



Full wwPDB EM Validation Report ⓘ

Jun 4, 2026 – 02:16 PM EDT

PDB ID : 9YRP / pdb_00009yrp
EMDB ID : EMD-73373
Title : Full-length human VPS13C in complex with calmodulin from the CryoEM composite map
Authors : Li, D.; Reinisch, K.M.
Deposited on : 2025-10-16
Resolution : 4.13 Å(reported)

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

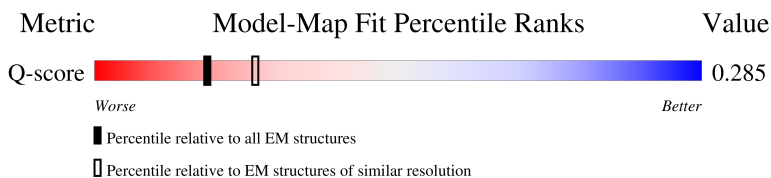
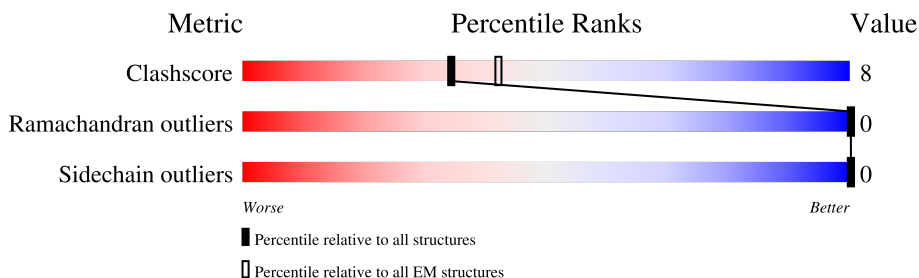
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.13 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	5607 (3.63 - 4.63)

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	149	<div> <div>52%</div> <div>91%</div> <div>8%</div> </div>
2	B	3777	<div> <div>15%</div> <div>64%</div> <div>14%</div> <div>22%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24677 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	148	Total	C	N	O	S	0	0
			1166	714	188	255	9		

- Molecule 2 is a protein called Intermembrane lipid transfer protein VPS13C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	2944	Total	C	N	O	S	0	0
			23511	15092	3941	4364	114		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3754	LEU	-	expression tag	UNP Q709C8
B	3755	GLU	-	expression tag	UNP Q709C8
B	3756	ASP	-	expression tag	UNP Q709C8
B	3757	TYR	-	expression tag	UNP Q709C8
B	3758	LYS	-	expression tag	UNP Q709C8
B	3759	ASP	-	expression tag	UNP Q709C8
B	3760	HIS	-	expression tag	UNP Q709C8
B	3761	ASP	-	expression tag	UNP Q709C8
B	3762	GLY	-	expression tag	UNP Q709C8
B	3763	ASP	-	expression tag	UNP Q709C8
B	3764	TYR	-	expression tag	UNP Q709C8
B	3765	LYS	-	expression tag	UNP Q709C8
B	3766	ASP	-	expression tag	UNP Q709C8
B	3767	HIS	-	expression tag	UNP Q709C8
B	3768	ASP	-	expression tag	UNP Q709C8
B	3769	ILE	-	expression tag	UNP Q709C8
B	3770	ASP	-	expression tag	UNP Q709C8
B	3771	TYR	-	expression tag	UNP Q709C8
B	3772	LYS	-	expression tag	UNP Q709C8
B	3773	ASP	-	expression tag	UNP Q709C8
B	3774	ASP	-	expression tag	UNP Q709C8

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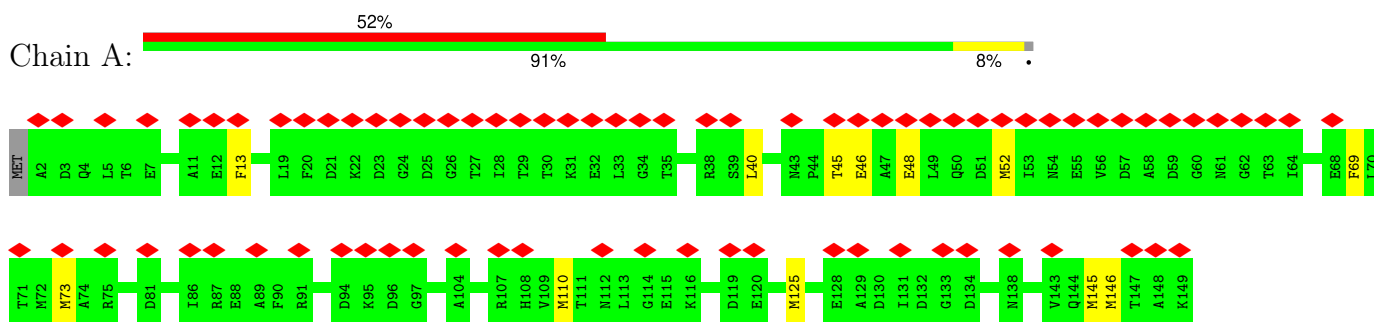
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Chain	Residue	Modelled	Actual	Comment	Reference
B	3775	ASP	-	expression tag	UNP Q709C8
B	3776	ASP	-	expression tag	UNP Q709C8
B	3777	LYS	-	expression tag	UNP Q709C8

