



## wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 09:52 AM UTC

PDB ID : 9I1I / pdb\_00009i1i  
EMDB ID : EMD-52570  
Title : Cryo-EM structure of mouse RNF213 (WB3/WB4 + ATP)  
Authors : Grabarczyk, D.B.; Ahel, J.; Clausen, T.  
Deposited on : 2025-01-16  
Resolution : 4.50 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
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

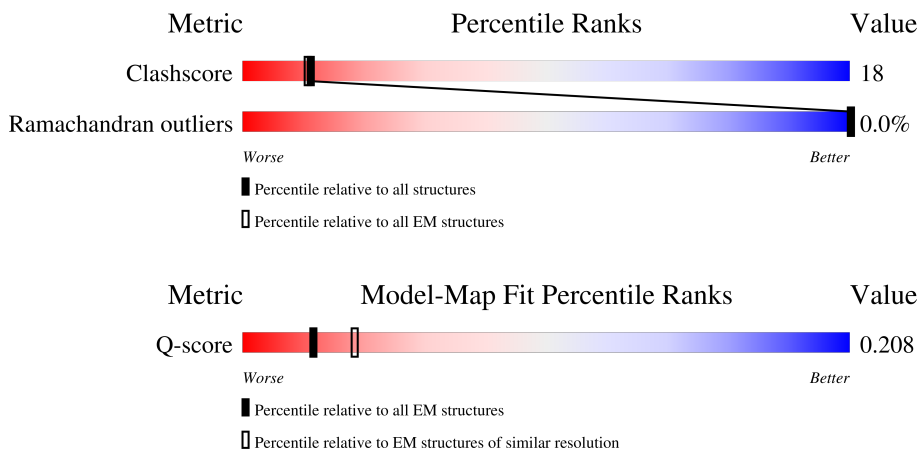
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	2937 ( 4.00 - 5.00 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5161	<div> <div>8%</div> <div>54%</div> <div>35%</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36852 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.

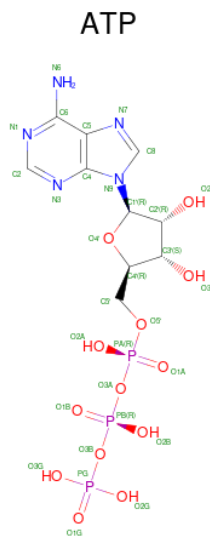
- Molecule 1 is a protein called E3 ubiquitin-protein ligase RNF213.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4584	Total	C	N	O	S	0	0
			36787	23443	6326	6799	219		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2449	GLN	GLU	engineered mutation	UNP E9Q555
A	2806	GLN	GLU	engineered mutation	UNP E9Q555
A	5149	GLY	-	expression tag	UNP E9Q555
A	5150	GLY	-	expression tag	UNP E9Q555
A	5151	GLY	-	expression tag	UNP E9Q555
A	5152	HIS	-	expression tag	UNP E9Q555
A	5153	HIS	-	expression tag	UNP E9Q555
A	5154	HIS	-	expression tag	UNP E9Q555
A	5155	HIS	-	expression tag	UNP E9Q555
A	5156	HIS	-	expression tag	UNP E9Q555
A	5157	HIS	-	expression tag	UNP E9Q555
A	5158	HIS	-	expression tag	UNP E9Q555
A	5159	HIS	-	expression tag	UNP E9Q555
A	5160	HIS	-	expression tag	UNP E9Q555
A	5161	HIS	-	expression tag	UNP E9Q555

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total 31	C 10	N 5	O 13	P 3	0
2	A	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	AltConf
4	A	2	Total Zn 2 2	0



