GLU:OE1	2.49	0.45
1:A:371:ILE:H	1:A:371:ILE:HD12	1.81	0.45
1:A:1113:ASP:N	1:A:1117:GLU:O	2.50	0.45
1:A:1206:MET:SD	1:A:1210:ARG:NH2	2.90	0.45
1:A:1371:ALA:HB1	1:A:1391:MET:HE1	1.98	0.45
1:A:1674:GLU:OE1	1:A:1676:GLY:N	2.50	0.45
1:A:1683:LYS:NZ	1:A:1685:THR:OG1	2.49	0.45
1:A:157:LYS:O	1:A:161:ILE:HG12	2.16	0.45
1:A:463:LEU:HD12	1:A:463:LEU:H	1.82	0.45
1:A:1807:ASP:OD1	1:A:1808:LEU:N	2.49	0.45
1:A:45:ARG:NH2	1:A:167:PRO:O	2.37	0.45
1:A:346:ASN:O	1:A:350:LYS:HE3	2.15	0.45
1:A:462:GLU:O	1:A:466:ILE:CD1	2.65	0.45
1:A:1000:ARG:C	1:A:1001:LEU:HD22	2.41	0.45
1:A:2808:PHE:CZ	1:A:2810:ALA:HB2	2.52	0.45
1:A:3224:ASN:C	1:A:3224:ASN:HD22	2.23	0.45
1:A:844:LEU:CB	1:A:889:ILE:HD11	2.46	0.45
1:A:1002:GLU:N	1:A:1002:GLU:OE1	2.49	0.45
1:A:4016:ASP:OD1	1:A:4017:ASP:N	2.46	0.45
1:A:1821:LEU:HD11	1:A:1823:VAL:CG2	2.46	0.45
1:A:1823:VAL:O	1:A:1842:ILE:N	2.45	0.45
1:A:4054:ILE:HB	1:A:4561:ILE:HB	1.99	0.45
1:A:209:LEU:HD12	1:A:241:SER:HB2	1.99	0.45
1:A:1456:ASP:OD1	1:A:1466:SER:OG	2.31	0.45
1:A:1803:TYR:CG	1:A:1803:TYR:O	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2730:ASP:OD1	1:A:2731:PHE:N	2.49	0.45
1:A:2865:ASN:OD1	1:A:2866:THR:N	2.50	0.45
1:A:627:VAL:O	1:A:628:MET:HE2	2.17	0.45
1:A:1534:THR:HG23	1:A:1534:THR:O	2.17	0.45
1:A:3658:HIS:O	1:A:3659:LEU:HD22	2.17	0.45
1:A:3909:VAL:N	1:A:3934:HIS:O	2.44	0.45
1:A:185:ASN:OD1	1:A:185:ASN:C	2.59	0.44
1:A:3594:TRP:CZ3	1:A:3626:THR:HG21	2.52	0.44
1:A:3828:PRO:HA	1:A:3840:LEU:HD12	1.99	0.44
1:A:49:LEU:N	1:A:84:VAL:O	2.51	0.44
1:A:268:LEU:HB2	1:A:269:PRO:HD3	1.98	0.44
1:A:1386:ARG:O	1:A:1387:ALA:C	2.59	0.44
1:A:1517:GLU:N	1:A:1517:GLU:OE1	2.49	0.44
1:A:2635:ASP:OD1	1:A:2638:ASN:ND2	2.50	0.44
1:A:3457:SER:O	1:A:3458:MET:HE2	2.17	0.44
1:A:1463:PRO:HG3	1:A:1492:VAL:HG13	1.97	0.44
1:A:265:HIS:C	1:A:266:LEU:HD22	2.42	0.44
1:A:924:PHE:O	1:A:1015:SER:HA	2.17	0.44
1:A:1635:LYS:HG3	1:A:1636:ILE:HD12	1.99	0.44
1:A:183:TYR:HE2	1:A:212:CYS:HB2	1.81	0.44
1:A:586:ASN:O	1:A:587:GLU:C	2.61	0.44
1:A:813:ILE:HD12	1:A:2240:LYS:CE	2.47	0.44
1:A:925:ILE:HG23	1:A:1013:GLN:NE2	2.33	0.44
1:A:416:ALA:HB2	1:A:444:ALA:HB1	1.98	0.44
1:A:1107:MET:HE2	1:A:1109:HIS:NE2	2.33	0.44
1:A:2040:LEU:HD21	1:A:2800:LYS:HZ2	1.81	0.44
1:A:2523:MET:HE2	1:A:2673:ILE:CG1	2.48	0.44
1:A:3188:ASN:N	1:A:3327:SER:O	2.43	0.44
1:A:3530:VAL:HB	1:A:3550:PHE:CE1	2.53	0.44
1:A:400:ARG:HA	1:A:400:ARG:NE	2.33	0.44
1:A:2171:LEU:HD13	1:A:2315:GLU:HB2	1.98	0.44
1:A:4036:LEU:HB3	1:A:4062:ALA:HB2	2.00	0.44
1:A:405:PRO:HA	1:A:408:ILE:HD12	2.00	0.43
1:A:629:ASP:OD1	1:A:630:PHE:N	2.51	0.43
1:A:755:MET:SD	1:A:2205:ILE:HG13	2.58	0.43
1:A:3258:VAL:HG13	1:A:3285:ILE:HG22	1.99	0.43
1:A:379:LEU:HD21	1:A:397:TRP:CE2	2.54	0.43
1:A:3153:TRP:NE1	1:A:3165:THR:HA	2.34	0.43
1:A:4395:GLY:O	1:A:4398:VAL:HG22	2.18	0.43
1:A:603:SER:CB	1:A:608:ILE:HG21	2.47	0.43
1:A:627:VAL:O	1:A:627:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ASN:N	1:A:939:GLY:O	2.51	0.43
1:A:1231:ILE:HG23	1:A:1255:LEU:HB3	2.00	0.43
1:A:1630:ILE:O	1:A:1631:LEU:HD22	2.18	0.43
1:A:1631:LEU:HD13	1:A:1640:ALA:HA	2.00	0.43
1:A:1890:LEU:HD12	1:A:1914:ASN:O	2.18	0.43
1:A:1971:LEU:HD12	1:A:2739:PRO:HD3	2.00	0.43
1:A:3685:TRP:O	1:A:3689:LYS:N	2.52	0.43
1:A:3937:GLU:N	1:A:3937:GLU:OE1	2.51	0.43
1:A:847:GLN:C	1:A:847:GLN:CD	2.86	0.43
1:A:1773:ILE:HD13	1:A:1779:PHE:HB2	2.00	0.43
1:A:4432:PHE:O	1:A:4436:LEU:HD23	2.18	0.43
1:A:424:GLN:O	1:A:427:ARG:N	2.51	0.43
1:A:845:GLN:C	1:A:889:ILE:HD12	2.44	0.43
1:A:993:TYR:N	1:A:994:PRO:HD2	2.34	0.43
1:A:1955:VAL:HG12	1:A:1956:SER:N	2.33	0.43
1:A:1971:LEU:HD12	1:A:2739:PRO:CD	2.48	0.43
1:A:1216:VAL:HG23	1:A:1219:THR:HG22	1.99	0.43
1:A:1614:LEU:N	1:A:1629:ASP:O	2.44	0.43
1:A:1641:HIS:ND1	1:A:1657:THR:O	2.50	0.43
1:A:2001:THR:HG22	1:A:2002:LYS:N	2.34	0.43
1:A:3495:SER:OG	1:A:3497:LYS:NZ	2.51	0.43
1:A:360:ASP:OD1	1:A:389:GLN:HB3	2.18	0.43
1:A:1136:GLU:N	1:A:1136:GLU:OE1	2.52	0.43
1:A:2872:GLY:N	1:A:2886:ASN:OD1	2.41	0.43
1:A:2905:ASP:C	1:A:2906:LEU:HD22	2.43	0.43
1:A:326:LEU:HD21	1:A:366:LEU:HD21	2.01	0.43
1:A:588:GLN:NE2	1:A:589:VAL:HG23	2.33	0.43
1:A:1926:GLN:OE1	1:A:1927:LEU:N	2.52	0.43
1:A:2565:ALA:O	1:A:2569:SER:N	2.52	0.43
1:A:2905:ASP:O	1:A:2906:LEU:HD22	2.19	0.43
1:A:3197:ILE:O	1:A:3201:ILE:HG12	2.19	0.43
1:A:3410:HIS:ND1	1:A:3427:THR:HG23	2.33	0.43
1:A:4089:HIS:HB3	1:A:4095:LEU:O	2.18	0.43
1:A:65:PRO:HD3	1:A:279:VAL:HG12	2.01	0.43
1:A:2211:SER:O	1:A:2215:HIS:ND1	2.52	0.43
1:A:4219:MET:SD	1:A:4219:MET:C	3.01	0.43
1:A:4422:HIS:O	1:A:4426:ILE:HG12	2.19	0.43
1:A:763:LYS:HE2	1:A:2208:LYS:HE3	2.01	0.43
1:A:2772:ASP:OD1	1:A:2796:LYS:HB2	2.19	0.43
1:A:3587:ALA:HB1	1:A:3600:VAL:HA	1.99	0.43
1:A:3602:VAL:HG23	1:A:3603:HIS:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3827:LEU:O	1:A:3828:PRO:C	2.61	0.43
1:A:123:ALA:HA	1:A:126:MET:HE2	2.00	0.42
1:A:896:ARG:HE	1:A:946:SER:C	2.27	0.42
1:A:1384:SER:HB3	1:A:1411:THR:HG23	2.00	0.42
1:A:1588:ASP:N	1:A:1588:ASP:OD1	2.51	0.42
1:A:1786:LEU:O	1:A:1787:GLN:NE2	2.52	0.42
1:A:2251:ASN:C	1:A:2251:ASN:HD22	2.24	0.42
1:A:3466:SER:O	1:A:3470:TYR:N	2.52	0.42
1:A:876:LYS:HA	1:A:910:GLY:HA3	2.02	0.42