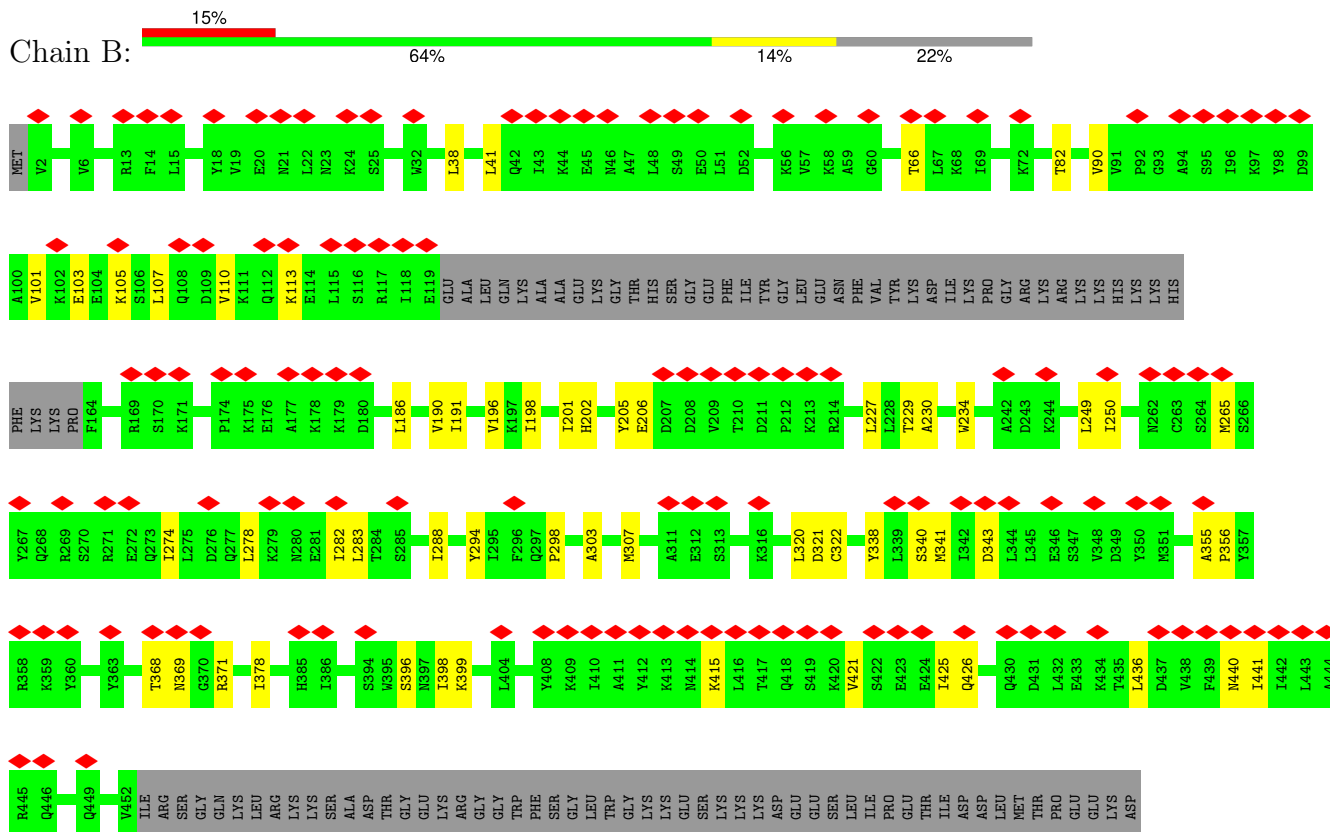
3 Residue-property plots

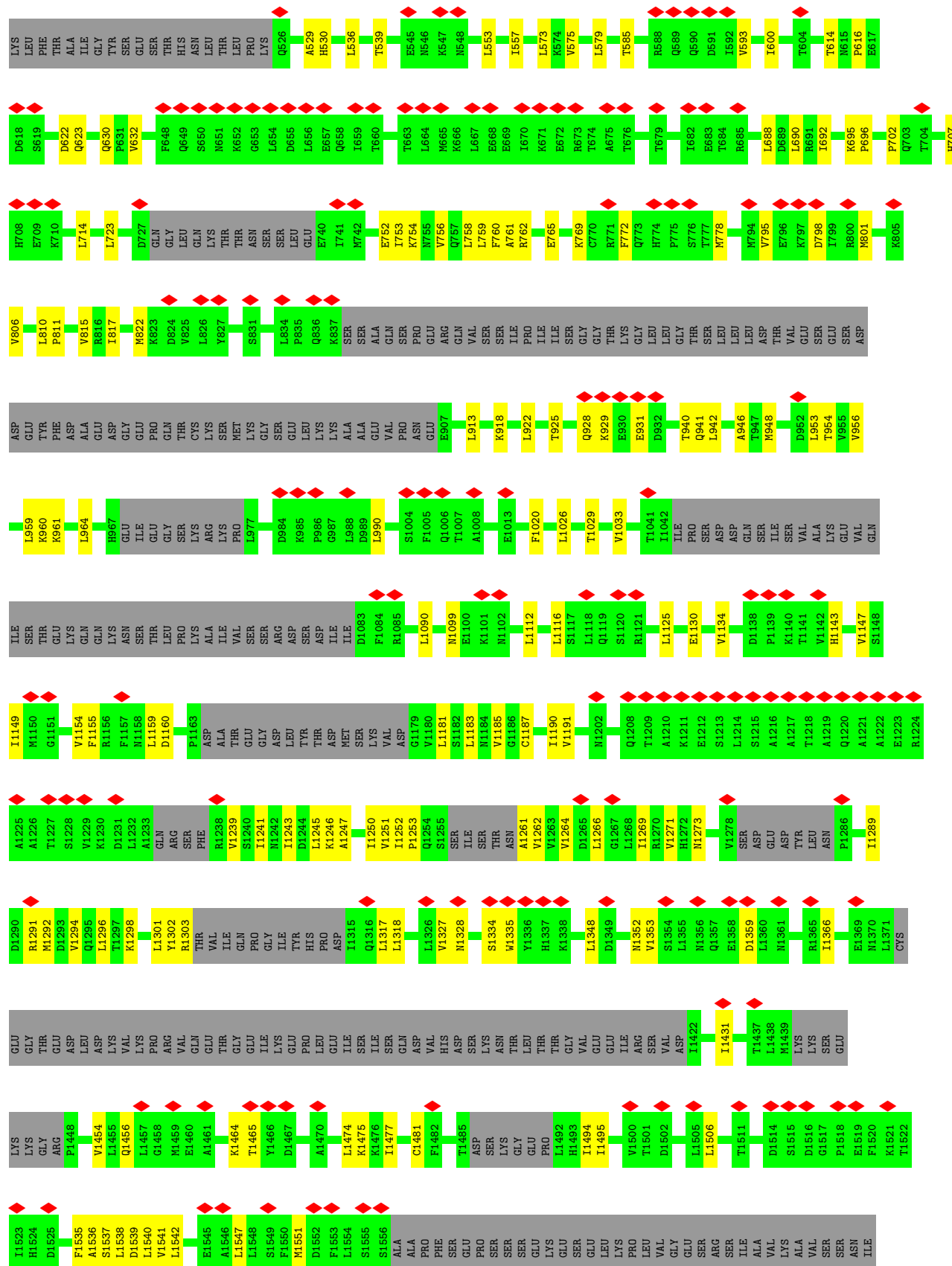
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



• Molecule 2: Intermembrane lipid transfer protein VPS13C





C2925	C2926	G2940	L2942	E2946	D2947	G2951	L2952	L2953	V2954	D2955	V2956	L2965	T2966	F2967	Y2970	H2971	E2972	G2973	S2974	A2975	P2976	L2978	L2979	N2980	N2981	W2985	L2988	Q2992	P2996	E2997	L3001	L3002	A3006	A3012	D3013	T3017	R3018	K3019	L3020	T3021	K3022	Y3024									
F2797	R2798	D2799	I2800	K2806	K2807	K2808	N2809	I2810	F2811	K2813	N2814	K2815	L2818	K2841	A2844	N2845	E2848	G2853	V2866	T2867	L2868	I2874	K2877	S2878	S2879	V2884	I2887	A2888	S2889	D2890	G2891	S2892	N2893	N2896	C2906	L2907	P2908	F2909	L2914	L2918	V2923	G2924									
T2671	L2672	R2673	N2674	L2675	L2676	P2677	V2678	G2679	L2680	L2683	L2693	Q2693	P2694	A2695	I2696	L2697	S2704	R2705	L2706	E2712	L2713	V2714	L2715	I2729	E2735	S2745	T2746	E2747	T2750	L2753	V2757	L2760	R2763	L2766	S2767	W2773	L2774	L2775	N2776	K2777	T2778	T2779	R2780	V2781	L2782	E2787	A2795	D2796			
L2567	E2568	R2569	I2570	H2580	V2581	P2582	L2583	I2592	G2593	P2594	A2595	G2596	L2597	L2598	E2599	I2609	S2610	E2613	E2614	L2615	H2616	R2617	S2618	R2619	E2620	V2621	L2625	S2633	P2636	L2637	A2643	E2647	L2648	S2649	Y2650	L2651	C2652	T2653	R2654	G2655	E2656	D2657	W2658	D2659	I2663	L2664	L2670				
SER	GLN	GLY	ASN	LEU	SER	ILE	LEU	SER	ARG	GLN	E2484	T2491	I2492	V2493	Y2497	T2498	E2499	V2500	A2501	N2502	I2503	P2504	I2505	P2508	G2509	R2510	R2511	L2512	Y2513	D2524	S2525	V2526	L2527	V2528	Q2529	I2530	D2531	A2532	T2533	E2534	G2535	V2538	L2541	R2542	L2545	Q2546	I2553	A2554	F2555	L2556	I2557
THR	SER	LYS	GLU	MET	GLU	ASN	LEU	TRP	GLY	ILE	LYS	SER	ILE	ASN	ASP	TYR	ASN	THR	TRP	PHE	GLY	VAL	ASP	THR	ALA	THR	GLU	ILE	THR	GLU	SER	PHE	LYS	GLY	ILE	GLU	HIS	SER	LEU	I2272	V2280	V2285	L2291	L2299	L2300	A2301	S2314	L2315	V2319	A2320	V2326
P2338	E2341	R2342	V2343	E2344	L2351	L2352	L2353	D2354	V2355	Q2361	ASP	LYS	SER	LEU	LEU	PRO	GLY	ASP	ASP	PHE	I2372	P2375	Q2376	N2377	N2385	T2386	N2387	L2388	T2389	T2390	I2391	S2392	T2410	F2414	D2415	Y2416	R2421	A2422	P2423	S2451	E2463	L2464	S2468	MET	VAL	PRO	SER				
A2107	P2112	L2120	P2126	F2132	L2136	K2142	W2146	V2151	A2158	V2173	C2177	S2178	L2179	E2182	A2187	I2193	V2197	K2198	E2199	F2200	T2201	I2202	I2207	T2211	V2212	L2213	A2217	A2218	L2219	SER	PRO	LYS	THR	LYS	GLU	ASP	GLY	SER	LYS	ASP	VAL	ARG	PRO	N2102							
N2019	N2023	N2024	W2027	L2028	S2031	Q2034	I2041	D2042	K2047	L2048	Y2049	V2050	C2051	D2062	F2063	F2064	V2068	PRO	GLN	SER	PRO	GLU	ASN	VAL	ALA	LYS	GLY	THR	GLN	ILE	PRO	ARG	GLN	THR	ALA	GLY	LYS	VAL	ILE	GLU	LYS	ASP	SER	VAL	ARG	PRO	N2102				
ASP	HIS	LEU	GLN	PHE	LEU	ASN	THR	THR	GLN	THR	ASN	THR	ALA	VAL	GLN	GLN	ASN	GLY	ASP	GLY	VAL	ALA	ALA	ASP	GLY	GLU	ALA	ASN	HIS	ASP	S1966	F1967	Q1968	S1988	L1995	T1999	L2000	D2002	D2003	L2003	R2004	E2005	G2006	I2007	E2008	R2013	M2014	K2018			
P1802	K1806	T1819	A1823	S1824	P1826	I1830	L1833	K1834	L1846	W1850	P1855	E1858	I1859	E1872	D1873	L1874	L1878	L1886	GLY	GLU	ALA	SER	GLN	PRO	SER	PRO	THR	GLN	VAL	GLN	THR	VAL	ARG	VAL	ARG	VAL	LYS	VAL	ASP	VAL	SER	SER	VAL	SER	VAL	PRO					
I1705	L1715	ASN	PHE	LEU	ASN	ASN	GLN	THR	THR	ALA	VAL	GLN	ALA	ALA	SER	SER	MET	LYS	ASP	ALA	GLU	ARG	ALA	ALA	ALA	ASP	LEU	GLN	K1750	I1758	N1759	L1760	K1761	I1766	I1767	I1778	L1783	V1793	P1794	M1795	E1796	H1797	Y1798	L1800	P1801						
SER	GLN	LYS	ASP	V1596	F1597	D1598	T1602	A1603	E1604	L1605	N1606	A1607	F1608	N1609	V1610	F1611	V1612	G1613	ASP	GLN	LYS	CYS	M1618	I1624	A1629	S1630	P1635	N1639	M1650	N1651	V1652	F1670	Q1673	D1679	A1680	T1681	E1682	G1683	E1684	A1685	V1686	A1687	L1696	V1700	G1702	I1703	Q1704				



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	392473	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.408	Depositor
Minimum map value	-0.447	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4239999, 1.4239999, 1.4239999	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	0.13	0/1178	0.28	0/1580
2	B	0.16	0/23945	0.35	0/32390
All	All	0.16	0/25123	0.35	0/33970

