



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:51 PM UTC

PDB ID : 6R9T / pdb_00006r9t
EMDB ID : EMD-4772
Title : Cryo-EM structure of autoinhibited human talin-1
Authors : Dedden, D.; Schumacher, S.; Zacharias, M.; Biertumpfel, C.; Mizuno, N.
Deposited on : 2019-04-04
Resolution : 6.20 Å (reported)
Based on initial models : 5IC1, 3DYJ, 1SJ8, 2L7A, 3IVF, 2L10, 2L7N, 2JSW, 2LQG, 2KVP

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

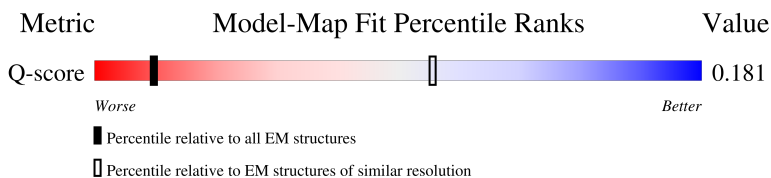
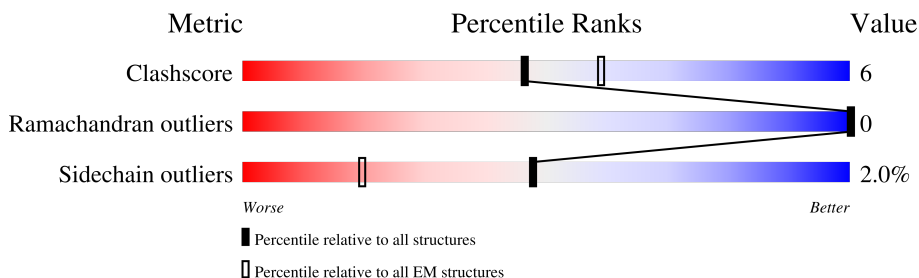
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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	537 (5.70 - 6.70)

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	2547	16% 71% 14% 14%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16011 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 Talin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2185	Total	C	N	O	S	0	0
			16011	9855	2859	3219	78		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2542	LEU	-	expression tag	UNP Q9Y490
A	2543	VAL	-	expression tag	UNP Q9Y490
A	2544	VAL	-	expression tag	UNP Q9Y490
A	2545	LEU	-	expression tag	UNP Q9Y490
A	2546	PHE	-	expression tag	UNP Q9Y490
A	2547	GLN	-	expression tag	UNP Q9Y490

A2403	T2404	L2407	N2412	A2413	A2414	V2415	Q2416	G2417	H2418	A2419	S2420	Q2421	E2422	K2423	S2427	V2431	A2432	A2441	C2442	K2443	D2447	Q2448	D2449	S2450	E2451	K2454	R2455	L2456	Q2457	N2461	A2462	N2469	L2470	A2473	A2474	Q2475	K2476	A2477	A2478	A2479	PHE	GLU	GLU	GLN	GLU	ASN	GLU	THR	VAL					
K2331	P2332	K2333	E2334	A2335	D2336	E2337	S2338	L2339	N2340	F2341	E2342	E2343	Q2344	L2345	L2346	E2347	S2351	A2354	A2355	A2358	L2359	S2364	Q2367	R2368	E2369	A2372	Q2373	Q2374	K2375	V2376	Q2377	A2378	L2379	P2380	A2381	N2382	A2383	L2384	D2385	D2386	G2387	Q2388	W2389	S2390	Q2391	L2392	L2393	L2394	S2395	R2398	A2402			
E2264	L2265	K2266	Q2267	Q2268	H2272	S2273	K2274	A2277	G2278	S2279	V2280	T2281	E2282	L2283	Q2284	Q2285	E2288	A2289	M2290	K2291	G2292	T2293	E2294	W2295	V2296	D2297	P2298	E2299	D2300	P2301	T2302	V2303	L2304	A2305	E2306	N2307	E2308	L2309	L2310	G2311	A2312	A2313	A2314	A2318	A2319	A2320	K2321	K2322	L2323	E2324	Q2325	P2326	R2329	A2330
F2160	C2161	S2162	E2163	P2165	P2166	A2167	K2168	T2169	E2177	H2178	T2179	K2180	A2192	G2193	N2194	S2195	C2196	E2197	Q2198	V2201	N2206	R2209	R2210	D2214	C2219	K2220	A2221	A2222	A2223	E2227	V2228	D2231	L2234	L2237	H2238	Y2239	G2240	G2246	H2253	L2258	Q2259	K2260	P2263											
P2074	E2075	Q2077	A2083	V2084	A2090	A2097	T2098	K2099	A2100	A2101	A2102	G2103	K2104	V2105	G2106	D2107	D2108	P2109	A2110	W2111	W2112	Q2113	L2114	K2115	N2116	S2117	A2118	V2122	S2127	L2128	L2129	K2130	T2131	V2132	K2133	E2136	D2137	E2138	A2139	T2140	K2141	G2142	T2143	R2144	T2149	R2154	Q2155	E2156	L2157					
E1952	R1955	R1956	V1957	K1960	V1964	L1965	R1973	A1984	G1987	D1991	T1995	F1998	A1999	T2000	A2001	G2002	T2003	L2004	N2005	R2006	E2007	G2008	T2009	E2010	T2011	H2015	R2016	E2017	G2018	I2019	L2020	V2025	V2034	Q2035	N2036	V2062	K2063	L2064	G2065	A2066	G2070	A2071	E2072	D2073										
G1826	S1830	I1831	T1832	Q1833	A1834	T1835	D1839	P1842	M1843	G1844	E1845	P1846	E1847	G1848	Y1853	V1858	R1859	A1886	M1887	L1889	T1890	Y1893	G1894	R1895	L1896	E1899	A1900	K1901	A1904	V1905	E1908	R1919	V1920	Q1921	H1925	T1932	L1937	Q1938	C1939	S1942	T1946	K1947												
L1675	A1682	A1688	P1689	R1690	E1691	G1692	I1693	H1699	A1719	A1722	E1723	A1724	S1725	Q1726	L1727	G1728	H1729	S1732	T1742	K1751	S1754	Q1757	Q1758	L1776	K1780	E1781	K1787	Q1788	T1792	A1799	V1800	Q1801	M1802	M1803	T1804	E1805	T1813	E1816	V1824	G1825														
M1538	L1539	V1540	T1541	T1542	I1543	K1544	A1545	L1546	E1547	G1548	A1549	F1550	T1551	E1552	E1553	R1554	A1555	Q1557	C1558	R1559	A1560	A1561	T1562	L1572	S1582	S1583	I1584	Q1587	V1600	R1618	P1624	R1625	D1626	P1627	V1632	H1636	S1637	T1648	M1651	K1654	A1655	P1656	G1657	Q1658	C1671	L1672								
Q1356	A1357	Q1360	K1361	E1375	E1378	M1387	S1388	Y1389	E1405	A1406	T1408	G1409	I1410	A1441	Q1442	V1449	S1450	Q1455	G1457	Q1458	Q1459	G1460	L1461	T1474	G1482	E1483	P1484	G1485	C1486	Q1490	V1498	L1511	A1512	S1513	A1514	R1515	T1516	Q1527	K1530	M1534														
S1225	D1226	S1227	L1228	P1229	P1230	T1231	T1232	G1233	F1235	Q1239	S1240	R1241	A1246	N1250	A1259	S1260	R1261	G1262	E1287	Q1291	A1292	P1293	E1296	D1297	R1298	V1301	T1303	Q1306	K1314	L1317	L1322	D1325	L1335	R1340	T1343	N1347	Q1348	L1349	T1350	T1351	Q1355													
1987	A988	Q991	M1000	V1001	L1027	C1045	M1050	D1051	L1054	G1081	E1082	T1095	S1099	I1102	N1113	E1114	Y1115	A1117	A1173	S1181	R1184	V1192	T1193	Q1194	A1195	L1196	N1197	R1198	L1203	Q1206	R1207	M1211	D1218	A1219	S1220	L1223	L1224																	
G876	A877	A878	A879	H880	P881	D882	S883	E884	Q885	Q886	Q887	Q888	R889	L890	R891	E892	A893	A894	E895	G896	L897	R898	M899	A900	T901	N902	Q906	N907	K910	K911	K912	L913	R916	A933	H937	S940	T941	P942	K943	A944	A946	G947	P948	Q949	L952	V953	C956	K957	L984					