1:A:3841:ASN:OD1	1:A:3852:LEU:N	2.53	0.42
1:A:3912:VAL:C	1:A:3913:LEU:HD22	2.45	0.42
1:A:4280:ALA:HA	1:A:4283:VAL:HG12	2.01	0.42
1:A:361:GLU:HA	1:A:364:THR:HG22	2.01	0.42
1:A:367:LEU:O	1:A:371:ILE:HD12	2.20	0.42
1:A:946:SER:O	1:A:947:THR:C	2.61	0.42
1:A:2988:ILE:CD1	1:A:3004:ALA:HB3	2.50	0.42
1:A:751:VAL:HG23	1:A:752:ASN:N	2.35	0.42
1:A:1775:SER:HB3	1:A:1778:LYS:HB3	2.01	0.42
1:A:2819:ILE:HG13	1:A:2821:PRO:HD3	2.01	0.42
1:A:174:LYS:O	1:A:175:GLN:C	2.62	0.42
1:A:496:GLY:O	1:A:500:GLU:HG3	2.19	0.42
1:A:3317:LEU:HD12	1:A:3317:LEU:C	2.45	0.42
1:A:3679:VAL:HG23	1:A:3680:TYR:N	2.35	0.42
1:A:4116:TYR:CD1	1:A:4488:ILE:HG22	2.54	0.42
1:A:200:ALA:HB3	1:A:203:ILE:HD11	2.02	0.42
1:A:403:ALA:O	1:A:408:ILE:HD11	2.20	0.42
1:A:588:GLN:HB2	1:A:634:SER:H	1.84	0.42
1:A:755:MET:CG	1:A:2205:ILE:HG13	2.50	0.42
1:A:759:GLU:HG2	1:A:2208:LYS:HE2	2.02	0.42
1:A:1543:SER:OG	1:A:1562:LYS:NZ	2.45	0.42
1:A:4474:GLN:O	1:A:4477:ILE:HG22	2.19	0.42
1:A:363:VAL:O	1:A:367:LEU:N	2.50	0.42
1:A:512:LYS:O	1:A:516:SER:N	2.53	0.42
1:A:910:GLY:O	1:A:911:LEU:HD22	2.19	0.42
1:A:108:GLU:HG2	1:A:110:LYS:HG2	2.02	0.42
1:A:779:ILE:CG1	1:A:784:LEU:HD11	2.50	0.42
1:A:823:ASN:O	1:A:860:ALA:N	2.47	0.42
1:A:993:TYR:CG	1:A:994:PRO:HD3	2.54	0.42
1:A:4356:LEU:HD23	1:A:4430:SER:HB2	2.00	0.42
1:A:3336:ASN:OD1	1:A:3337:ILE:N	2.53	0.41
1:A:3590:GLU:O	1:A:3591:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3650:LEU:C	1:A:3650:LEU:HD23	2.45	0.41
1:A:174:LYS:O	1:A:174:LYS:HD3	2.20	0.41
1:A:1054:ASN:O	1:A:1058:MET:N	2.53	0.41
1:A:1204:LEU:HD13	1:A:1263:LEU:HB2	2.01	0.41
1:A:2190:ASP:OD1	1:A:2191:LEU:HD12	2.20	0.41
1:A:1115:LYS:NZ	1:A:1116:GLU:OE1	2.37	0.41
1:A:1587:MET:CE	1:A:1598:LEU:HD12	2.51	0.41
1:A:4126:ILE:O	1:A:4129:ARG:HG2	2.20	0.41
1:A:4356:LEU:HD21	1:A:4429:ALA:HB3	2.03	0.41
1:A:379:LEU:O	1:A:383:VAL:HG22	2.19	0.41
1:A:807:GLN:HA	1:A:2232:PHE:CD1	2.55	0.41
1:A:1057:SER:C	1:A:1058:MET:SD	3.03	0.41
1:A:4218:THR:O	1:A:4222:ARG:HG2	2.20	0.41
1:A:4326:ILE:O	1:A:4329:ILE:HG22	2.20	0.41
1:A:185:ASN:O	1:A:186:CYS:SG	2.79	0.41
1:A:439:ARG:NH2	1:A:791:ASP:OD1	2.53	0.41
1:A:972:GLY:O	1:A:973:LEU:HD22	2.20	0.41
1:A:1066:ILE:HB	1:A:1071:VAL:HB	2.03	0.41
1:A:1200:TYR:CZ	1:A:1204:LEU:HD11	2.56	0.41
1:A:1415:LYS:O	1:A:1415:LYS:HD3	2.20	0.41
1:A:1785:ASN:C	1:A:1786:LEU:HD22	2.45	0.41
1:A:3635:ASN:OD1	1:A:3636:GLU:N	2.54	0.41
1:A:341:ASN:HA	1:A:344:ARG:HG2	2.03	0.41
1:A:1215:ARG:HE	1:A:1220:ASP:HA	1.86	0.41
1:A:2611:THR:HG22	1:A:2630:GLN:NE2	2.35	0.41
1:A:3076:LEU:HD12	1:A:3084:GLN:O	2.21	0.41
1:A:3475:GLY:HA3	1:A:3500:VAL:HA	2.02	0.41
1:A:4486:LYS:NZ	1:A:4490:ASP:OD2	2.44	0.41
1:A:535:GLU:O	1:A:536:PRO:C	2.63	0.41
1:A:975:TYR:HA	1:A:1005:LEU:HD13	2.02	0.41
1:A:1250:THR:OG1	1:A:1270:ASP:OD2	2.36	0.41
1:A:3508:GLU:O	1:A:3539:ASP:N	2.49	0.41
1:A:3922:GLN:N	1:A:3922:GLN:CD	2.79	0.41
1:A:3937:GLU:HG2	1:A:3937:GLU:O	2.21	0.41
1:A:4528:TYR:CE1	1:A:4532:LEU:HD11	2.56	0.41
1:A:341:ASN:OD1	1:A:341:ASN:O	2.39	0.41
1:A:352:VAL:O	1:A:355:LEU:HB3	2.21	0.41
1:A:416:ALA:CB	1:A:444:ALA:HB1	2.50	0.41
1:A:424:GLN:C	1:A:428:GLU:OE1	2.64	0.41
1:A:1097:GLN:HB3	1:A:1100:LYS:HA	2.03	0.41
1:A:1116:GLU:O	1:A:1141:TRP:N	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:TYR:HB3	1:A:1201:PRO:HD3	2.02	0.41
1:A:1596:ALA:HB3	1:A:1619:LEU:HD21	2.02	0.41
1:A:1665:LEU:HD12	1:A:1689:ARG:O	2.20	0.41
1:A:2436:VAL:O	1:A:2439:THR:OG1	2.29	0.41
1:A:2764:ILE:HD13	1:A:2771:LEU:HB3	2.02	0.41
1:A:3564:GLU:OE1	1:A:3584:THR:CG2	2.69	0.41
1:A:4482:ILE:HG23	1:A:4483:ALA:N	2.36	0.41
1:A:115:LYS:NZ	1:A:119:SER:OG	2.42	0.41
1:A:885:THR:HB	1:A:901:MET:HB2	2.01	0.41
1:A:1416:ASN:O	1:A:1444:GLY:N	2.53	0.41
1:A:3004:ALA:HB1	1:A:3017:PHE:CE2	2.56	0.41
1:A:4038:ILE:HD13	1:A:4062:ALA:CB	2.48	0.41
1:A:4224:VAL:HG21	1:A:4288:GLN:OE1	2.21	0.41
1:A:463:LEU:HB3	1:A:502:LEU:CD1	2.51	0.40
1:A:1462:GLY:O	1:A:1463:PRO:C	2.63	0.40
1:A:2336:ALA:O	1:A:2340:LYS:HG2	2.21	0.40
1:A:3215:ALA:O	1:A:3219:VAL:HG23	2.21	0.40
1:A:3593:PRO:O	1:A:3594:TRP:HB3	2.21	0.40
1:A:469:TYR:O	1:A:473:GLN:HG2	2.22	0.40
1:A:832:MET:HE3	1:A:852:GLY:HA3	2.03	0.40
1:A:833:GLU:OE2	1:A:835:ALA:N	2.55	0.40
1:A:1389:TYR:HE2	1:A:1404:VAL:HG12	1.86	0.40
1:A:3891:SER:OG	1:A:3894:TYR:O	2.14	0.40
1:A:3980:SER:O	1:A:3983:PHE:O	2.40	0.40
1:A:1287:TYR:HD1	1:A:1356:LEU:HA	1.86	0.40
1:A:1641:HIS:C	1:A:1642:LYS:HD3	2.46	0.40
1:A:1644:THR:O	1:A:1645:LEU:HD22	2.22	0.40
1:A:2164:LYS:HB2	1:A:2322:ILE:HD13	2.01	0.40
1:A:2800:LYS:HD3	1:A:2800:LYS:N	2.36	0.40
1:A:51:LYS:HA	1:A:82:LEU:O	2.22	0.40
1:A:832:MET:SD	1:A:852:GLY:N	2.95	0.40
1:A:2055:VAL:O	1:A:2763:LYS:N	2.51	0.40
1:A:2408:SER:O	1:A:2412:PHE:N	2.40	0.40
1:A:3226:THR:O	1:A:3227:LYS:C	2.64	0.40
1:A:3653:ASP:O	1:A:3712:LYS:NZ	2.44	0.40
1:A:4084:TYR:CE1	1:A:4088:TYR:HE2	2.38	0.40
1:A:100:LYS:HB3	1:A:113:LEU:HB3	2.02	0.40
1:A:484:TYR:O	1:A:488:ILE:HG12	2.22	0.40
1:A:575:ASN:HA	1:A:618:ALA:HB1	2.03	0.40
1:A:1434:ASN:N	1:A:1456:ASP:O	2.44	0.40
1:A:2059:LYS:HB2	1:A:2759:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2971:ASN:OD1	1:A:2972:GLN:N	2.55	0.40
1:A:3519:THR:HG23	1:A:3528:SER:OG	2.21	0.40
1:A:3957:GLU:OE1	1:A:3979:LYS:NZ	2.50	0.40