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	1166	0	1093	10	0
2	B	23511	0	24031	394	0
All	All	24677	0	25124	401	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (401) 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:B:1995:LEU:HB3	2:B:2028:ILE:HG22	1.65	0.78
2:B:1026:LEU:HD23	2:B:1026:LEU:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3328:PHE:CE2	2:B:3397:LEU:HD21	2.20	0.77
2:B:2202:ILE:CG2	2:B:2285:VAL:HG12	2.14	0.77
2:B:2351:LEU:HD12	2:B:2351:LEU:O	1.86	0.74
2:B:1262:VAL:HG23	2:B:1366:ILE:HD13	1.72	0.71
2:B:1618:ASN:HB2	2:B:1652:VAL:HG11	1.73	0.71
2:B:2609:ILE:HD11	2:B:2664:ILE:HG21	1.73	0.71
2:B:1538:LEU:HD23	2:B:1608:PHE:HE2	1.54	0.70
2:B:1154:VAL:O	2:B:1185:VAL:HG23	1.91	0.70
2:B:817:ILE:HG21	2:B:822:MET:SD	2.32	0.69
2:B:3225:VAL:HG22	2:B:3269:ALA:HB2	1.75	0.69
2:B:1143:HIS:HE1	2:B:1252:ILE:HG23	1.59	0.68
2:B:1264:VAL:HG22	2:B:1301:LEU:CD1	2.24	0.68
2:B:2884:VAL:HG13	2:B:2918:LEU:HD11	1.76	0.68
2:B:3654:LEU:HD13	2:B:3670:GLN:HB3	1.77	0.67
2:B:1348:LEU:HD23	2:B:1431:ILE:HD12	1.76	0.66
2:B:1271:VAL:HG13	2:B:1294:VAL:HG22	1.78	0.65
2:B:2782:LEU:HD22	2:B:2818:LEU:HD11	1.79	0.65
2:B:3328:PHE:HE2	2:B:3397:LEU:HD21	1.61	0.64
2:B:1540:LEU:HB2	2:B:1610:VAL:HG22	1.79	0.64
2:B:557:ILE:HG23	2:B:579:LEU:HD11	1.80	0.64
2:B:1833:LEU:HD23	2:B:1834:LYS:O	1.98	0.63
2:B:3204:LEU:HD23	2:B:3205:TYR:N	2.13	0.63
2:B:2000:LEU:HD23	2:B:2000:LEU:O	2.00	0.62
2:B:2556:ILE:HD12	2:B:2599:GLU:CD	2.24	0.62
2:B:1703:ILE:HG22	2:B:1705:ILE:HD11	1.81	0.61
2:B:2285:VAL:CG2	2:B:2301:ALA:HB3	2.30	0.61
2:B:2942:LEU:HD23	2:B:2976:PRO:HD3	1.82	0.61
2:B:1159:LEU:HD23	2:B:1160:ASP:N	2.16	0.61
2:B:2285:VAL:HG22	2:B:2301:ALA:HB3	1.83	0.61
1:A:145:MET:HE1	2:B:378:ILE:HD11	1.84	0.60
2:B:2314:SER:C	2:B:2315:LEU:HD12	2.26	0.60
2:B:2014:MET:HE1	2:B:2120:LEU:HD21	1.84	0.60
2:B:2207:ILE:HD11	2:B:2416:TYR:CE1	2.37	0.59
1:A:45:THR:HG22	1:A:46:GLU:H	1.68	0.59
2:B:3382:LEU:HD23	2:B:3412:GLN:OE1	2.02	0.59
2:B:1241:ILE:HG22	2:B:1273:ASN:HB3	1.85	0.59
2:B:942:LEU:HD13	2:B:959:LEU:HD12	1.85	0.59
2:B:1538:LEU:HD23	2:B:1608:PHE:CE2	2.37	0.59
2:B:38:LEU:HD21	2:B:41:LEU:HD21	1.85	0.59
2:B:2343:VAL:HG21	2:B:2385:ASN:HB3	1.84	0.58
2:B:371:ARG:O	2:B:371:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2782:LEU:CD1	2:B:2868:LEU:HD13	2.34	0.58
2:B:573:LEU:HD21	2:B:575:VAL:HG23	1.86	0.57
2:B:1298:LYS:HD2	2:B:1298:LYS:O	2.04	0.57
2:B:2132:PHE:CD2	2:B:2151:VAL:HG13	2.40	0.57
2:B:3023:THR:HG23	2:B:3027:ASN:O	2.04	0.57
2:B:573:LEU:HB3	2:B:614:THR:HG22	1.87	0.56
2:B:1262:VAL:HG23	2:B:1366:ILE:CD1	2.34	0.56
2:B:198:ILE:HG22	2:B:201:ILE:HD11	1.89	0.56
2:B:2556:ILE:HD12	2:B:2599:GLU:OE2	2.06	0.56
2:B:1874:ASP:O	2:B:1878:LEU:HD23	2.05	0.55
2:B:191:ILE:HG21	2:B:307:MET:HE2	1.89	0.55
2:B:2197:VAL:HG11	2:B:2200:PHE:CE2	2.41	0.55
2:B:2493:VAL:HG22	2:B:2499:GLU:OE1	2.07	0.55
2:B:1269:ILE:HD11	2:B:1296:LEU:HD13	1.88	0.55
2:B:3220:VAL:HG23	2:B:3220:VAL:O	2.07	0.55
2:B:3325:PHE:CZ	2:B:3397:LEU:HD22	2.41	0.55
2:B:2463:GLU:C	2:B:2464:LEU:HD12	2.32	0.55
2:B:714:LEU:HD12	2:B:759:LEU:O	2.07	0.55
2:B:1481:CYS:HB2	2:B:1494:ILE:HD11	1.89	0.54
2:B:1541:VAL:HG22	2:B:1611:PHE:CE1	2.41	0.54
2:B:1793:VAL:HG13	2:B:1795:MET:HE1	1.88	0.54
2:B:2556:ILE:HD13	2:B:2569:ARG:HH12	1.71	0.54
2:B:2202:ILE:HG21	2:B:2285:VAL:HG12	1.87	0.54
2:B:2701:VAL:HG13	2:B:2704:SER:HB3	1.89	0.54
1:A:13:PHE:CD2	1:A:73:MET:HE3	2.42	0.54
2:B:815:VAL:HB	2:B:922:LEU:HD23	1.90	0.54
2:B:990:LEU:HD11	2:B:1020:PHE:CE1	2.43	0.54
2:B:1541:VAL:HG13	2:B:1611:PHE:CE2	2.43	0.53
2:B:196:VAL:HG12	2:B:227:LEU:HB3	1.89	0.53
2:B:2729:ILE:O	2:B:2729:ILE:HG13	2.09	0.53
2:B:2527:LEU:HD23	2:B:2542:ARG:NH2	2.24	0.53
2:B:2893:MET:HE2	2:B:2893:MET:HA	1.91	0.53
2:B:3221:VAL:HG21	2:B:3276:PHE:CE2	2.44	0.52
2:B:714:LEU:HD11	2:B:758:LEU:HD21	1.89	0.52
1:A:69:PHE:O	1:A:73:MET:HG2	2.09	0.52
2:B:2980:MET:SD	2:B:3063:LEU:HD23	2.49	0.52
2:B:806:VAL:HG23	2:B:913:LEU:HA	1.90	0.52
2:B:2674:ASN:HB2	2:B:2693:LEU:HD22	1.91	0.52
2:B:2207:ILE:HD11	2:B:2416:TYR:CD1	2.44	0.52
2:B:2554:ALA:HB3	2:B:2595:ALA:HB3	1.91	0.52
2:B:2002:ASP:C	2:B:2003:LEU:HD22	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2146:MET:HA	2:B:2146:MET:HE2	1.92	0.52
2:B:3017:THR:HG22	2:B:3019:LYS:H	1.75	0.52
2:B:3654:LEU:HD13	2:B:3670:GLN:CB	2.40	0.52
2:B:3281:ILE:HD11	2:B:3361:VAL:HG21	1.92	0.52
1:A:145:MET:CE	2:B:378:ILE:HD11	2.41	0.51
2:B:2884:VAL:CG1	2:B:2918:LEU:HD11	2.39	0.51
1:A:45:THR:HG22	1:A:46:GLU:N	2.25	0.51
2:B:3086:GLU:O	2:B:3086:GLU:HG3	2.11	0.51
1:A:146:MET:HA	1:A:146:MET:HE3	1.92	0.51
2:B:2107:ALA:HB3	2:B:2136:LEU:HB3	1.93	0.51
2:B:2670:LEU:O	2:B:2701:VAL:HG12	2.11	0.51
2:B:2988:LEU:HD21	2:B:3064:PHE:CZ	2.46	0.51
2:B:3068:VAL:O	2:B:3071:VAL:HG22	2.11	0.51
2:B:3211:ASN:HB2	2:B:3221:VAL:HG23	1.93	0.51
2:B:1318:LEU:HD13	2:B:1353:VAL:HG22	1.94	0.50
2:B:2583:LEU:O	2:B:2583:LEU:HD23	2.12	0.50
2:B:2610:SER:O	2:B:2621:VAL:HG11	2.12	0.50
2:B:3021:THR:HG22	2:B:3030:GLU:HG3	1.93	0.50
2:B:320:LEU:HD21	2:B:322:CYS:HB2	1.94	0.50
2:B:2853:VAL:HG22	2:B:2868:LEU:HD23	1.94	0.50
2:B:2853:VAL:HG22	2:B:2868:LEU:CD2	2.41	0.50
2:B:1245:LEU:HB3	2:B:1269:ILE:HB	1.93	0.50
2:B:3371:THR:HG23	2:B:3371:THR:O	2.12	0.50
2:B:1191:VAL:HA	2:B:1250:ILE:HG23	1.94	0.49
2:B:1143:HIS:CE1	2:B:1252:ILE:HG23	2.45	0.49
2:B:2042:ASP:OD1	2:B:2042:ASP:C	2.55	0.49
2:B:2299:LEU:HD21	2:B:2326:VAL:CG1	2.42	0.49
2:B:2319:VAL:HG12	2:B:2320:ALA:N	2.27	0.49
2:B:2782:LEU:HD22	2:B:2818:LEU:CD1	2.43	0.49
2:B:2942:LEU:HD22	2:B:2970:TYR:CE1	2.46	0.49
2:B:2341:GLU:OE1	2:B:2388:ASN:O	2.30	0.49
2:B:1608:PHE:HB3	2:B:1624:ILE:HG12	1.93	0.49
2:B:2706:ILE:O	2:B:2706:ILE:HG13	2.12	0.49
2:B:1317:LEU:HD21	2:B:1359:ASP:HB3	1.95	0.48
2:B:2491:THR:HG22	2:B:2501:ALA:HB1	1.95	0.48
2:B:593:VAL:O	2:B:593:VAL:HG13	2.13	0.48
2:B:1029:THR:O	2:B:1033:VAL:HG23	2.13	0.48
2:B:1704:GLN:OE1	2:B:1766:ILE:HD12	2.13	0.48
2:B:2954:VAL:HG23	2:B:2967:PHE:CE1	2.49	0.48
2:B:3055:LEU:HD11	2:B:3060:ARG:NH2	2.28	0.48
2:B:2528:VAL:HG12	2:B:2541:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3240:PHE:O	2:B:3241:ILE:C	2.56	0.48
2:B:229:THR:HG22	2:B:230:ALA:N	2.29	0.48
2:B:1147:VAL:HG22	2:B:1190:ILE:HA	1.95	0.48
2:B:3328:PHE:CZ	2:B:3397:LEU:HD11	2.49	0.48
2:B:1243:ILE:HB	2:B:1271:VAL:HB	1.96	0.48
2:B:536:LEU:HD22	2:B:539:THR:OG1	2.14	0.48
2:B:2567:LEU:HD23	2:B:2567:LEU:H	1.77	0.48