VAL	VAL	LYS	GLU	LYS	MET	VAL	GLY	ILE	ALA	GLN	ILE	ILE	ALA	GLN	GLU	MET	LEU	LYS	ARG	ARG	GLU	LEU	GLU	GLU	ALA	ARG	LYS	LYS	LEU	ALA	GLN	ILE	ARG	GLN	GLN	TYR	LYS	PHE	LEU	PRO	SER	GLU	LEU	ARG	ASP	GLU	HIS	LEU	VAL	VAL	LEU	PHE	GLN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30438	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	76.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.089	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0232	Depositor
Map size (Å)	237.43999, 237.43999, 237.43999	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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	0/16192	0.37	0/21946

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	16011	0	16175	197	0
All	All	16011	0	16175	197	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 6.

All (197) 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:280:PHE:O	1:A:283:HIS:HB2	1.97	0.65
1:A:1998:PHE:HB3	1:A:2004:LEU:HB2	1.80	0.63
1:A:1919:ARG:HB3	1:A:1964:VAL:HG12	1.82	0.61
1:A:608:LEU:HG	1:A:654:GLN:HB3	1.84	0.60
1:A:2020:LEU:HD22	1:A:2129:LEU:HD23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLY:HA3	1:A:722:VAL:HA	1.86	0.58
1:A:2142:GLY:H	1:A:2198:GLN:HB3	1.69	0.58
1:A:329:LEU:HB2	1:A:340:VAL:HB	1.85	0.57
1:A:244:GLN:NE2	1:A:289:MET:O	2.38	0.57
1:A:1246:ALA:O	1:A:1250:ASN:ND2	2.38	0.56
1:A:1937:LEU:HD13	1:A:1946:THR:HB	1.88	0.56
1:A:262:LEU:HD11	1:A:276:GLU:HB2	1.88	0.56
1:A:2034:VAL:HG12	1:A:2114:LEU:HG	1.88	0.56
1:A:2108:ASP:HB3	1:A:2111:VAL:HG23	1.88	0.55
1:A:2075:GLU:O	1:A:2206:ASN:ND2	2.39	0.55
1:A:1654:LYS:HE2	1:A:1656:PRO:HB3	1.88	0.54
1:A:2210:ARG:NH1	1:A:2214:ASP:OD2	2.40	0.54
1:A:1690:ARG:HD2	1:A:1693:ILE:HB	1.88	0.54
1:A:797:ARG:NH1	1:A:1045:CYS:SG	2.81	0.54
1:A:2130:LYS:NZ	1:A:2144:ARG:O	2.40	0.54
1:A:1632:VAL:O	1:A:1636:HIS:ND1	2.39	0.54
1:A:221:ASP:O	1:A:225:ASN:ND2	2.42	0.53
1:A:660:THR:OG1	1:A:665:GLN:NE2	2.41	0.53
1:A:1351:THR:HA	1:A:1361:LYS:HE3	1.90	0.53
1:A:1113:ASN:ND2	1:A:1173:ALA:O	2.42	0.53
1:A:1816:GLU:OE2	1:A:1887:ASN:ND2	2.41	0.53
1:A:2113:GLN:HA	1:A:2116:ASN:HB3	1.90	0.53
1:A:503:MET:HG2	1:A:623:LEU:HD13	1.91	0.53
1:A:2329:ARG:NH1	1:A:2412:ASN:OD1	2.42	0.53
1:A:623:LEU:O	1:A:627:GLN:NE2	2.41	0.53
1:A:1360:GLN:HB3	1:A:1618:ARG:HE	1.73	0.53
1:A:685:LYS:HE2	1:A:765:ARG:HH21	1.73	0.52
1:A:1355:GLN:HG2	1:A:1357:ALA:H	1.74	0.52
1:A:515:ASP:O	1:A:592:LYS:NZ	2.42	0.52
1:A:561:THR:O	1:A:634:ARG:NH1	2.43	0.52
1:A:2149:THR:HA	1:A:2209:ARG:HH11	1.75	0.52
1:A:2228:VAL:HG13	1:A:2290:MET:HB2	1.92	0.52
1:A:1340:ARG:NH1	1:A:1343:THR:OG1	2.43	0.52
1:A:543:ILE:HA	1:A:546:GLN:HE21	1.73	0.51
1:A:1224:LEU:HD21	1:A:1306:LYS:HD3	1.92	0.51
1:A:741:ARG:NH2	1:A:1939:CYS:SG	2.83	0.51
1:A:952:LEU:O	1:A:956:CYS:N	2.41	0.51
1:A:661:ASP:OD2	1:A:663:HIS:ND1	2.43	0.51
1:A:1203:LEU:O	1:A:1206:GLN:NE2	2.43	0.51
1:A:550:ILE:HA	1:A:580:ILE:HG12	1.92	0.50
1:A:2389:TRP:NE1	1:A:2441:ALA:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2407:LEU:HD22	1:A:2431:VAL:HG11	1.93	0.50
1:A:2413:ALA:HB1	1:A:2418:HIS:HB3	1.93	0.50
1:A:1952:GLU:HA	1:A:1955:ARG:HE	1.77	0.50
1:A:702:VAL:HG22	1:A:753:ALA:HB1	1.94	0.50
1:A:1534:ASN:O	1:A:1538:ASN:ND2	2.45	0.49
1:A:852:ASN:O	1:A:856:LEU:N	2.46	0.49
1:A:1693:ILE:O	1:A:1751:LYS:NZ	2.46	0.49
1:A:2179:THR:HG22	1:A:2280:VAL:HG13	1.93	0.49
1:A:1458:GLN:HB3	1:A:1584:ILE:HD12	1.93	0.49
1:A:1407:MET:HE3	1:A:1637:SER:HB2	1.94	0.49
1:A:2282:GLU:OE1	1:A:2285:GLN:NE2	2.44	0.49
1:A:1671:CYS:HB2	1:A:1742:THR:HG21	1.93	0.49
1:A:1788:GLN:HE21	1:A:1792:THR:HG21	1.77	0.49
1:A:367:THR:HA	1:A:378:TYR:O	2.12	0.48
1:A:1682:ALA:O	1:A:1758:GLN:NE2	2.46	0.48
1:A:1001:VAL:HG22	1:A:1027:LEU:HD13	1.96	0.48
1:A:1558:CYS:O	1:A:1562:THR:OG1	2.31	0.48