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	4524/4563 (99%)	4338 (96%)	182 (4%)	4 (0%)	48 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3828	PRO
1	A	1477	GLN
1	A	3906	ALA
1	A	1804	ASN

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	4051/4080 (99%)	4051 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	402	HIS
1	A	1056	GLN
1	A	1209	ASN
1	A	1349	GLN
1	A	1368	ASN
1	A	1377	ASN
1	A	1414	HIS
1	A	1416	ASN
1	A	1478	HIS
1	A	1489	GLN
1	A	1580	ASN
1	A	1953	HIS
1	A	2279	GLN
1	A	2287	GLN
1	A	2353	GLN
1	A	2382	GLN
1	A	2497	GLN
1	A	2908	ASN
1	A	2942	HIS
1	A	3051	ASN
1	A	3073	ASN
1	A	3167	GLN
1	A	3207	HIS
1	A	3213	ASN
1	A	3224	ASN
1	A	3308	HIS
1	A	3420	ASN
1	A	3701	HIS
1	A	3929	ASN
1	A	4375	GLN
1	A	4449	GLN

5.3.3 RNA ⓘ

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](#)

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.

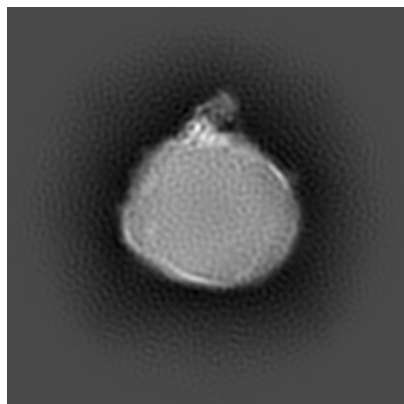
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47801. These allow visual inspection of the internal detail of the map and identification of artifacts.

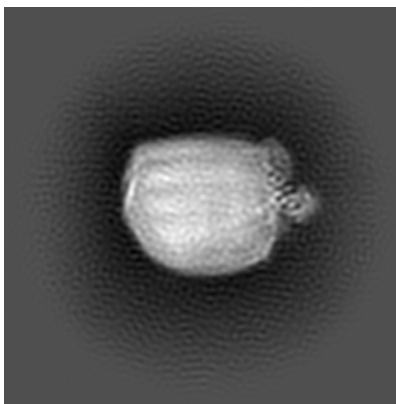
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