2:B:1247:ALA:HB1	2:B:1266:LEU:HB3	1.95	0.48
2:B:1778:ILE:HD12	2:B:1819:THR:HG21	1.96	0.48
2:B:2906:CYS:C	2:B:2907:LEU:HD22	2.39	0.48
2:B:3319:MET:N	2:B:3319:MET:HE2	2.29	0.48
2:B:1950:TYR:HA	2:B:1968:GLN:HA	1.96	0.47
2:B:283:LEU:HD12	2:B:288:ILE:HA	1.96	0.47
2:B:2992:GLN:HE22	2:B:3012:ALA:H	1.61	0.47
2:B:1090:LEU:HB3	2:B:1112:LEU:HB3	1.96	0.47
2:B:234:TRP:HD1	2:B:249:LEU:HD21	1.79	0.47
2:B:3088:THR:HG22	2:B:3089:LEU:N	2.30	0.47
2:B:282:ILE:HG22	2:B:282:ILE:O	2.14	0.47
2:B:2299:LEU:HD21	2:B:2326:VAL:HG13	1.97	0.47
2:B:2513:TYR:HA	2:B:2652:CYS:HB2	1.96	0.47
2:B:2637:LEU:HD23	2:B:2637:LEU:O	2.15	0.47
2:B:2678:TYR:HB2	2:B:2715:LEU:HD11	1.96	0.47
2:B:2874:ILE:HD13	2:B:2965:ILE:HB	1.95	0.47
2:B:3635:HIS:HB3	2:B:3647:MET:HG3	1.97	0.47
2:B:695:LYS:HB3	2:B:696:PRO:CD	2.45	0.47
2:B:1261:ALA:O	2:B:1303:ARG:HA	2.15	0.47
2:B:1541:VAL:HG22	2:B:1611:PHE:CZ	2.49	0.47
2:B:338:TYR:O	2:B:341:MET:HG3	2.15	0.47
2:B:2757:VAL:HG12	2:B:2766:LEU:CD2	2.45	0.47
2:B:913:LEU:HD23	2:B:946:ALA:HB3	1.97	0.47
2:B:1029:THR:HG21	2:B:1099:ASN:CG	2.39	0.47
2:B:2527:LEU:HD23	2:B:2542:ARG:CZ	2.45	0.47
2:B:3019:LYS:HE3	2:B:3030:GLU:HB3	1.98	0.47
2:B:2512:LEU:HD11	2:B:2525:SER:HB3	1.97	0.46
2:B:3656:ILE:HD12	2:B:3667:VAL:HA	1.97	0.46
2:B:3692:LYS:HD2	2:B:3692:LYS:C	2.41	0.46
2:B:956:VAL:HG23	2:B:956:VAL:O	2.15	0.46
2:B:340:SER:O	2:B:343:ASP:OD1	2.33	0.46
2:B:2285:VAL:O	2:B:2285:VAL:HG23	2.14	0.46
2:B:2814:ASN:O	2:B:2815:LYS:HB2	2.14	0.46
2:B:3281:ILE:CD1	2:B:3361:VAL:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1539:ASP:C	2:B:1540:LEU:HD12	2.41	0.46
2:B:690:LEU:HD11	2:B:692:ILE:CG1	2.46	0.46
2:B:1181:LEU:HB2	2:B:1239:VAL:HG13	1.98	0.46
2:B:2014:MET:HE1	2:B:2120:LEU:HD11	1.97	0.46
2:B:415:LYS:NZ	2:B:421:VAL:HG13	2.31	0.46
2:B:1149:ILE:HG23	2:B:1149:ILE:O	2.16	0.46
2:B:1767:ILE:HG23	2:B:1767:ILE:O	2.16	0.46
2:B:2112:PRO:HD2	2:B:2132:PHE:O	2.16	0.46
2:B:2542:ARG:NH1	2:B:2546:GLN:HG3	2.30	0.46
2:B:2650:TYR:HA	2:B:3744:VAL:HG13	1.96	0.46
2:B:2676:LEU:HD11	2:B:2753:LEU:HD13	1.97	0.46
2:B:2781:VAL:O	2:B:2781:VAL:HG23	2.15	0.46
2:B:3067:ASP:HB2	2:B:3070:LEU:HD12	1.98	0.46
2:B:1187:CYS:HA	2:B:1246:LYS:O	2.16	0.46
2:B:2503:ILE:HG13	2:B:2503:ILE:O	2.16	0.46
2:B:2774:LEU:HD23	2:B:2866:VAL:HB	1.98	0.46
2:B:1700:VAL:HG12	2:B:1701:GLY:O	2.16	0.46
2:B:2648:LEU:HD12	2:B:2651:ILE:HD11	1.97	0.46
2:B:2200:PHE:HD2	2:B:2280:VAL:HG11	1.80	0.46
2:B:723:LEU:C	2:B:723:LEU:HD23	2.41	0.45
2:B:1154:VAL:HG12	2:B:1155:PHE:HD1	1.80	0.45
2:B:2497:TYR:OH	2:B:2583:LEU:HD22	2.15	0.45
2:B:2531:ASP:OD2	2:B:2538:VAL:HB	2.16	0.45
2:B:2592:ILE:HD11	2:B:2625:LEU:HD22	1.99	0.45
2:B:2750:THR:HG23	2:B:2806:LYS:HE2	1.98	0.45
2:B:206:GLU:HB3	2:B:265:MET:HE3	1.98	0.45
2:B:368:THR:O	2:B:369:ASN:CG	2.59	0.45
2:B:529:ALA:O	2:B:530:HIS:CG	2.70	0.45
2:B:1859:ILE:HD12	2:B:1936:LEU:HD11	1.98	0.45
2:B:2501:ALA:O	2:B:2502:ASN:OD1	2.33	0.45
2:B:2583:LEU:HD23	2:B:2583:LEU:C	2.42	0.45
2:B:2782:LEU:HD12	2:B:2868:LEU:HD13	1.98	0.45
2:B:2953:LEU:HD23	2:B:2953:LEU:H	1.81	0.45
2:B:925:THR:HG21	2:B:931:GLU:HA	1.98	0.45
2:B:1464:LYS:HG2	2:B:1465:THR:H	1.81	0.45
2:B:2014:MET:HA	2:B:2051:CYS:HB3	1.98	0.45
2:B:2291:LEU:C	2:B:2291:LEU:HD23	2.41	0.45
2:B:2524:ASP:HB3	2:B:2583:LEU:HD21	1.99	0.45
2:B:2553:ILE:HD12	2:B:2594:PRO:HB2	1.99	0.45
2:B:3106:GLU:O	2:B:3106:GLU:HG2	2.16	0.45
2:B:3689:ILE:HG22	2:B:3691:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:LYS:HZ3	2:B:421:VAL:HG13	1.81	0.45
2:B:954:THR:HG23	2:B:954:THR:O	2.15	0.45
2:B:1454:VAL:HG13	2:B:1477:ILE:CD1	2.46	0.45
2:B:2545:LEU:O	2:B:2581:VAL:HG22	2.17	0.45
2:B:202:HIS:HE2	2:B:278:LEU:HD22	1.81	0.45
2:B:1292:MET:N	2:B:1292:MET:HE2	2.32	0.45
2:B:2422:ALA:O	2:B:2423:PRO:C	2.60	0.45
2:B:2942:LEU:HD22	2:B:2970:TYR:CZ	2.51	0.45
2:B:1454:VAL:HG13	2:B:1474:LEU:HD11	1.98	0.45
2:B:2651:ILE:HD12	2:B:3744:VAL:O	2.17	0.45
2:B:1185:VAL:CG1	2:B:1245:LEU:HB2	2.46	0.45
2:B:1950:TYR:O	2:B:2063:PHE:CZ	2.70	0.45
2:B:2198:LYS:HG3	2:B:2199:GLU:N	2.32	0.45
2:B:2985:TRP:HB2	2:B:3024:TYR:OH	2.16	0.45
2:B:3661:ILE:HG13	2:B:3662:LEU:H	1.81	0.45
2:B:2906:CYS:O	2:B:2907:LEU:HD22	2.17	0.45
2:B:1547:LEU:O	2:B:1551:MET:HG2	2.18	0.44
2:B:2338:PRO:HB2	2:B:2341:GLU:HG3	1.99	0.44
2:B:2680:LEU:HD21	2:B:2713:LEU:HD22	1.98	0.44
2:B:3023:THR:HA	2:B:3027:ASN:O	2.17	0.44
2:B:369:ASN:OD1	2:B:369:ASN:O	2.36	0.44
2:B:573:LEU:HD23	2:B:573:LEU:C	2.43	0.44
2:B:778:MET:CG	2:B:778:MET:O	2.65	0.44
2:B:798:ASP:HB3	2:B:801:MET:HE3	1.97	0.44
2:B:2775:ILE:HD11	2:B:2867:THR:HG22	1.99	0.44
2:B:110:VAL:O	2:B:113:LYS:HG3	2.17	0.44
2:B:1761:LYS:HE3	2:B:1783:LEU:HD12	2.00	0.44
2:B:1830:ILE:HG23	2:B:1830:ILE:O	2.18	0.44
2:B:2354:ASP:OD1	2:B:2355:VAL:N	2.51	0.44
2:B:2815:LYS:HE3	2:B:3421:ASP:HB2	1.99	0.44
2:B:3206:TRP:O	2:B:3208:GLN:N	2.51	0.44
2:B:3365:LEU:HD11	2:B:3372:LEU:H	1.81	0.44
2:B:3413:MET:O	2:B:3417:VAL:HG12	2.17	0.44
2:B:3661:ILE:HG13	2:B:3662:LEU:N	2.33	0.44
2:B:2064:PHE:O	2:B:2068:VAL:HG12	2.17	0.44
2:B:2527:LEU:HD11	2:B:2648:LEU:HD22	1.99	0.44
2:B:2556:ILE:HD13	2:B:2569:ARG:NH1	2.33	0.44
2:B:753:ILE:HG22	2:B:756:VAL:CG2	2.48	0.44
2:B:1766:ILE:HG12	2:B:1778:ILE:HG12	2.00	0.44
2:B:2505:VAL:HG12	2:B:2505:VAL:O	2.17	0.44
2:B:229:THR:HG22	2:B:230:ALA:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:GLU:OE1	2:B:769:LYS:HA	2.18	0.44
2:B:795:VAL:HG12	2:B:801:MET:SD	2.57	0.44
2:B:2773:TRP:HB3	2:B:2800:ILE:HG21	2.00	0.44
2:B:191:ILE:HG21	2:B:307:MET:CE	2.47	0.43
2:B:250:ILE:HB	2:B:303:ALA:HB3	1.99	0.43
2:B:2782:LEU:HD22	2:B:2818:LEU:CG	2.48	0.43
2:B:283:LEU:HD22	2:B:298:PRO:CG	2.48	0.43
2:B:695:LYS:HB3	2:B:696:PRO:HD2	2.00	0.43
2:B:758:LEU:O	2:B:759:LEU:HD12	2.18	0.43
2:B:2782:LEU:HB3	2:B:2818:LEU:HD11	2.00	0.43
2:B:2887:ILE:HD13	2:B:2893:MET:HE1	2.00	0.43
1:A:40:LEU:HD22	2:B:398:ILE:HG23	1.99	0.43
2:B:758:LEU:C	2:B:759:LEU:HD12	2.44	0.43
2:B:2841:LYS:HG2	2:B:2848:GLU:OE2	2.19	0.43
2:B:2887:ILE:HG23	2:B:2892:SER:O	2.18	0.43
2:B:1334:SER:HG	2:B:1335:TRP:CD1	2.36	0.43
2:B:2207:ILE:HD12	2:B:2414:PHE:CE2	2.53	0.43
2:B:2158:ALA:H	2:B:2173:VAL:HG23	1.82	0.43
2:B:1454:VAL:HG13	2:B:1477:ILE:HD11	2.01	0.43
2:B:1535:PHE:HB3	2:B:1605:LEU:HA	2.01	0.43
2:B:1872:GLU:HB2	2:B:2063:PHE:CE1	2.53	0.43
2:B:3185:SER:O	2:B:3186:GLY:C	2.62	0.43
2:B:3318:ASP:C	2:B:3319:MET:HE2	2.44	0.43
2:B:355:ALA:N	2:B:356:PRO:HD2	2.33	0.43
2:B:2031:SER:O	2:B:2041:ILE:HA	2.18	0.43