1:A:2274:LYS:O	1:A:2278:GLY:N	2.45	0.48
1:A:243:CYS:SG	1:A:283:HIS:NE2	2.84	0.48
1:A:275:GLY:O	1:A:278:LYS:HB3	2.12	0.48
1:A:1405:GLU:O	1:A:1409:GLY:N	2.46	0.48
1:A:1474:ILE:HG12	1:A:1498:VAL:HG13	1.95	0.48
1:A:2201:VAL:HG21	1:A:2258:LEU:HD21	1.96	0.48
1:A:1858:VAL:HG12	1:A:1965:LEU:HD22	1.94	0.48
1:A:277:ARG:O	1:A:281:GLN:N	2.44	0.48
1:A:289:MET:SD	1:A:297:ARG:NH1	2.87	0.48
1:A:517:ASP:HA	1:A:596:ALA:HB2	1.96	0.48
1:A:2227:GLU:HB3	1:A:2292:GLY:HA3	1.96	0.48
1:A:1181:SER:HA	1:A:1184:ARG:HE	1.78	0.47
1:A:1512:ALA:O	1:A:1516:THR:OG1	2.29	0.47
1:A:1824:VAL:HG21	1:A:1932:THR:HA	1.95	0.47
1:A:1648:ILE:HA	1:A:1651:MET:HE2	1.96	0.47
1:A:229:PRO:HD2	1:A:307:THR:HB	1.95	0.47
1:A:953:VAL:HA	1:A:956:CYS:HB2	1.96	0.47
1:A:621:GLU:OE2	1:A:624:ARG:NH2	2.43	0.47
1:A:794:PRO:HA	1:A:912:LYS:HD3	1.96	0.47
1:A:2118:ALA:O	1:A:2122:VAL:N	2.46	0.47
1:A:748:GLU:HA	1:A:751:VAL:HG12	1.97	0.47
1:A:1527:GLN:HA	1:A:1530:LYS:HB3	1.97	0.47
1:A:2101:ALA:HA	1:A:2104:LYS:HD2	1.97	0.47
1:A:913:LEU:HA	1:A:916:ARG:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1672:LEU:HD23	1:A:1675:LEU:HD12	1.97	0.47
1:A:1835:ILE:HG12	1:A:1921:GLN:HG2	1.97	0.47
1:A:272:LYS:HD2	1:A:2288:GLU:HG2	1.97	0.46
1:A:1455:GLN:HB3	1:A:1587:GLN:HB3	1.97	0.46
1:A:2001:ALA:HA	1:A:2443:LYS:HD3	1.97	0.46
1:A:840:ILE:HG23	1:A:856:LEU:HB3	1.95	0.46
1:A:1114:GLU:HG2	1:A:1116:TYR:H	1.80	0.46
1:A:1987:GLY:O	1:A:1991:ASP:N	2.47	0.46
1:A:1723:GLU:HG3	1:A:1726:GLN:H	1.81	0.46
1:A:274:LYS:HD2	1:A:2285:GLN:HB3	1.98	0.46
1:A:937:HIS:O	1:A:941:THR:OG1	2.33	0.46
1:A:2138:GLU:HA	1:A:2141:LYS:HB2	1.97	0.46
1:A:786:LYS:HA	1:A:789:ALA:HB3	1.97	0.46
1:A:1356:GLN:HG2	1:A:1361:LYS:HD3	1.98	0.46
1:A:748:GLU:OE2	1:A:1942:SER:OG	2.34	0.46
1:A:848:SER:O	1:A:1956:ARG:NH2	2.49	0.46
1:A:1000:MET:HE2	1:A:1000:MET:HB3	1.76	0.46
1:A:1450:SER:HA	1:A:1725:SER:HB2	1.97	0.46
1:A:1511:LEU:O	1:A:1515:ARG:NH2	2.48	0.46
1:A:2177:ARG:HD3	1:A:2388:GLN:HB3	1.97	0.46
1:A:1957:VAL:HA	1:A:1960:LYS:HB2	1.96	0.46
1:A:1241:ARG:NH2	1:A:1287:GLU:OE1	2.45	0.46
1:A:1347:ASN:O	1:A:1351:THR:OG1	2.34	0.46
1:A:1455:GLN:NE2	1:A:1456:ALA:O	2.43	0.46
1:A:2253:HIS:NE2	1:A:2268:GLN:OE1	2.41	0.45
1:A:2240:GLY:HA2	1:A:2283:LEU:HD11	1.98	0.45
1:A:1192:VAL:O	1:A:1196:LEU:N	2.46	0.45
1:A:1051:ASP:N	1:A:1051:ASP:OD1	2.48	0.45
1:A:2194:ASN:HA	1:A:2266:LYS:HD3	1.98	0.45
1:A:550:ILE:HG12	1:A:580:ILE:HA	1.99	0.45
1:A:683:VAL:HG22	1:A:706:ALA:HB1	1.98	0.45
1:A:2193:GLY:O	1:A:2266:LYS:NZ	2.48	0.45
1:A:984:LEU:HD23	1:A:987:ILE:HD12	1.98	0.45
1:A:266:LEU:HD13	1:A:270:TYR:HB3	1.98	0.45
1:A:1886:ALA:HA	1:A:1889:LEU:HD12	1.99	0.45
1:A:2160:PHE:O	1:A:2220:LYS:NZ	2.50	0.45
1:A:1261:ARG:NH2	1:A:1378:GLU:O	2.50	0.45
1:A:1540:VAL:HA	1:A:1543:ILE:HB	1.99	0.45
1:A:1826:GLY:O	1:A:1830:SER:N	2.50	0.45
1:A:1947:LYS:NZ	1:A:2334:GLU:OE2	2.45	0.45
1:A:1194:GLN:OE1	1:A:1198:ARG:NH2	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HE3	1:A:2296:VAL:HG11	1.98	0.44
1:A:1095:THR:HG23	1:A:1196:LEU:HD22	1.99	0.44
1:A:912:LYS:HE3	1:A:916:ARG:HE	1.83	0.44
1:A:1830:SER:HA	1:A:1833:GLN:HB2	1.98	0.44
1:A:250:HIS:CG	1:A:283:HIS:HB3	2.53	0.44
1:A:1314:LYS:HD3	1:A:1317:LEU:HD12	1.99	0.44
1:A:1832:THR:HA	1:A:1835:ILE:HB	1.99	0.44
1:A:1893:TYR:HA	1:A:1896:LEU:HD12	1.99	0.44
1:A:2062:VAL:HG21	1:A:2084:VAL:HG11	2.00	0.44
1:A:1301:VAL:HG13	1:A:1349:LEU:HD11	2.00	0.44
1:A:2140:THR:HB	1:A:2144:ARG:HD3	1.99	0.44
1:A:2309:LEU:HD22	1:A:2367:GLN:HB3	1.99	0.44
1:A:279:ILE:O	1:A:283:HIS:ND1	2.47	0.43
1:A:582:SER:HB3	1:A:933:ALA:HB1	2.00	0.43
1:A:352:ASN:ND2	1:A:354:THR:OG1	2.51	0.43
1:A:1389:TYR:OH	1:A:1651:MET:O	2.36	0.43
1:A:599:GLU:HA	1:A:603:GLY:HA2	1.99	0.43
1:A:1886:ALA:O	1:A:1890:THR:N	2.52	0.43