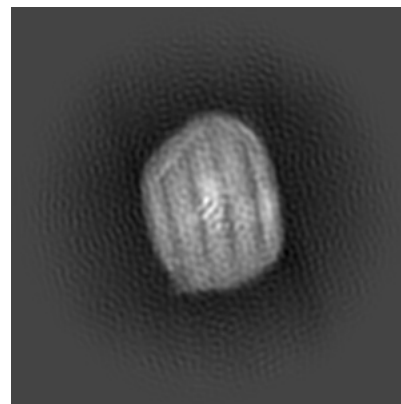
6.1.1 Primary map



X

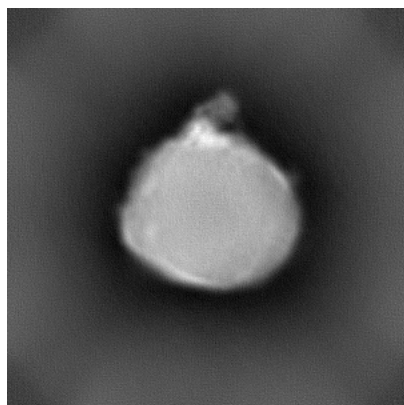


Y

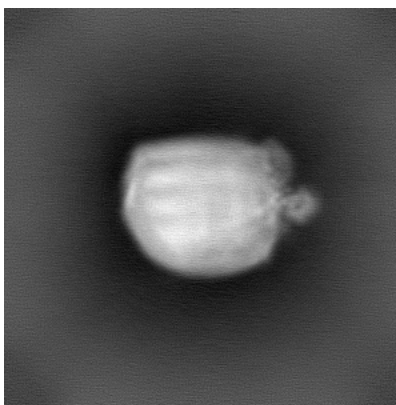


Z

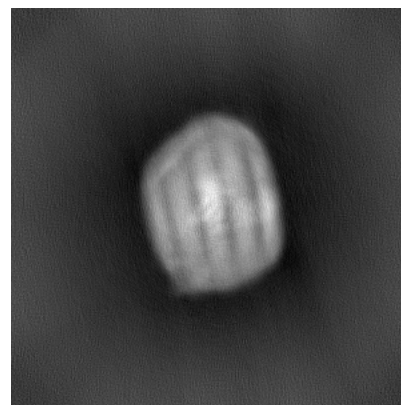
6.1.2 Raw map



X



Y

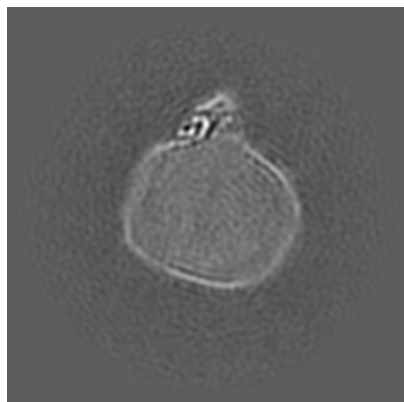


Z

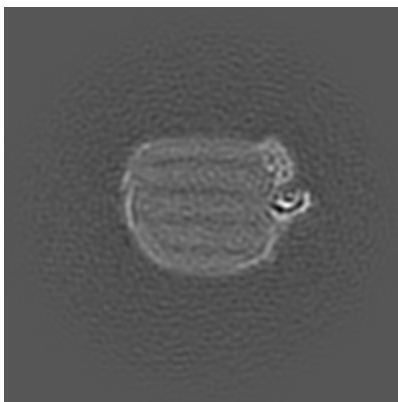
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

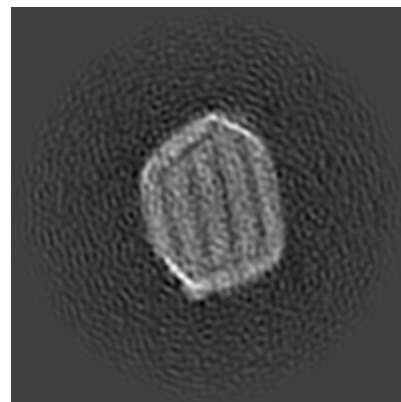
6.2.1 Primary map



X Index: 225

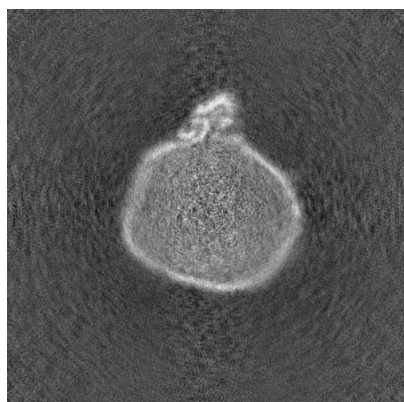


Y Index: 225

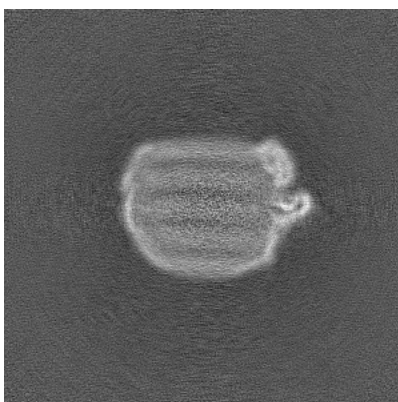


Z Index: 225

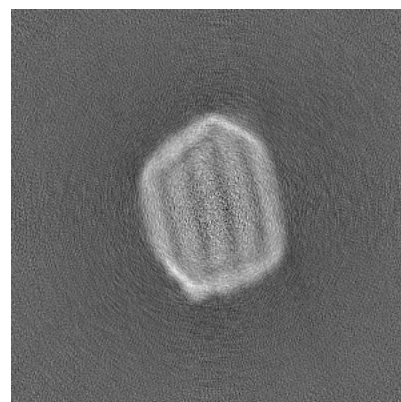
6.2.2 Raw map



X Index: 225



Y Index: 225

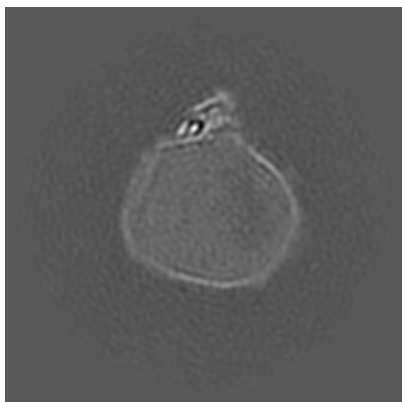


Z Index: 225

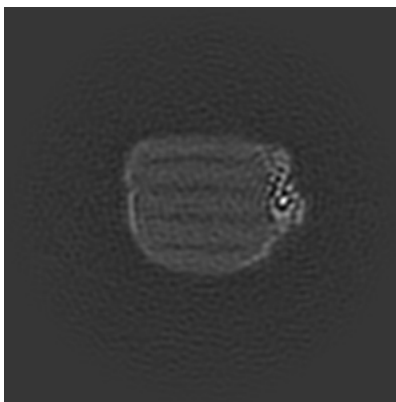
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

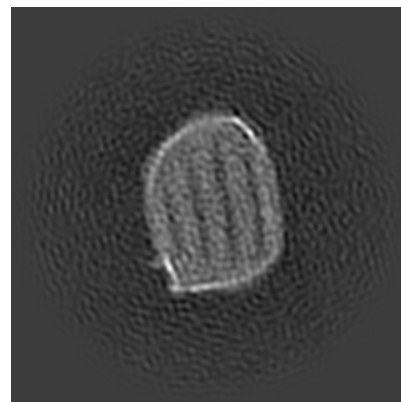
6.3.1 Primary map



X Index: 230

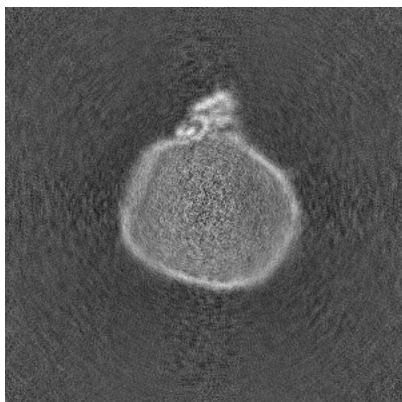


Y Index: 213

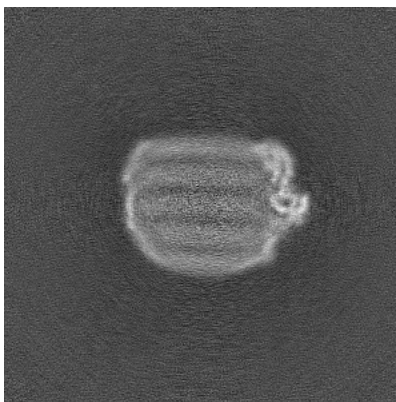


Z Index: 196

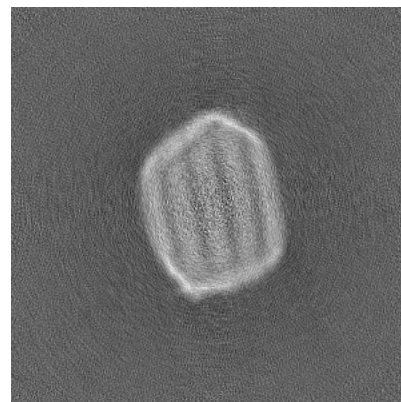
6.3.2 Raw map



X Index: 227



Y Index: 219

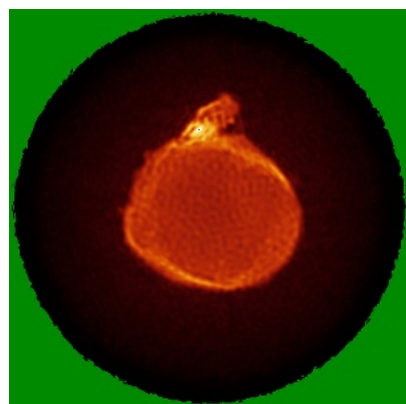


Z Index: 219

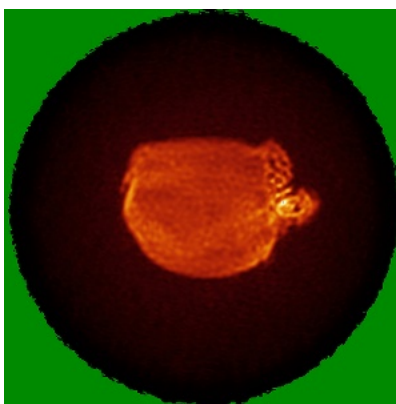
The images above show the largest variance slices of the map in three orthogonal directions.