2:B:2375:PRO:HB2	2:B:3085:TYR:HA	2.01	0.43
2:B:2557:ILE:O	2:B:2570:ILE:HG12	2.19	0.43
2:B:3634:TYR:O	2:B:3648:VAL:HG22	2.19	0.43
2:B:274:ILE:O	2:B:278:LEU:HG	2.19	0.43
2:B:1134:VAL:HB	2:B:1147:VAL:HB	2.01	0.43
2:B:2974:SER:N	2:B:3059:GLN:OE1	2.52	0.43
2:B:3382:LEU:HD22	2:B:3408:GLN:HB3	2.00	0.43
2:B:283:LEU:HD13	2:B:294:TYR:HE2	1.84	0.43
2:B:1650:MET:HE1	2:B:1652:VAL:HG22	2.00	0.43
2:B:2542:ARG:HD2	2:B:2580:HIS:ND1	2.34	0.43
2:B:3742:SER:O	2:B:3746:LEU:HG	2.19	0.43
2:B:752:GLU:HB3	2:B:754:LYS:HE3	2.00	0.42
2:B:1542:LEU:HD12	2:B:1612:VAL:HG22	1.99	0.42
2:B:2062:ASP:OD1	2:B:2063:PHE:N	2.51	0.42
2:B:2177:CYS:SG	2:B:2197:VAL:HG13	2.59	0.42
2:B:425:ILE:HG23	2:B:426:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:948:MET:HB2	2:B:953:LEU:HD13	2.02	0.42
2:B:1291:ARG:C	2:B:1292:MET:HE2	2.44	0.42
2:B:941:GLN:HB2	2:B:960:LYS:HB2	2.00	0.42
2:B:964:LEU:O	2:B:964:LEU:HG	2.19	0.42
2:B:1495:ILE:CG2	2:B:1538:LEU:HD11	2.48	0.42
2:B:2673:ARG:HB3	2:B:2767:SER:HA	2.01	0.42
2:B:600:ILE:HG22	2:B:600:ILE:O	2.19	0.42
2:B:2018:LYS:HB3	2:B:2047:LYS:HB3	2.01	0.42
2:B:2200:PHE:CD2	2:B:2280:VAL:HG11	2.54	0.42
2:B:3099:VAL:HA	2:B:3106:GLU:HA	2.02	0.42
2:B:1758:ILE:CG2	2:B:1760:LEU:HG	2.49	0.42
2:B:2636:PRO:HB2	2:B:2705:ARG:NH2	2.35	0.42
2:B:3052:VAL:HG11	2:B:3074:ALA:HB2	2.01	0.42
2:B:2501:ALA:O	2:B:2502:ASN:C	2.63	0.42
2:B:2981:ASN:HB3	2:B:3001:LEU:HD22	2.02	0.42
2:B:553:LEU:HD23	2:B:585:THR:O	2.20	0.42
2:B:1292:MET:HB2	2:B:1327:VAL:HB	2.01	0.42
2:B:1536:ALA:O	2:B:1606:ASN:HB3	2.18	0.42
2:B:1825:LEU:HG	2:B:1826:PRO:HD2	2.01	0.42
2:B:2546:GLN:HB2	2:B:2663:ILE:HG12	2.02	0.42
2:B:3365:LEU:HA	2:B:3368:ILE:HD12	2.02	0.42
2:B:3680:PRO:HB2	2:B:3687:LEU:HD11	2.01	0.42
1:A:110:MET:HE1	1:A:125:MET:SD	2.59	0.42
2:B:616:PRO:HD3	2:B:622:ASP:O	2.20	0.42
2:B:1951:ASN:HA	2:B:2063:PHE:CE1	2.55	0.42
2:B:2182:GLU:O	2:B:2193:ILE:HA	2.20	0.42
2:B:2735:GLU:HA	2:B:2757:VAL:HG22	2.01	0.42
2:B:2760:ILE:O	2:B:2760:ILE:HG13	2.20	0.42
2:B:283:LEU:HD22	2:B:298:PRO:HG2	2.01	0.42
2:B:702:PRO:HG3	2:B:707:HIS:HB2	2.00	0.42
2:B:817:ILE:HG21	2:B:822:MET:CE	2.49	0.42
2:B:928:GLN:C	2:B:929:LYS:HD3	2.44	0.42
2:B:1020:PHE:HD2	2:B:1090:LEU:HG	1.84	0.42
2:B:2202:ILE:HG23	2:B:2285:VAL:HG12	1.98	0.42
2:B:2389:ILE:HG22	2:B:2390:THR:N	2.35	0.42
2:B:2392:SER:HA	2:B:3099:VAL:O	2.20	0.42
2:B:321:ASP:OD1	2:B:321:ASP:C	2.63	0.42
2:B:369:ASN:OD1	2:B:369:ASN:C	2.62	0.42
2:B:1183:LEU:O	2:B:1243:ILE:HA	2.20	0.42
2:B:3013:ASP:OD1	2:B:3013:ASP:O	2.37	0.42
2:B:810:LEU:C	2:B:810:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2213:LEU:HD12	2:B:2410:THR:HG22	2.02	0.41
2:B:3144:LYS:HA	2:B:3147:ILE:HG12	2.02	0.41
2:B:3686:VAL:HG11	2:B:3710:LYS:HG3	2.02	0.41
2:B:227:LEU:HD13	2:B:250:ILE:HG13	2.02	0.41
2:B:234:TRP:CD1	2:B:249:LEU:HD21	2.54	0.41
2:B:2343:VAL:HG21	2:B:2385:ASN:CB	2.50	0.41
2:B:2813:LYS:HB2	2:B:2815:LYS:HZ3	1.85	0.41
2:B:2956:VAL:HG13	2:B:2956:VAL:O	2.19	0.41
2:B:3638:ILE:CD1	2:B:3711:VAL:HG13	2.50	0.41
2:B:761:ALA:HB1	2:B:772:PHE:CD1	2.55	0.41
2:B:1264:VAL:HG22	2:B:1301:LEU:HD13	2.01	0.41
2:B:1670:PHE:CB	2:B:1700:VAL:HG22	2.49	0.41
2:B:2023:ASN:OD1	2:B:2024:ASN:N	2.53	0.41
2:B:2508:PRO:HA	2:B:2530:ILE:HB	2.02	0.41
2:B:2570:ILE:HD12	2:B:2582:PRO:HD2	2.02	0.41
2:B:630:GLN:O	2:B:632:VAL:HG23	2.19	0.41
2:B:1130:GLU:C	2:B:1154:VAL:HG23	2.45	0.41
2:B:1251:VAL:HG12	2:B:1253:PRO:HD3	2.02	0.41
2:B:1318:LEU:HD12	2:B:1352:ASN:O	2.20	0.41
2:B:1537:SER:HA	2:B:1607:ALA:O	2.20	0.41
2:B:1995:LEU:O	2:B:2027:MET:N	2.53	0.41
2:B:2387:MET:HE2	2:B:2387:MET:HB3	1.99	0.41
2:B:436:LEU:HD23	2:B:441:ILE:HG13	2.02	0.41
2:B:623:GLN:O	2:B:688:LEU:HD12	2.20	0.41
2:B:1999:THR:HG22	2:B:2013:ARG:NH1	2.34	0.41
2:B:2621:VAL:HB	2:B:2643:ALA:HB3	2.03	0.41
2:B:2779:THR:O	2:B:2795:ALA:HB1	2.20	0.41
2:B:186:LEU:O	2:B:190:VAL:HG23	2.19	0.41
2:B:436:LEU:HD21	2:B:440:ASN:HB2	2.01	0.41
2:B:1872:GLU:HB3	2:B:1952:ASN:HA	2.01	0.41
2:B:940:THR:OG1	2:B:961:LYS:HB2	2.21	0.41
2:B:1190:ILE:O	2:B:1250:ILE:HG12	2.20	0.41
2:B:1474:LEU:HB3	2:B:1506:LEU:HG	2.03	0.41
2:B:1673:GLN:O	2:B:1696:LEU:HD12	2.20	0.41
2:B:1988:SER:HA	2:B:2034:GLN:O	2.20	0.41
2:B:2813:LYS:HB2	2:B:2815:LYS:NZ	2.35	0.41
2:B:3654:LEU:HD12	2:B:3656:ILE:HD11	2.03	0.41
2:B:1116:LEU:HD22	2:B:1125:LEU:HD22	2.03	0.41
2:B:1181:LEU:HD13	2:B:1239:VAL:HG11	2.01	0.41
2:B:1596:VAL:HG22	2:B:1635:PRO:HG3	2.03	0.41
2:B:2377:MET:O	2:B:3085:TYR:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2649:SER:O	2:B:2650:TYR:HD1	2.04	0.41
2:B:2671:THR:HG21	2:B:2763:ARG:NH2	2.35	0.41
2:B:3328:PHE:CE2	2:B:3397:LEU:HD11	2.56	0.41
2:B:101:VAL:O	2:B:105:LYS:HD3	2.20	0.41
2:B:760:PHE:HE2	2:B:762:ARG:HE	1.68	0.41
2:B:811:PRO:O	2:B:918:LYS:HB2	2.21	0.41
2:B:1262:VAL:HG22	2:B:1303:ARG:HH12	1.85	0.41
2:B:1456:GLN:HB2	2:B:1475:LYS:CB	2.50	0.41
2:B:2049:TYR:O	2:B:2049:TYR:CG	2.73	0.41
2:B:2126:PRO:HB2	2:B:2211:THR:HG23	2.02	0.41
2:B:103:GLU:O	2:B:107:LEU:HG	2.21	0.41
2:B:396:SER:O	2:B:399:LYS:HG2	2.21	0.41
2:B:1289:ILE:HG23	2:B:1328:ASN:OD1	2.21	0.41
2:B:1778:ILE:CD1	2:B:1819:THR:HG21	2.51	0.41
2:B:2179:LEU:HD12	2:B:2179:LEU:O	2.20	0.41
2:B:2197:VAL:HB	2:B:2280:VAL:HG22	2.03	0.41
2:B:3002:LEU:HD12	2:B:3002:LEU:O	2.20	0.41
2:B:1020:PHE:CD2	2:B:1090:LEU:HG	2.56	0.40
2:B:1802:PRO:HG3	2:B:1850:TRP:CH2	2.56	0.40
2:B:3119:TRP:CE3	2:B:3179:ILE:HD12	2.56	0.40
2:B:90:VAL:HG23	2:B:205:TYR:CD1	2.56	0.40
2:B:1302:TYR:C	2:B:1303:ARG:HE	2.29	0.40
2:B:2343:VAL:HG12	2:B:2344:GLU:HG3	2.02	0.40
2:B:2351:LEU:HD12	2:B:2353:LEU:CD1	2.52	0.40
2:B:3727:GLU:HA	2:B:3730:GLN:HG2	2.03	0.40
2:B:798:ASP:HB3	2:B:801:MET:HG2	2.04	0.40
2:B:3186:GLY:O	2:B:3187:ILE:C	2.64	0.40
1:A:48:GLU:O	1:A:52:MET:HG2	2.22	0.40
2:B:66:THR:HB	2:B:82:THR:OG1	2.21	0.40
2:B:2874:ILE:HG12	2:B:2909:PHE:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	146/149 (98%)	145 (99%)	1 (1%)	0	100	100
2	B	2892/3777 (77%)	2667 (92%)	225 (8%)	0	100	100
All	All	3038/3926 (77%)	2812 (93%)	226 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	126/127 (99%)	126 (100%)	0	100	100
2	B	2671/3385 (79%)	2671 (100%)	0	100	100
All	All	2797/3512 (80%)	2797 (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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
2	B	385	HIS
2	B	566	GLN
2	B	615	ASN
2	B	651	ASN
2	B	658	GLN
2	B	927	GLN
2	B	1119	GLN
2	B	1370	ASN
2	B	1709	HIS
2	B	2327	HIS
2	B	2348	GLN
2	B	2358	ASN