1:A:2066:ALA:O	1:A:2077:GLN:NE2	2.51	0.43
1:A:489:THR:HG23	1:A:492:GLN:H	1.83	0.43
1:A:2234:LEU:HA	1:A:2237:LEU:HB2	2.00	0.43
1:A:519:LEU:HD12	1:A:520:PRO:HD2	2.01	0.43
1:A:2398:ARG:O	1:A:2402:ALA:N	2.52	0.43
1:A:2342:GLU:HG2	1:A:2415:VAL:HA	1.99	0.43
1:A:2443:LYS:HD2	1:A:2448:GLN:HG3	2.01	0.43
1:A:632:GLU:OE1	1:A:636:ASN:ND2	2.52	0.42
1:A:1050:MET:HE2	1:A:1117:ALA:HB3	2.00	0.42
1:A:1921:GLN:O	1:A:1925:HIS:ND1	2.47	0.42
1:A:1799:ALA:HA	1:A:1802:MET:HB2	2.01	0.42
1:A:278:LYS:O	1:A:281:GLN:HB3	2.19	0.42
1:A:2127:SER:O	1:A:2131:THR:N	2.49	0.42
1:A:2277:ALA:HA	1:A:2280:VAL:HB	2.00	0.42
1:A:519:LEU:HD22	1:A:596:ALA:HB1	2.02	0.42
1:A:618:ALA:HB1	1:A:644:VAL:HG22	2.01	0.42
1:A:1322:LEU:HD22	1:A:1335:LEU:HD13	2.02	0.42
1:A:2019:ILE:HG22	1:A:2128:LEU:HD21	2.02	0.42
1:A:683:VAL:O	1:A:687:LYS:N	2.53	0.42
1:A:2166:PRO:HG2	1:A:2221:GLU:HA	2.01	0.42
1:A:291:GLU:HG2	1:A:295:LYS:HE3	2.01	0.42
1:A:318:LYS:HD2	1:A:323:ASN:HA	2.00	0.42
1:A:1947:LYS:HB3	1:A:1947:LYS:HE2	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:OD1	1:A:372:ASP:N	2.51	0.42
1:A:504:GLN:O	1:A:507:GLN:NE2	2.53	0.42
1:A:1229:PRO:HA	1:A:1230:PRO:HD3	1.94	0.41
1:A:1551:THR:HB	1:A:1554:ASN:HB2	2.02	0.41
1:A:2355:ALA:O	1:A:2359:LEU:N	2.52	0.41
1:A:276:GLU:O	1:A:280:PHE:N	2.48	0.41
1:A:1218:ASP:N	1:A:1218:ASP:OD1	2.53	0.41
1:A:1688:ALA:HA	1:A:1689:PRO:HD3	1.94	0.41
1:A:2180:LYS:NZ	1:A:2381:ALA:O	2.53	0.41
1:A:2309:LEU:HD21	1:A:2364:SER:HA	2.02	0.41
1:A:988:ALA:O	1:A:991:GLN:NE2	2.50	0.41
1:A:1729:HIS:O	1:A:1732:SER:OG	2.36	0.41
1:A:1754:SER:HB3	1:A:1757:GLN:HB2	2.03	0.41
1:A:507:GLN:H	1:A:507:GLN:HG3	1.68	0.41
1:A:2336:ASP:HB2	1:A:2417:GLY:HA3	2.02	0.41
1:A:1099:SER:HA	1:A:1102:ILE:HD12	2.02	0.41
1:A:1387:MET:O	1:A:1442:GLN:NE2	2.54	0.41
1:A:2099:LYS:HE2	1:A:2099:LYS:HB3	1.88	0.40
1:A:1800:VAL:O	1:A:1804:THR:OG1	2.35	0.40
1:A:2165:PRO:HA	1:A:2166:PRO:HD3	1.90	0.40
1:A:1901:LYS:HE2	1:A:1901:LYS:HB3	1.88	0.40
1:A:2109:PRO:O	1:A:2113:GLN:N	2.52	0.40
1:A:680:ALA:HA	1:A:683:VAL:HB	2.03	0.40
1:A:1658:GLN:HE22	1:A:1780:LYS:HG2	1.85	0.40
1:A:2345:ILE:HG23	1:A:2470:LEU:HD11	2.04	0.40
1:A:801:ALA:HB3	1:A:836:LEU:HB2	2.03	0.40
1:A:897:LEU:O	1:A:901:THR:OG1	2.34	0.40
1:A:1556:ALA:HA	1:A:1559:ARG:HB2	2.04	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	2181/2547 (86%)	2150 (99%)	31 (1%)	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	1668/1992 (84%)	1635 (98%)	33 (2%)	48	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	SER
1	A	369	ASP
1	A	380	VAL
1	A	515	ASP
1	A	517	ASP
1	A	522	LEU
1	A	525	ASP
1	A	627	GLN
1	A	726	THR
1	A	727	ILE
1	A	736	LEU
1	A	778	LEU
1	A	1051	ASP
1	A	1054	LEU
1	A	1223	LEU
1	A	1405	GLU
1	A	1410	ILE
1	A	1449	VAL
1	A	1542	THR
1	A	1562	THR
1	A	1572	LEU
1	A	1600	VAL
1	A	1776	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1813	THR
1	A	1905	VAL
1	A	1964	VAL
1	A	1995	THR
1	A	2025	VAL
1	A	2111	VAL
1	A	2295	TRP
1	A	2297	ASP
1	A	2347	GLU
1	A	2418	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	GLN
1	A	225	ASN
1	A	352	ASN
1	A	390	GLN
1	A	500	ASN
1	A	507	GLN
1	A	510	GLN
1	A	524	GLN
1	A	546	GLN
1	A	583	ASN
1	A	636	ASN
1	A	665	GLN
1	A	788	HIS
1	A	825	GLN
1	A	838	ASN
1	A	949	GLN
1	A	974	GLN
1	A	1019	GLN
1	A	1026	ASN
1	A	1065	GLN
1	A	1113	ASN
1	A	1133	GLN
1	A	1236	GLN
1	A	1239	GLN
1	A	1250	ASN
1	A	1265	GLN
1	A	1360	GLN
1	A	1416	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1453	ASN
1	A	1459	GLN
1	A	1488	GLN
1	A	1538	ASN
1	A	1658	GLN
1	A	1669	ASN
1	A	1869	GLN
1	A	1909	ASN
1	A	1921	GLN
1	A	1963	HIS
1	A	2036	ASN
1	A	2077	GLN
1	A	2113	GLN
1	A	2116	ASN
1	A	2388	GLN
1	A	2406	ASN
1	A	2418	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