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

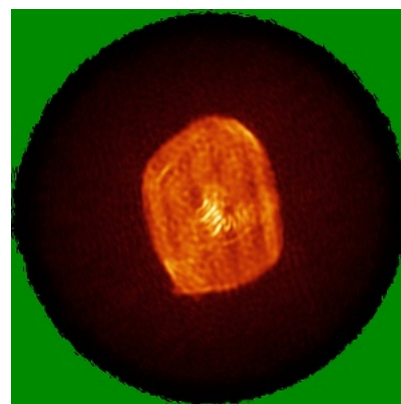
6.4.1 Primary map



X

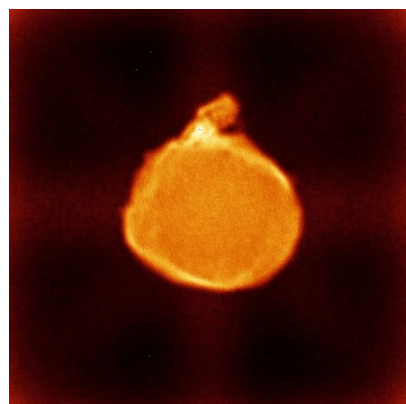


Y

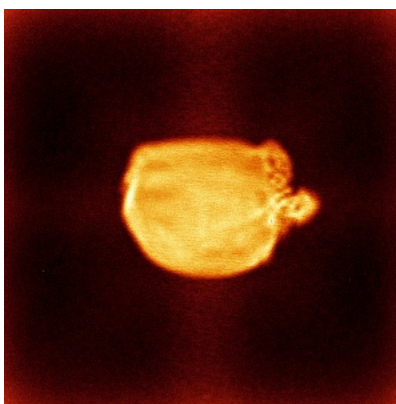


Z

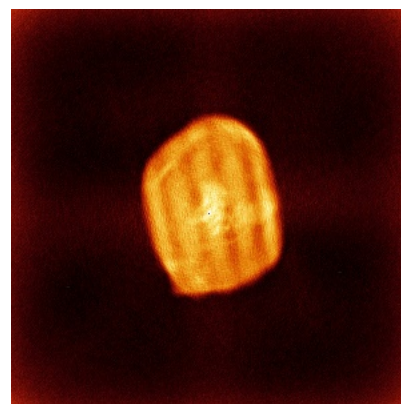
6.4.2 Raw map



X



Y

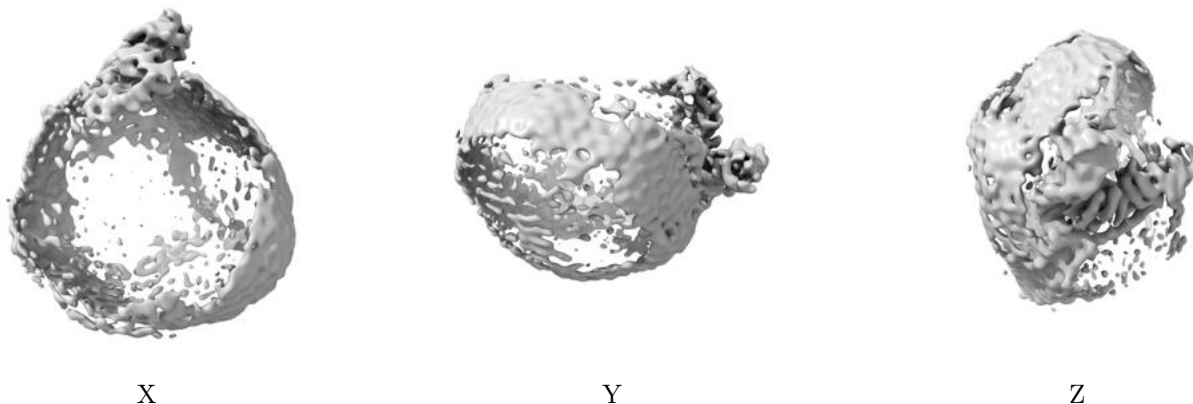


Z

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.

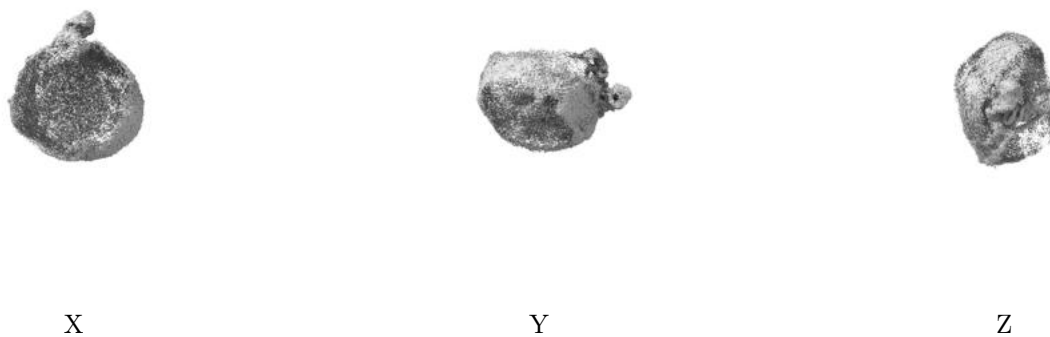
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.182. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

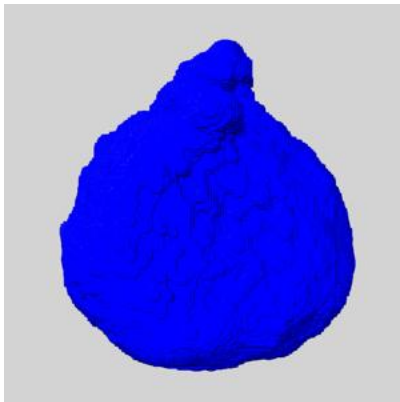
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

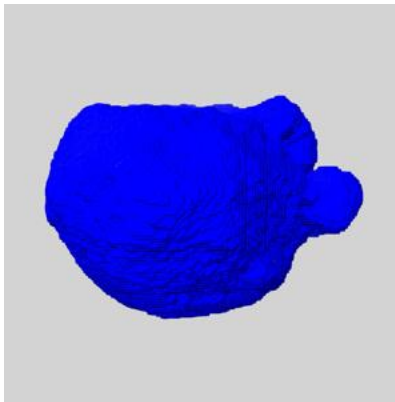
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

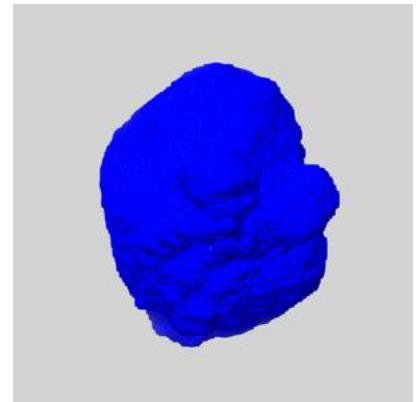
6.6.1 emd_47801_msk_1.map [i](#)