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Mol	Chain	Res	Type
2	B	2522	HIS
2	B	2529	GLN
2	B	2546	GLN
2	B	2600	HIS
2	B	2719	GLN
2	B	3143	GLN
2	B	3145	HIS
2	B	3223	HIS
2	B	3301	GLN
2	B	3336	HIS
2	B	3404	HIS
2	B	3705	GLN

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](#)

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.

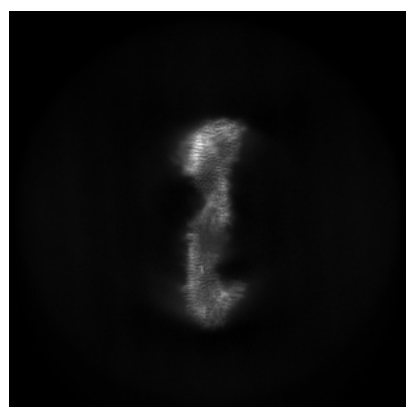
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73373. These allow visual inspection of the internal detail of the map and identification of artifacts.

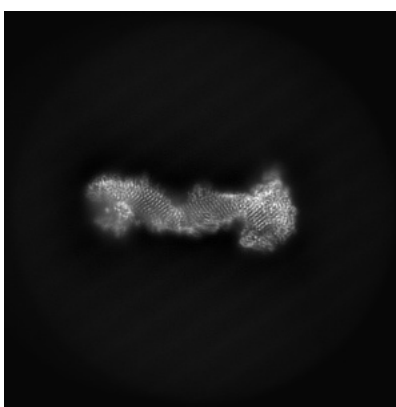
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

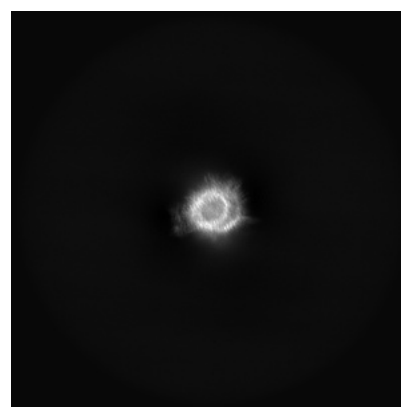
6.1.1 Primary map



X



Y



Z

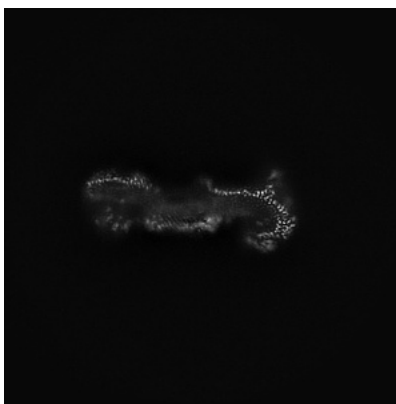
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

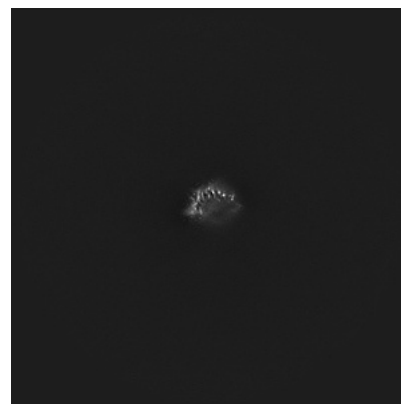
6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

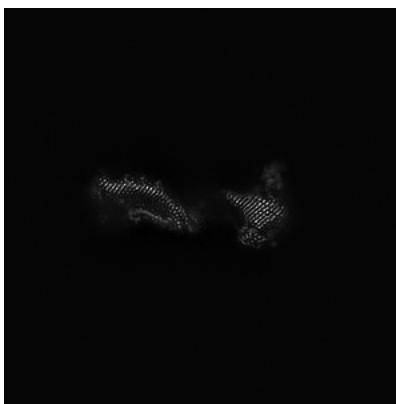
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

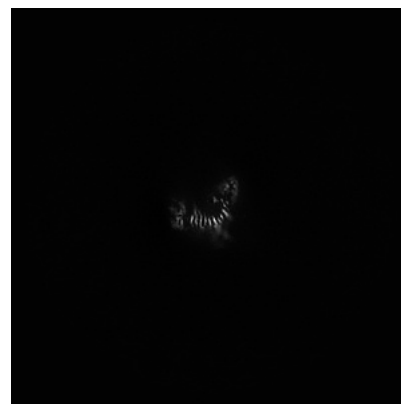
6.3.1 Primary map



X Index: 206



Y Index: 179



Z Index: 245

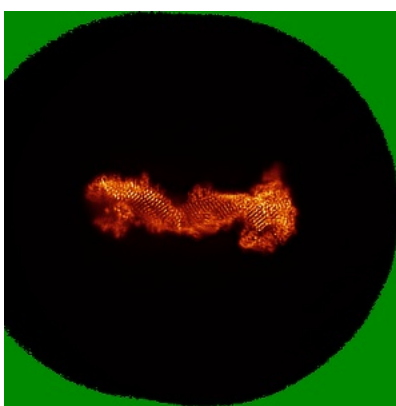
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