There are no chain breaks in this entry.

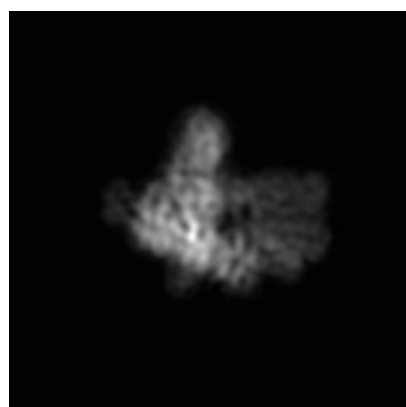
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4772. These allow visual inspection of the internal detail of the map and identification of artifacts.

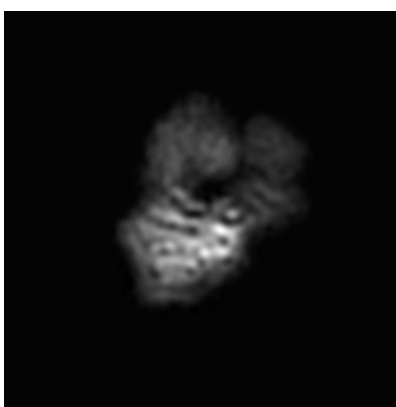
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

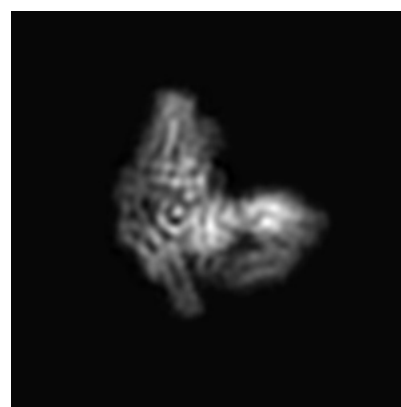
6.1.1 Primary map



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: 112



Y Index: 112



Z Index: 112

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

6.3 Largest variance slices [i](#)

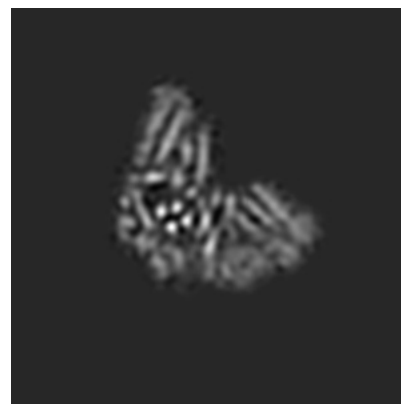
6.3.1 Primary map



X Index: 89



Y Index: 102

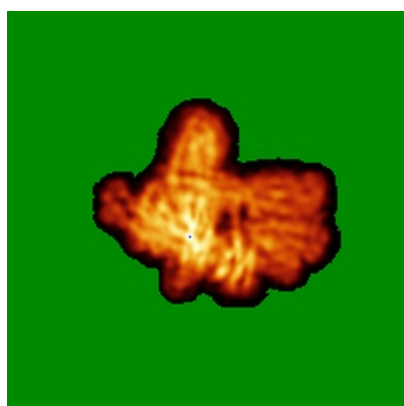


Z Index: 94

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

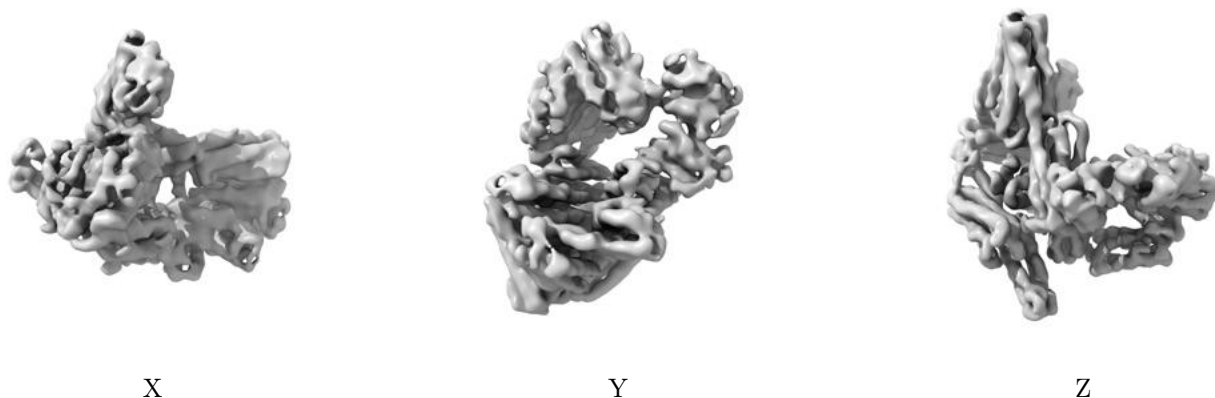


Z

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 0.0232. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