X



Y

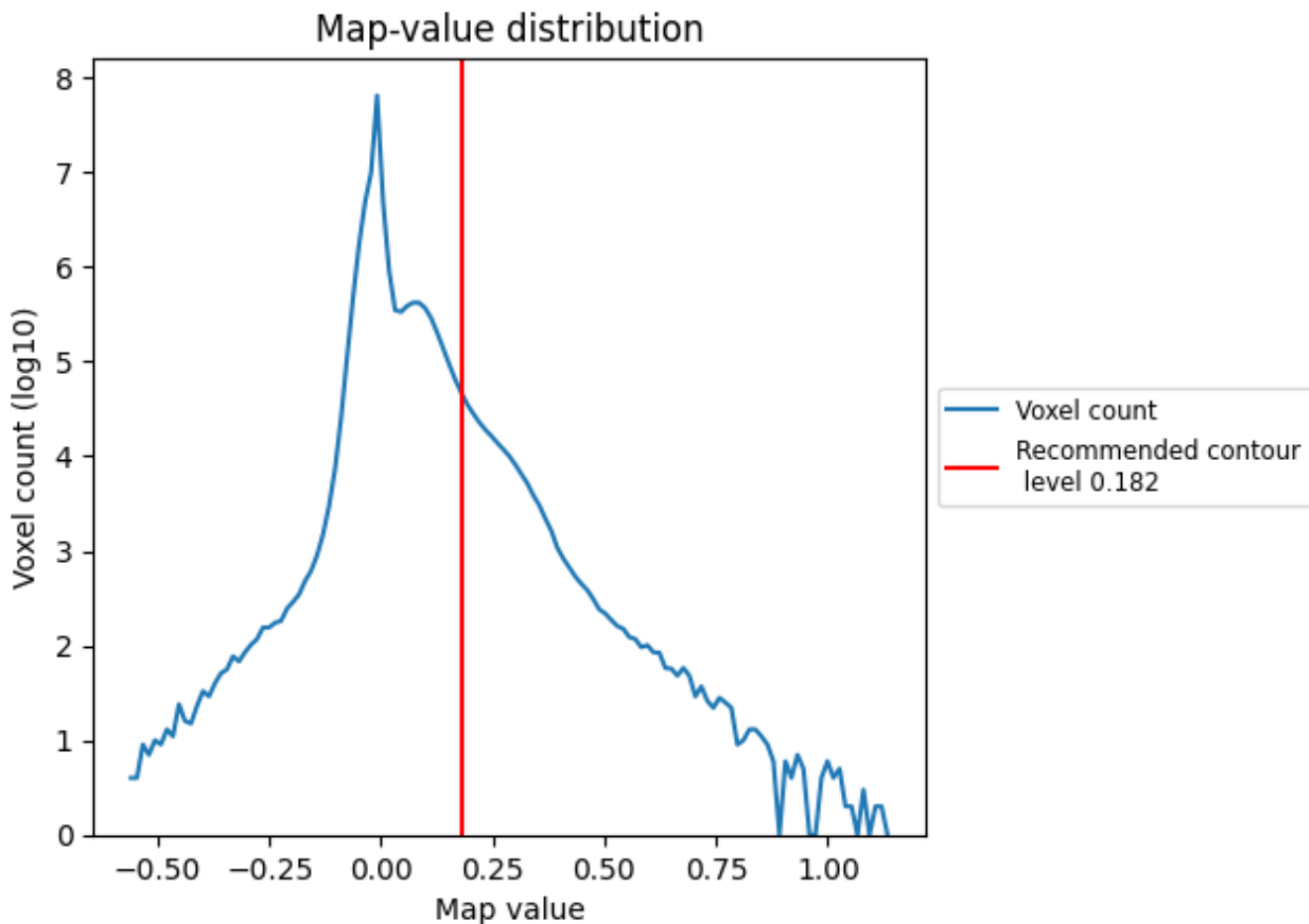


Z

7 Map analysis [i](#)

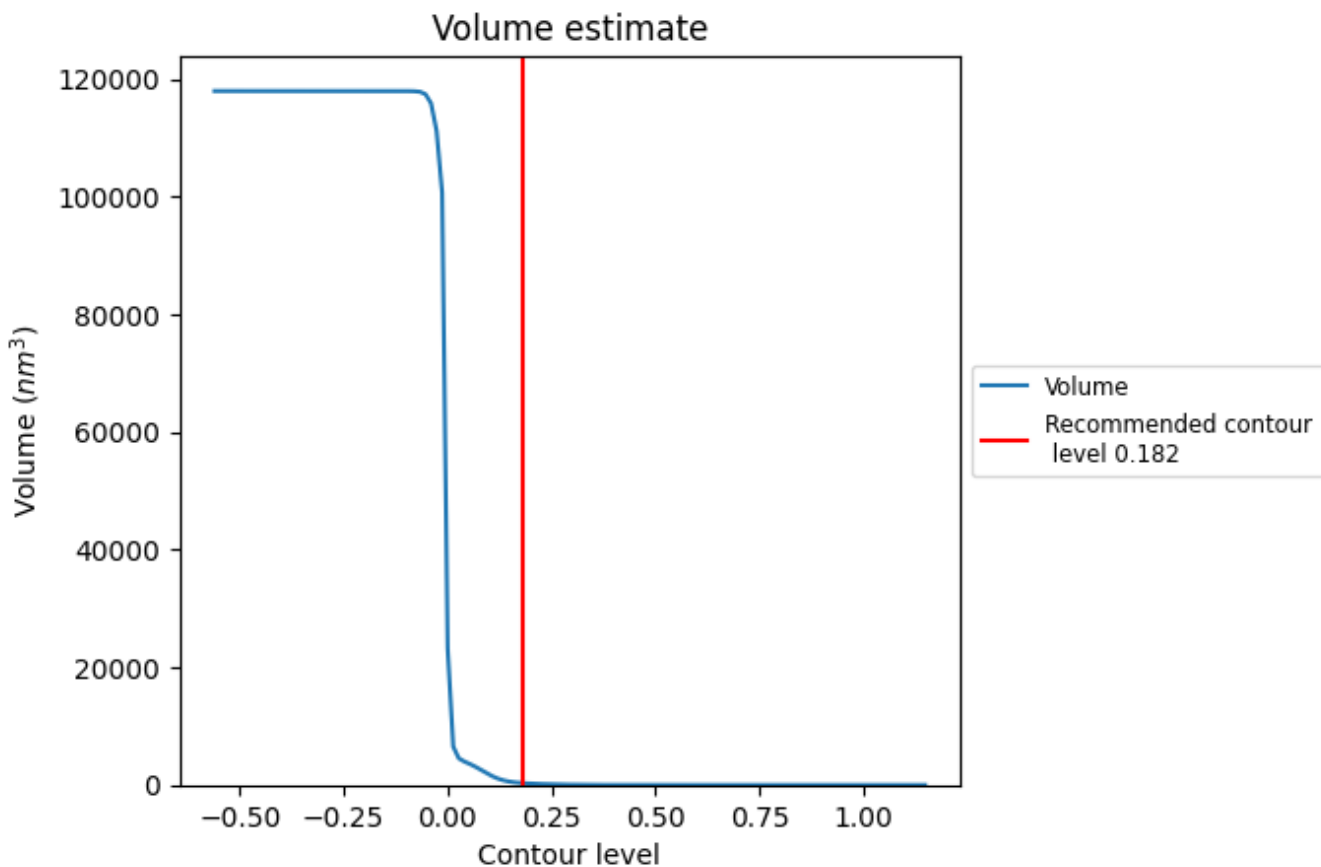
This section contains the results of statistical analysis of the map.

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.