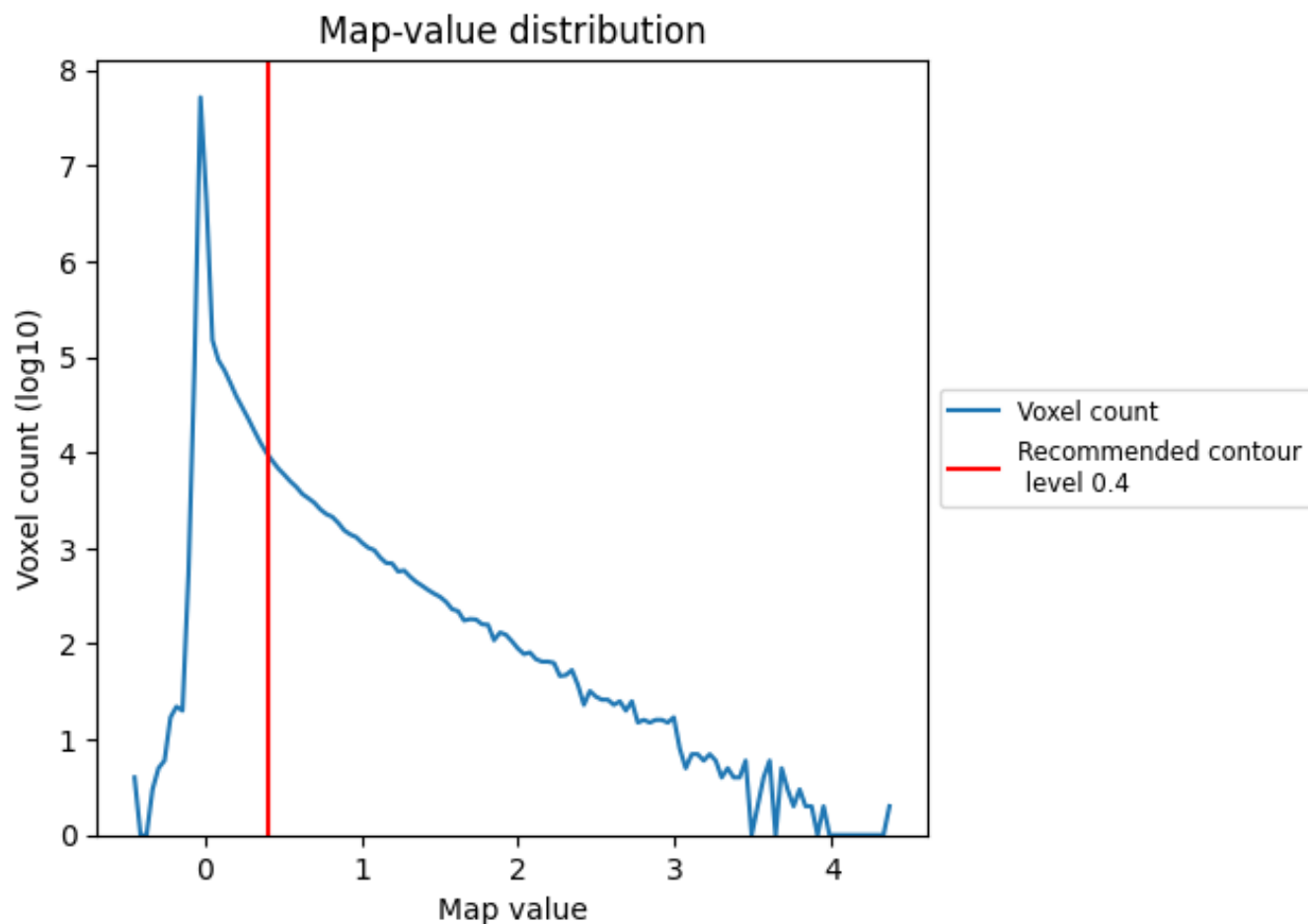
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

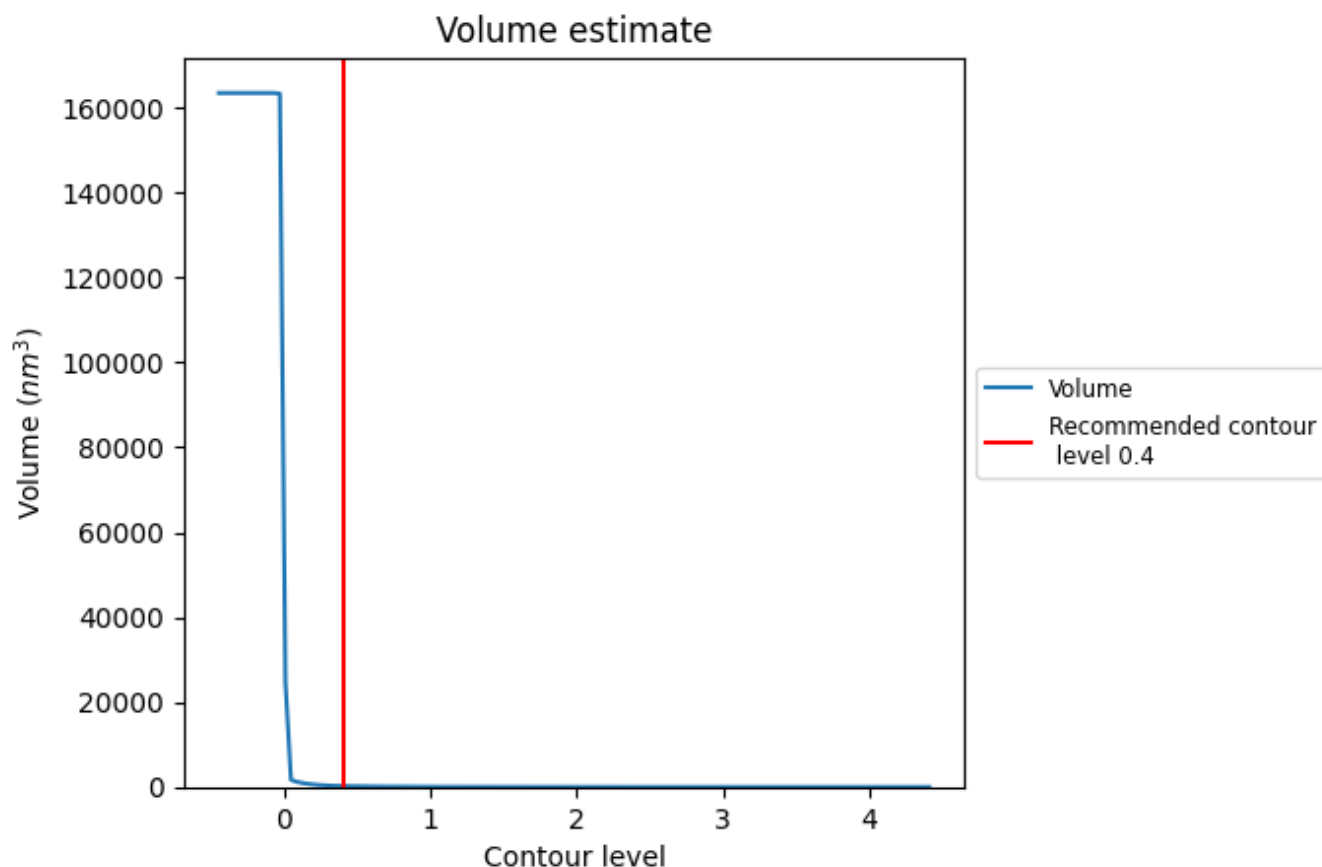
This section contains the results of statistical analysis of the map.

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.

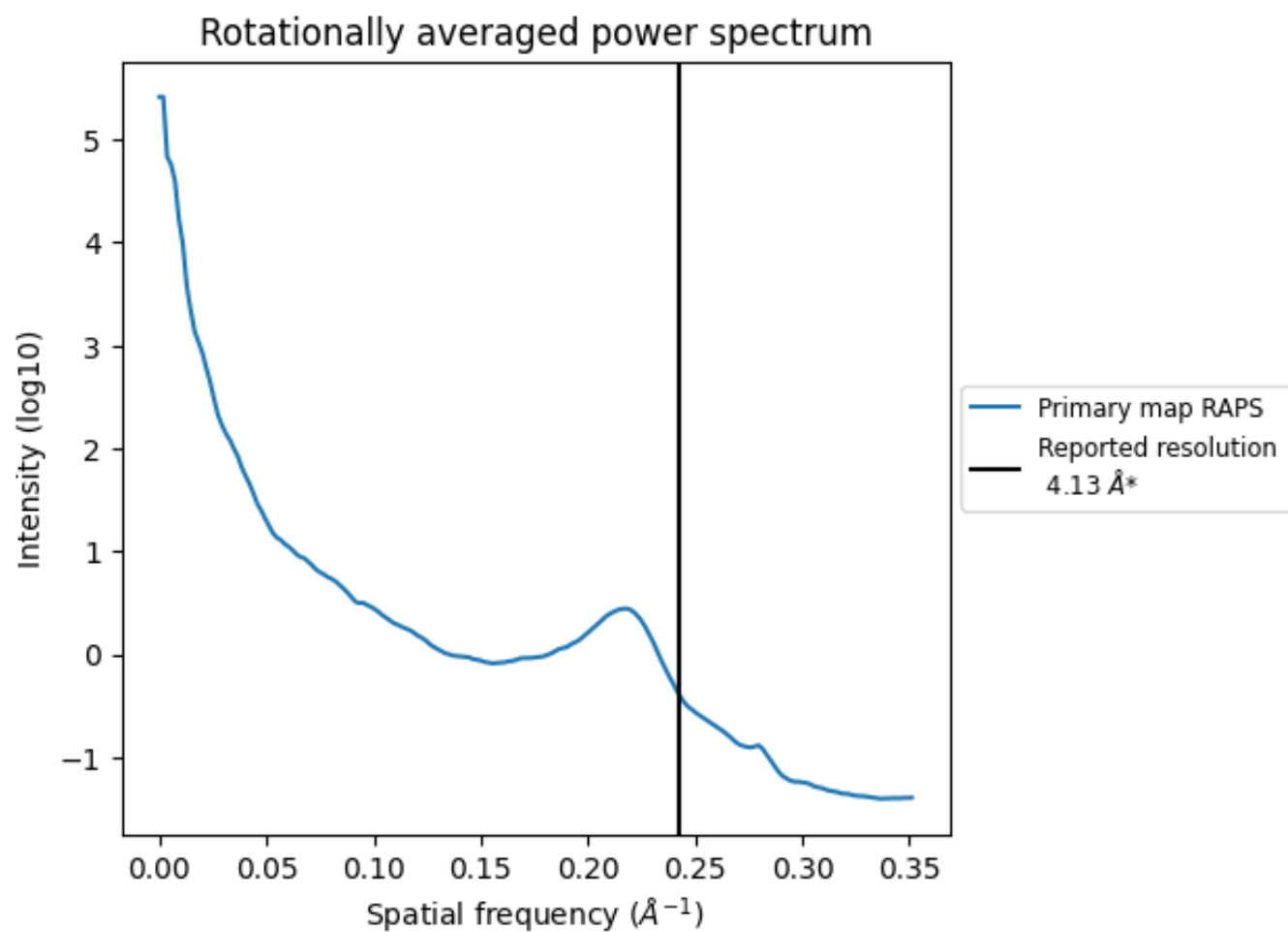
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 213 nm^3 ; this corresponds to an approximate mass of 192 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 0.242 Å⁻¹