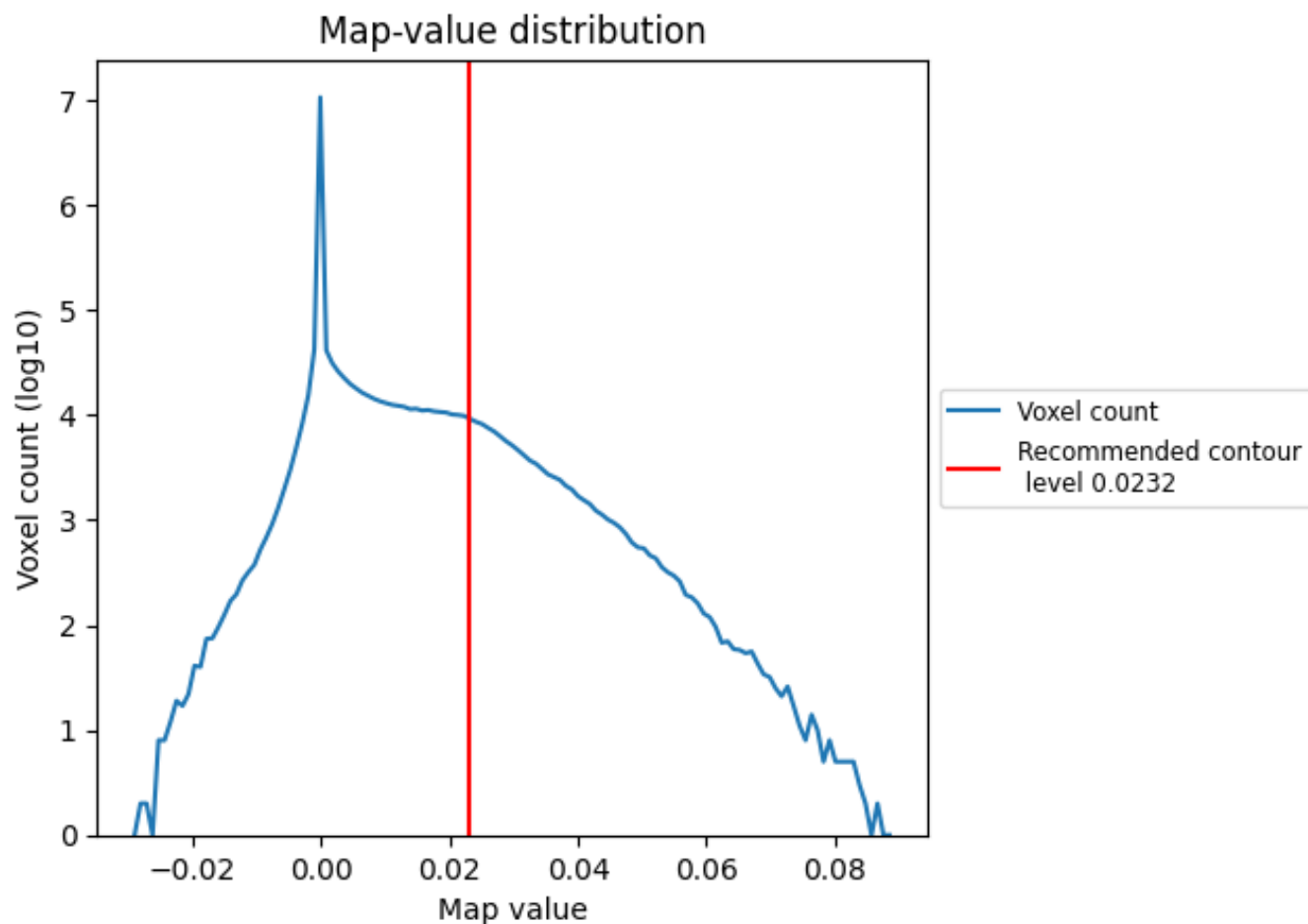
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

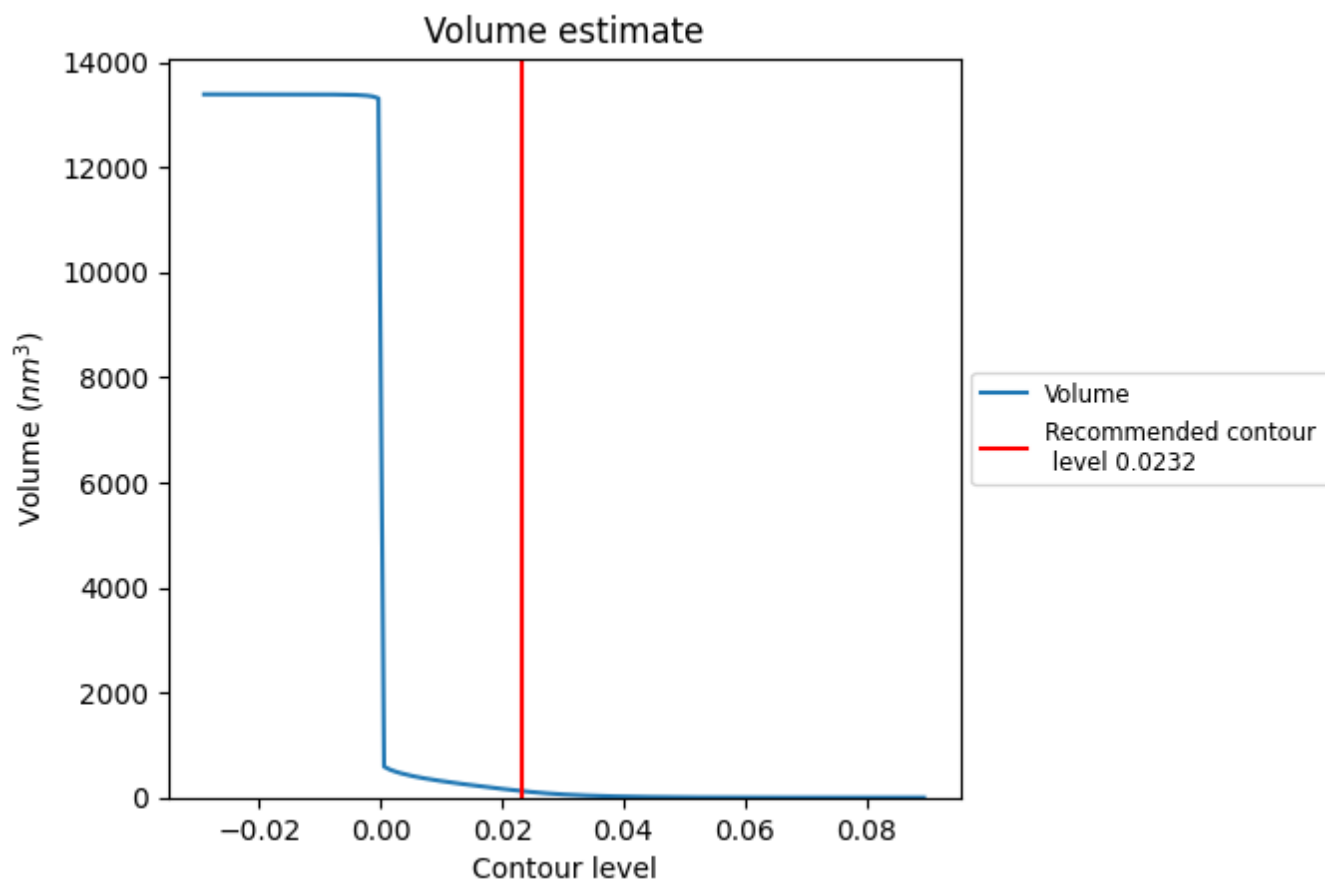
This section contains the results of statistical analysis of the map.