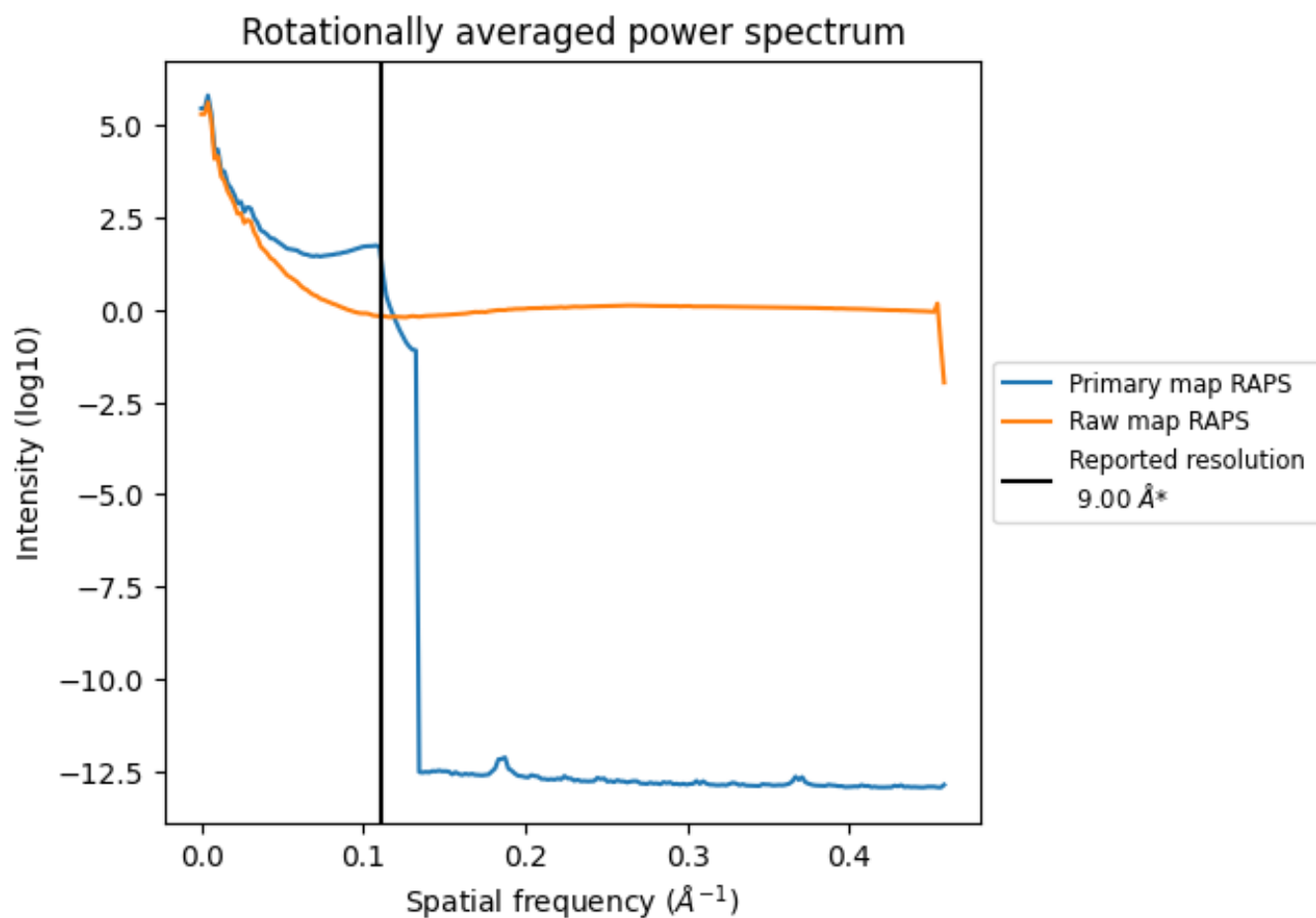
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 304 nm^3 ; this corresponds to an approximate mass of 275 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](#)

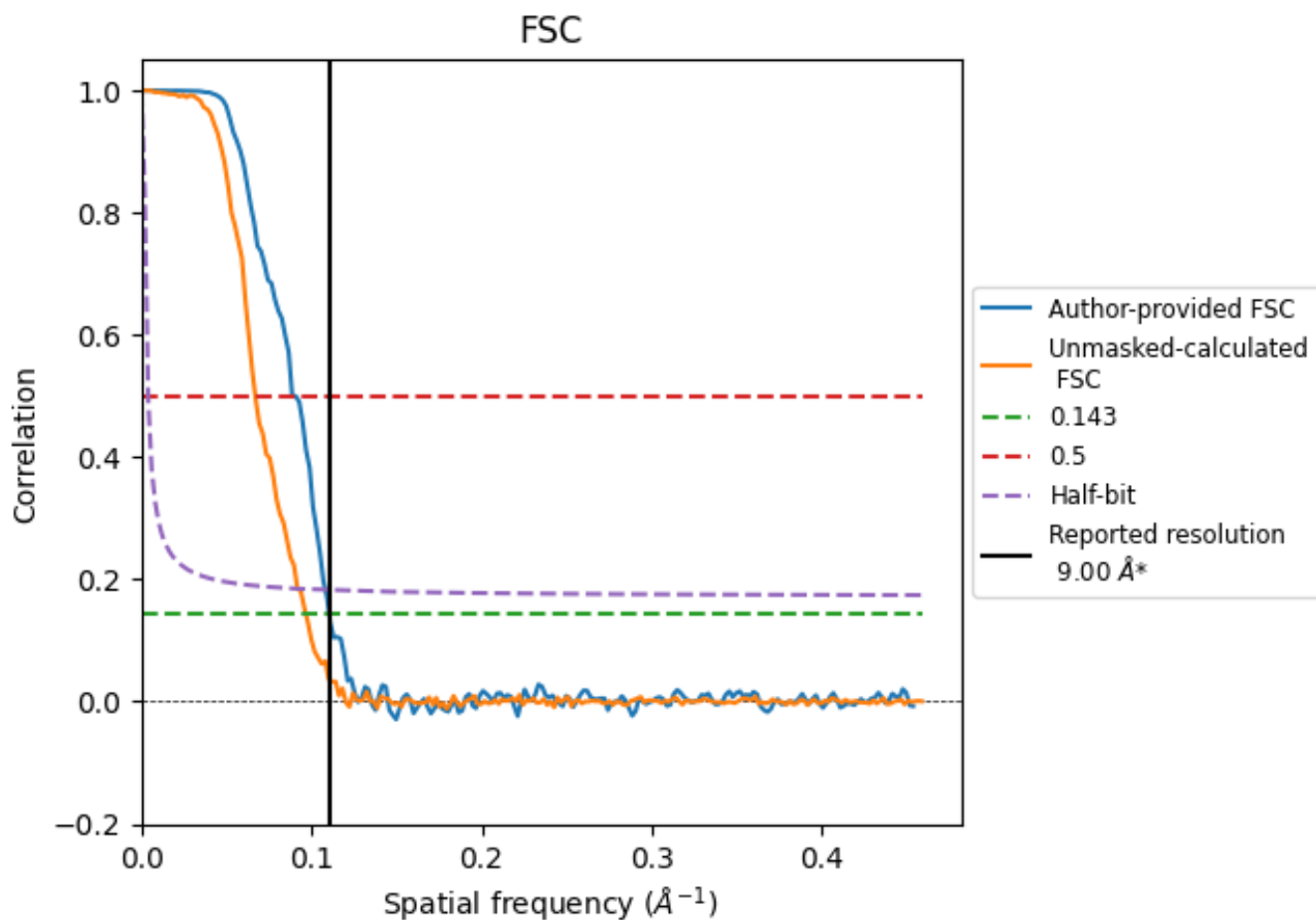


*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.111 Å⁻¹

8.2 Resolution estimates [i](#)

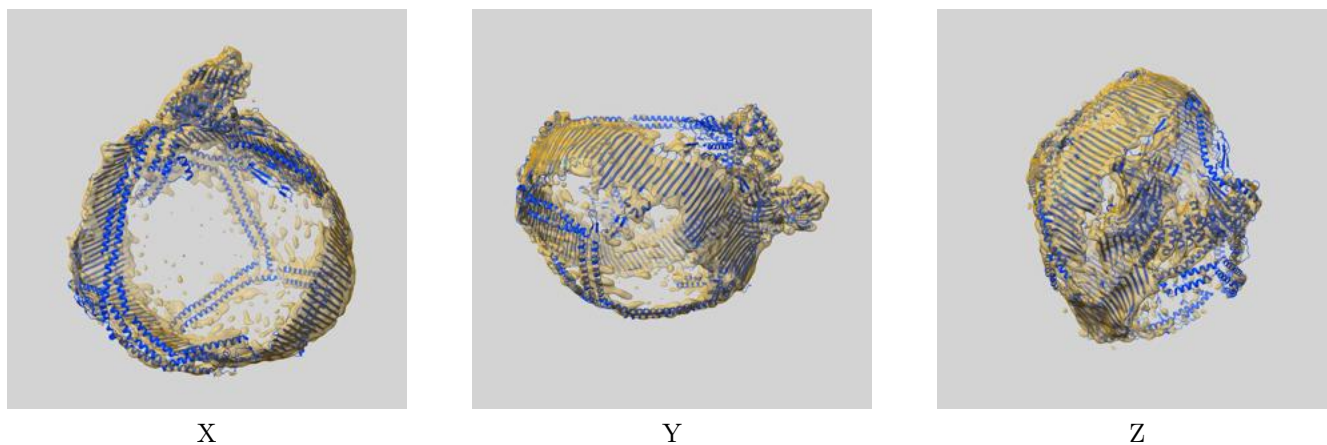
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.00	-	-
Author-provided FSC curve	9.06	11.27	9.24
Unmasked-calculated*	10.34	14.93	10.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 10.34 differs from the reported value 9.0 by more than 10 %