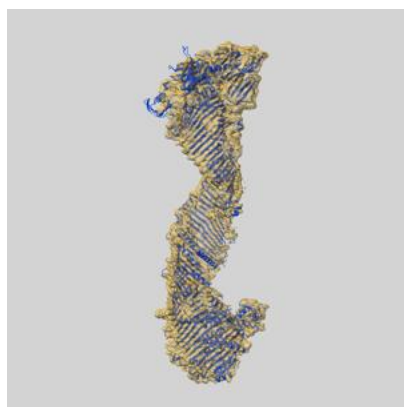
8 Fourier-Shell correlation

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

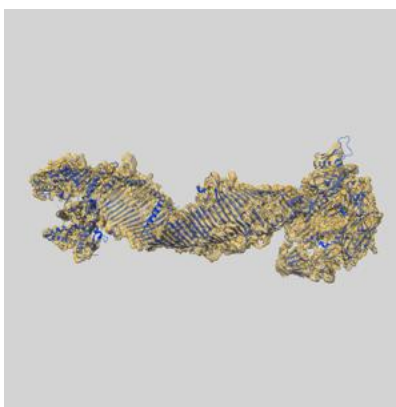
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73373 and PDB model 9YRP. Per-residue inclusion information can be found in section [3](#) on page [5](#).

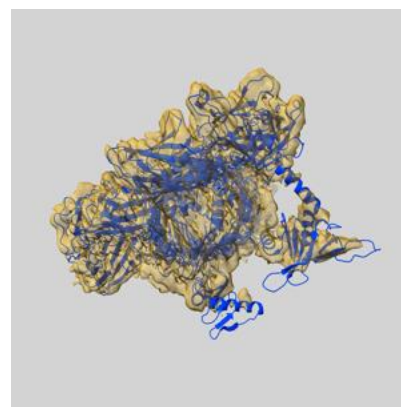
9.1 Map-model overlay [i](#)



X



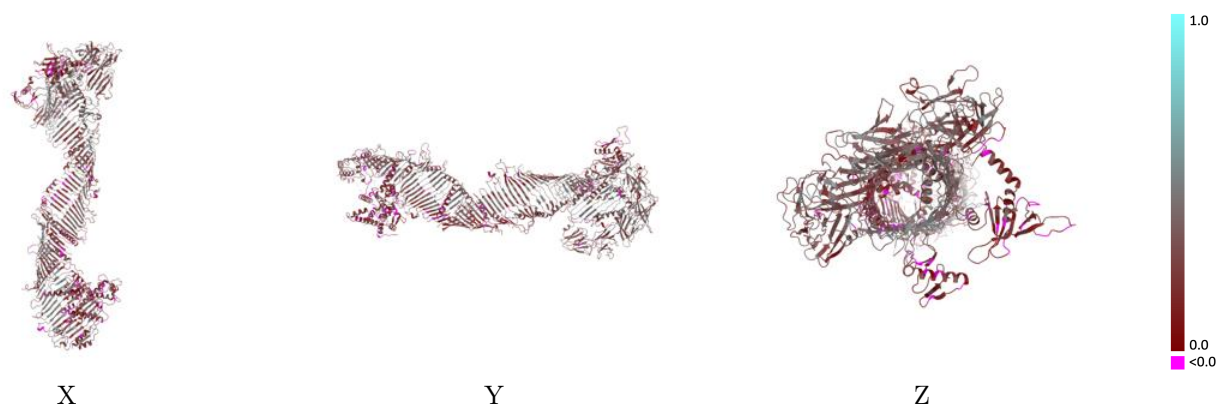
Y



Z

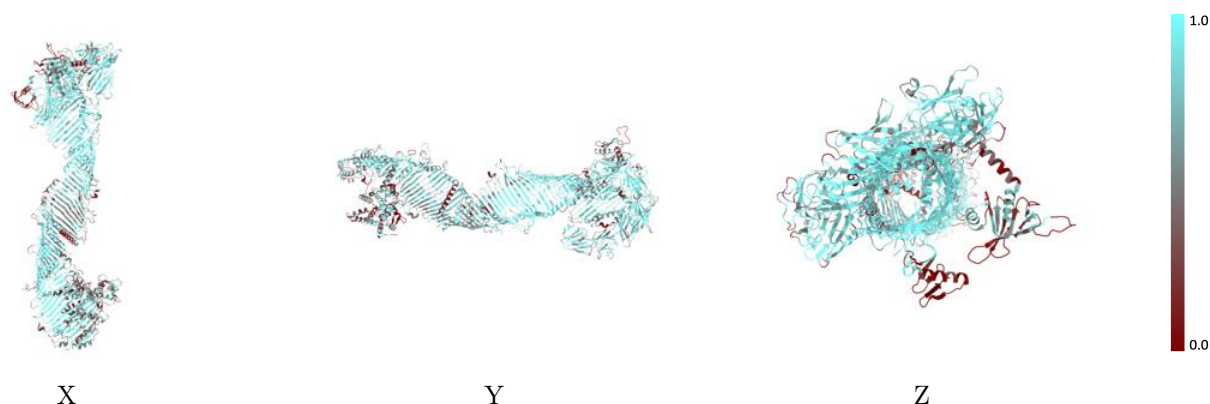
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



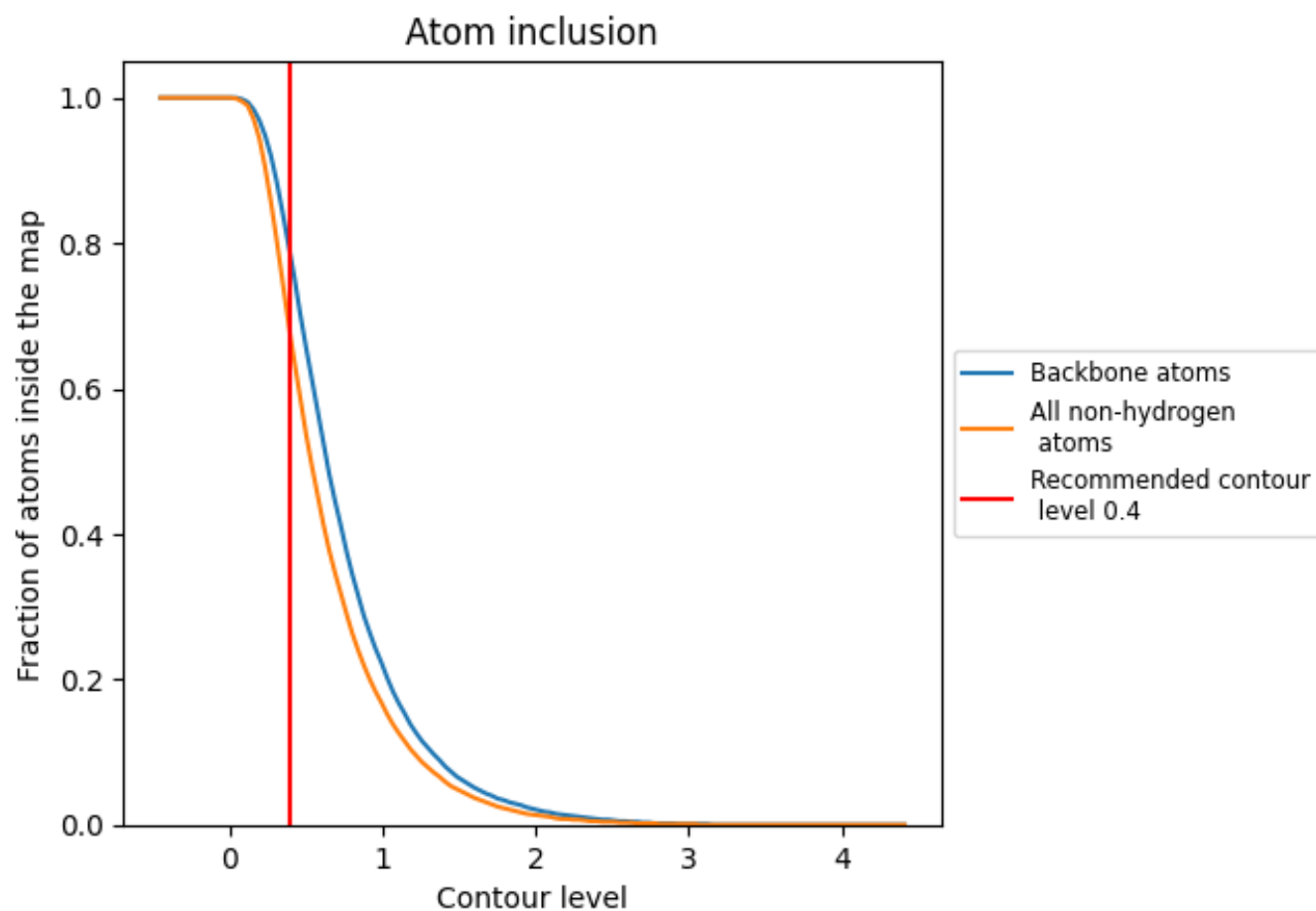
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6720	<div></div> 0.2850
A	<div></div> 0.4110	<div></div> 0.1850
B	<div></div> 0.6850	<div></div> 0.2900