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.

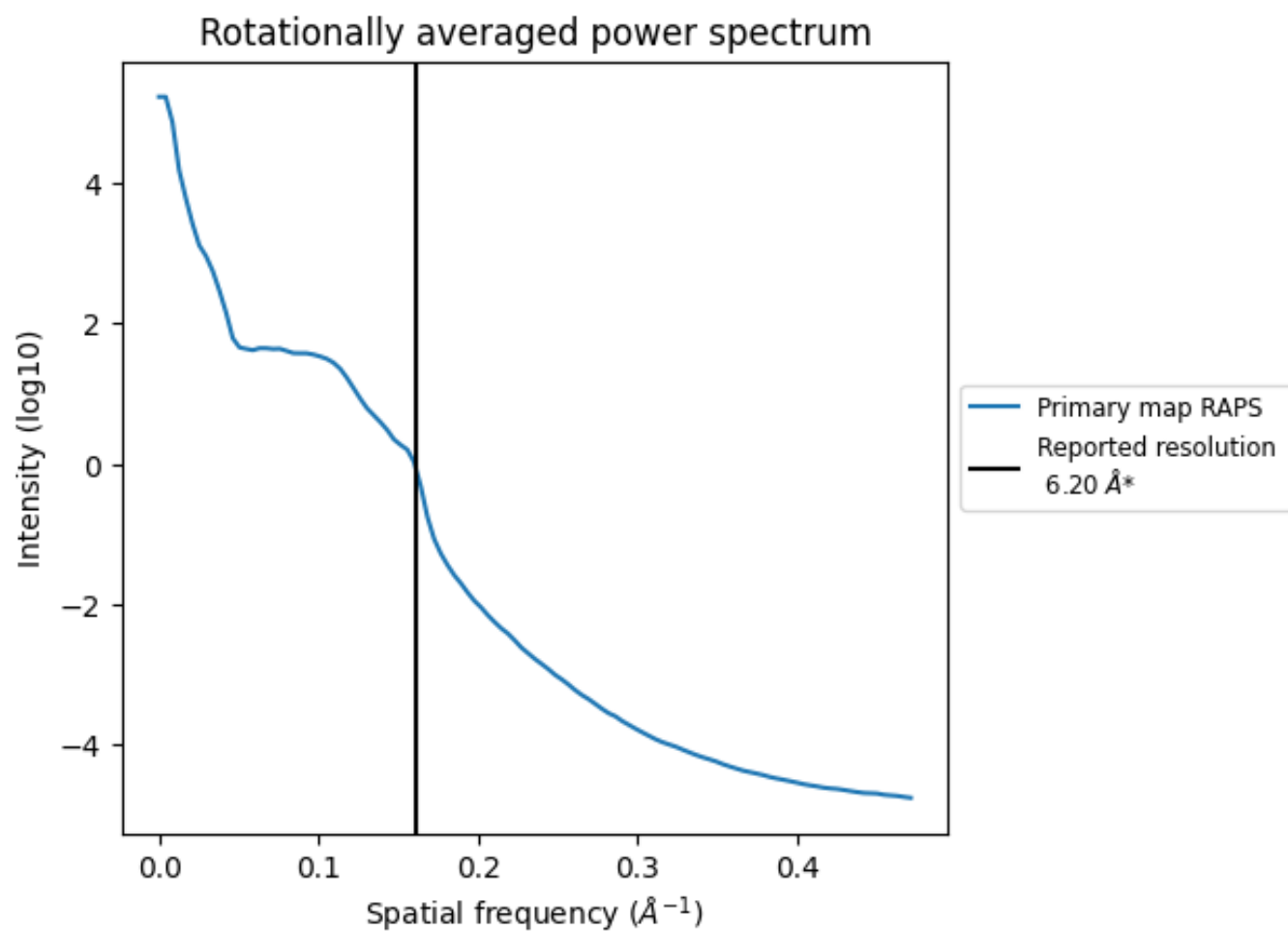
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 125 nm^3 ; this corresponds to an approximate mass of 113 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 0.161 Å⁻¹

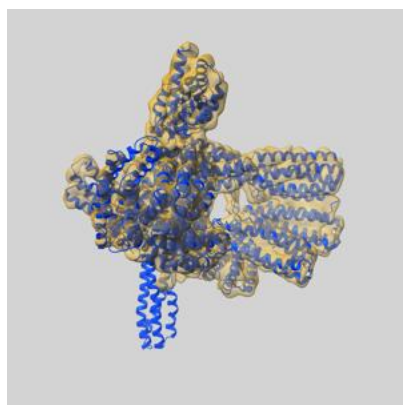
8 Fourier-Shell correlation

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

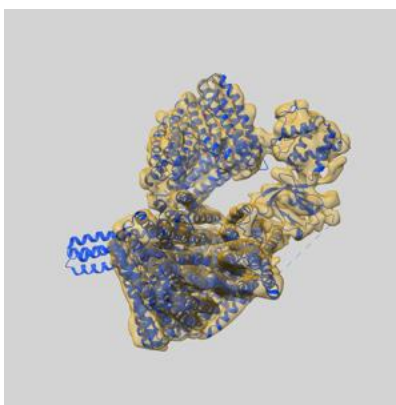
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4772 and PDB model 6R9T. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

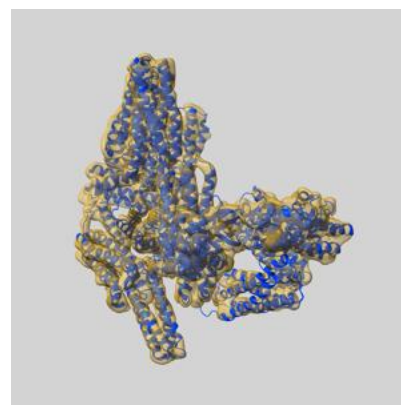
9.1 Map-model overlay [i](#)