9 Map-model fit [i](#)

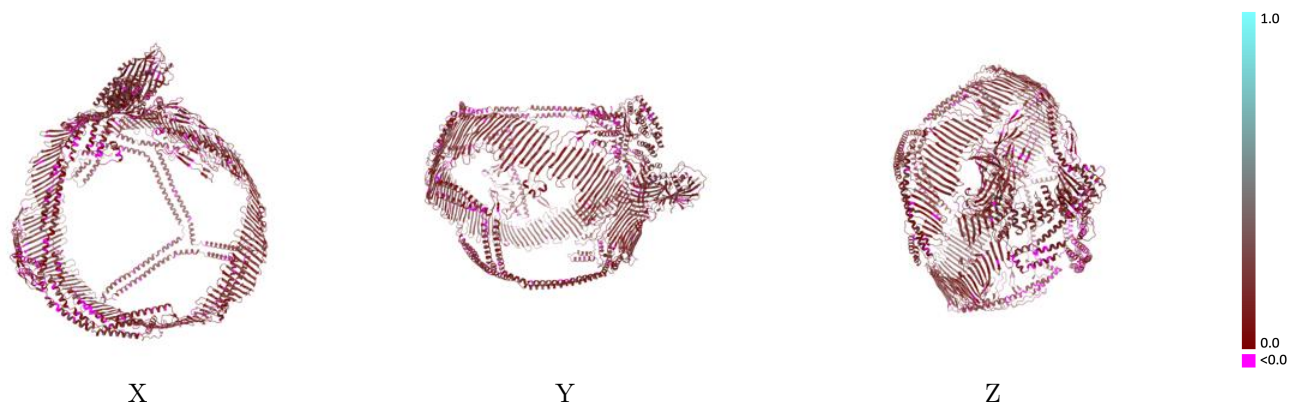
This section contains information regarding the fit between EMDB map EMD-47801 and PDB model 9EA7. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



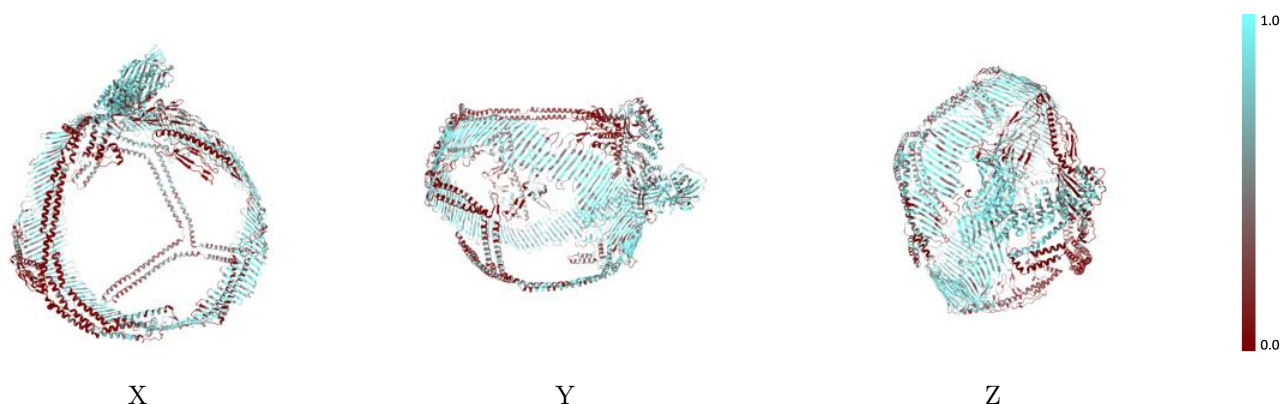
The images above show the 3D surface view of the map at the recommended contour level 0.182 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



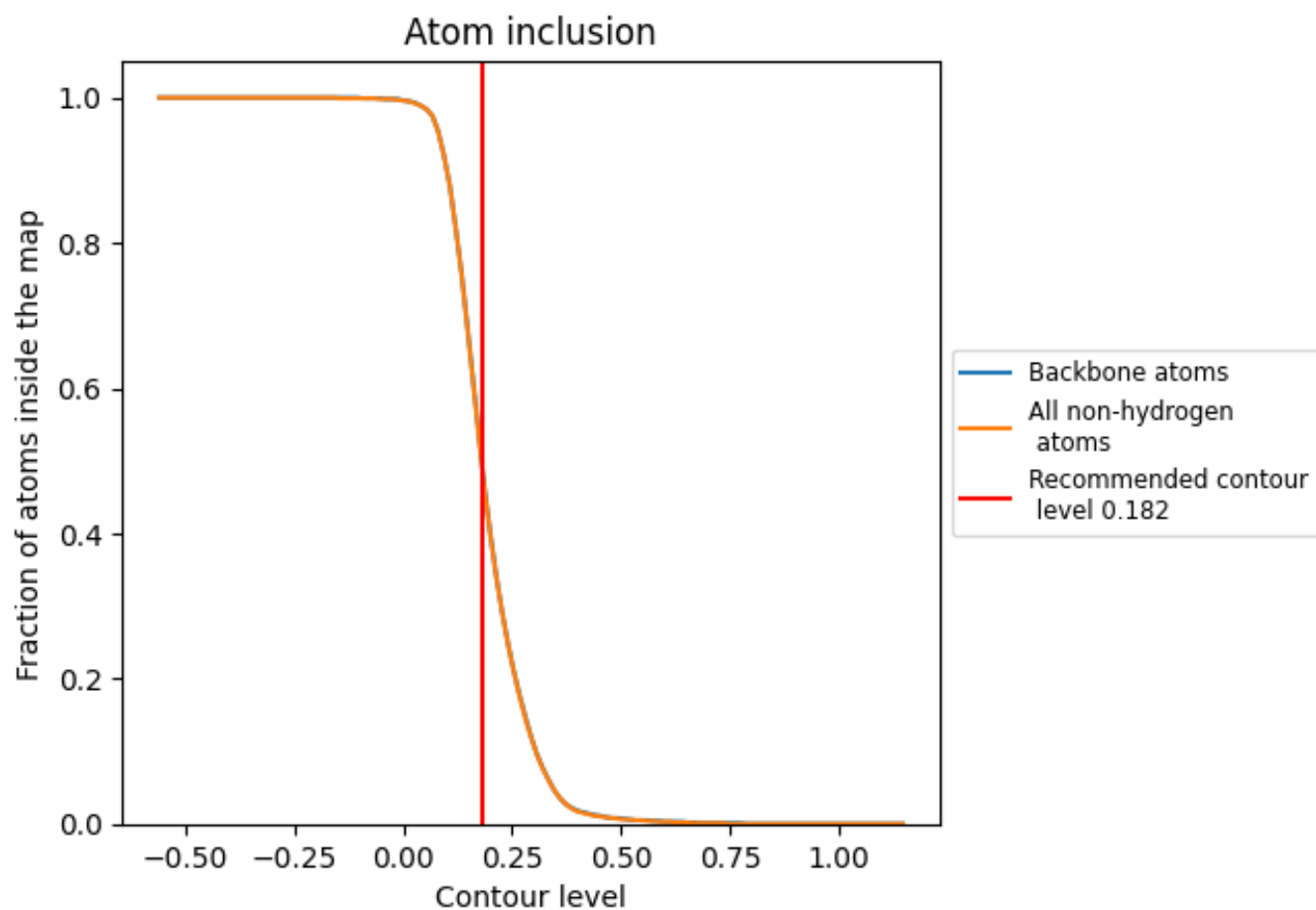
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.182).





9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 49% 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 (0.182) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4860	 0.1580
A	 0.4930	 0.1580