X



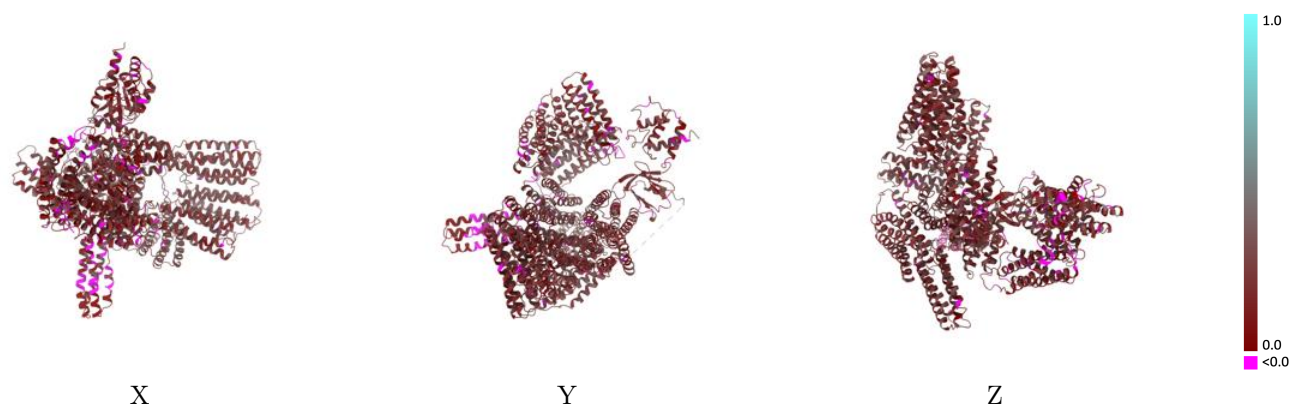
Y



Z

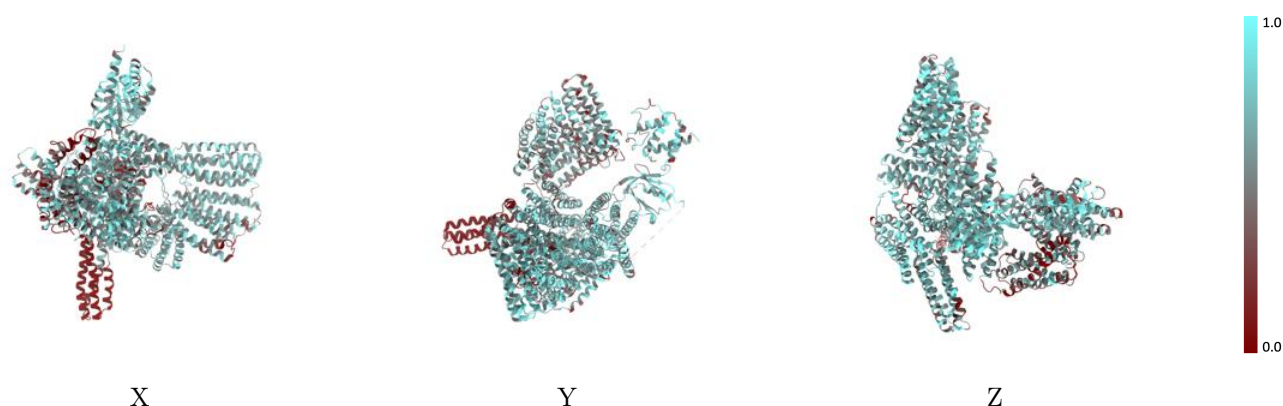
The images above show the 3D surface view of the map at the recommended contour level 0.0232 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



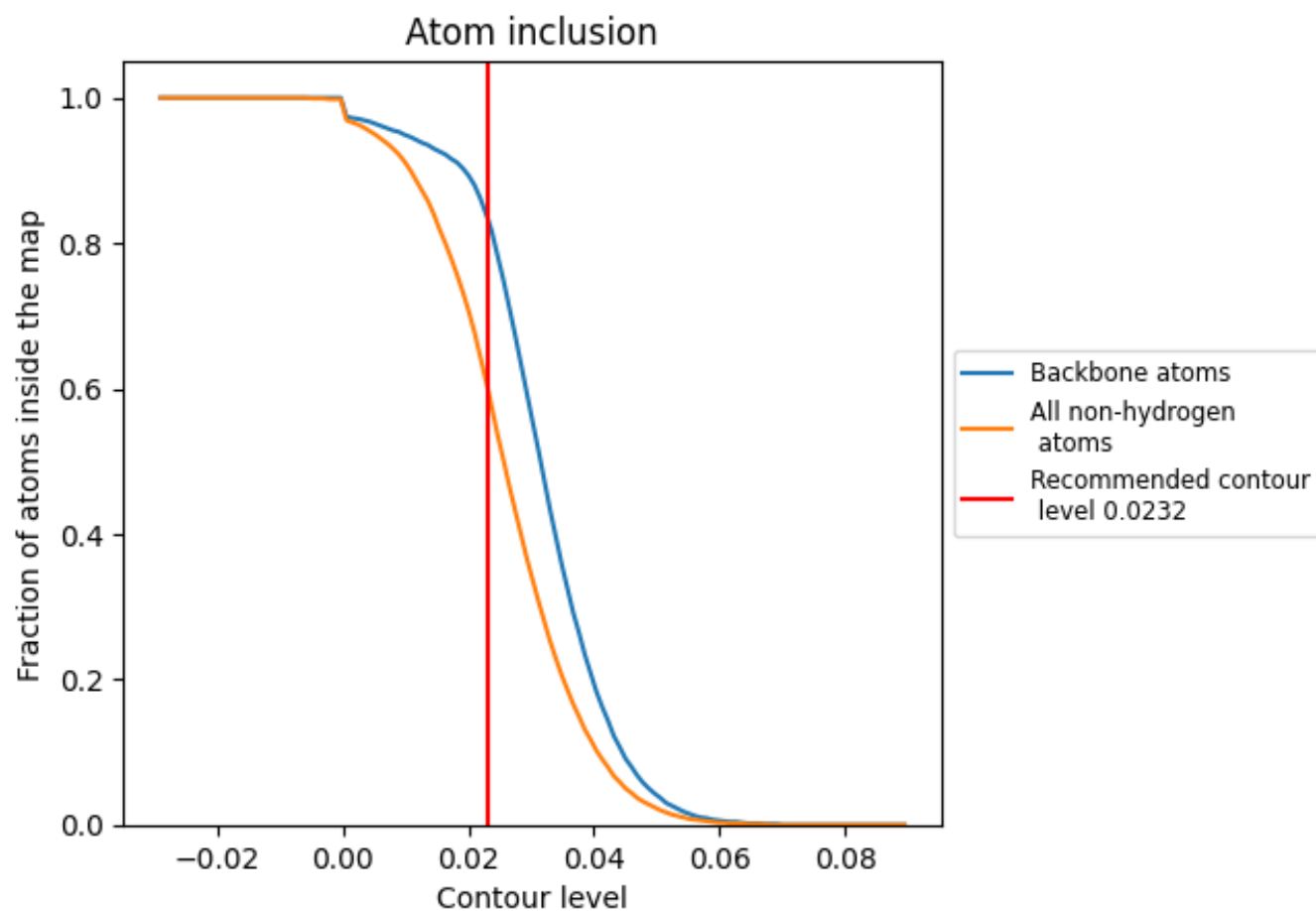
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0232).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 60% 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 (0.0232) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5960	0.1810
A	0.5960	0.1810