E1685	A1686	A1687	L1688	M1689	M1690	L1691	S1692	K1697	K1698	T1699	V1700	V1704	Q1705	A1706	T1707	C1710	K1713	A1714	D1715	Y1717	C1718	L1719	L1720	E1721	V1722	M1723	K1724	K1725	Q1729	L1730	E1733	L1736	M1737	G1738	K1739	L1740	V1742	A1743	M1744	S1747	L1748	V1749	Y1750	M1751	S1752	A1753	L1754	L1755	P1756				
R1599	T1600	W1601	T1602	N1616	F1617	G1618	L1619	E1620	L1621	S1622	Q1623	L1624	E1625	D1630	V1631	T1632	Q1633	C1639	R1640	E1643	D1644	L1645	L1646	E1649	V1650	V1652	K1656	R1657	A1658	E1659	H1660	F1661	Y1662	L1663	N1664	Y1666	L1667	A1668	E1669	Q1670	L1671	V1672	Y1673	L1674	S1675	E1676	S1677	L1678	R1679	K1680	S1684		
G1416	E1417	N1418	D1419	H1429	Q1433	G1434	Y1435	R1445	D1450	H1454	L1455	Q1456	E1457	L1458	W1459	R1460	L1468	P1469	D1470	K1471	D1474	S1475	A1476	R1477	N1478	W1481	L1482	K1483	T1484	H1489	G1490	S1491	V1492	E1493	L1494	S1495	S1498	L1499	T1503	V1508	Y1509	V1510	H1511	E1512	G1517								
I1520	R1527	L1528	L1529	L1530	P1531	D1532	GLY	HIS	GLY	TYR	P1537	E1538	A1539	L1540	Y1543	L1548	K1549	E1550	L1551	L1552	M1553	K1554	L1555	M1556	L1557	M1558	S1559	G1560	K1561	H1564	S1565	N1566	T1567	L1568	E1569	V1570	E1571	E1575	M1580	Q1581	R1582	H1585	I1588	K1589	L1590	H1591	M1596	L1597	F1598				
R1599	T1600	W1601	T1602	N1616	F1617	G1618	L1619	E1620	L1621	S1622	Q1623	L1624	E1625	D1630	V1631	T1632	Q1633	C1639	R1640	E1643	D1644	L1645	L1646	E1649	V1650	V1652	K1656	R1657	A1658	E1659	H1660	F1661	Y1662	L1663	N1664	Y1666	L1667	A1668	E1669	Q1670	L1671	V1672	Y1673	L1674	S1675	E1676	S1677	L1678	R1679	K1680	S1684		
E1685	A1686	A1687	L1688	M1689	M1690	L1691	S1692	K1697	K1698	T1699	V1700	V1704	Q1705	A1706	T1707	C1710	K1713	A1714	D1715	Y1717	C1718	L1719	L1720	E1721	V1722	M1723	K1724	K1725	Q1729	L1730	E1733	L1736	M1737	G1738	K1739	L1740	V1742	A1743	M1744	S1747	L1748	V1749	Y1750	M1751	S1752	A1753	L1754	L1755	P1756				
G767	I768	S770	R771	L772	P773	G774	ASP	R776	K777	I778	S779	N780	M783	K784	L785	D786	E787	E788	N789	K792	M793	L794	M795	H796	L797	I800	Y801	Q802	H803	R804	F806	L815	T816	E817	C818	L819	H822	E823	N827	I828	T829	A830	N831	H832	Q833	F834	F835	L844	I845	C846			
K847	L848	L849	P854	GLY	HIS	THR	GLU	GLY	LEU	PRO	E863	K864	Y866	V870	T871	S872	T873	L874	Q875	E876	A877	L878	A879	T880	T881	W884	L885	Q886	S887	L888	F889	K890	S891	R892	M893	L894	S895	I896	S897	S898	A899	Y901	R902	L903	T904	Y905	E908	M909	A910	I1006	V911	W912	R913
R914	E917	E922	K923	K927	G932	D933	M934	E935	G936	L937	L938	K939	Q940	E941	P942	P943	R944	L945	Q946	I947	F950	C955	H961	E969	K970	C971	L972	I973	C980	Q983	T984	E988	G989	L990	S991	Q996	K997	F998	L1001	L1002	S1003	A1004	V1005	I1006	T1007	K1008							
S1009	W1010	V1011	V1012	H1013	N1014	G1015	E1016	P1017	V1018	F1019	D1020	V1021	F1025	K1026	Y1027	L1028	L1029	K1030	W1031	D1032	P1033	V1034	L1037	L1040	T1043	M1044	E1045	K1046	D1049	M1050	T1051	T1052	R1056	M1059	V1065	V1069	A1070	L1073	G1076	T1077	V1080	G1081	L1083	E1084	L1085	I1086							
L1087	E1088	H1089	Q1090	S1091	Q1092	F1093	I1096	W1097	R1101	R1102	R1103	LEU	PRO	SER	GLN	GLU	LYS	ALA	CYS	D1112	V1113	R1114	S1115	K1118	R1119	R1120	R1121	L1124	L1127	K1128	Q1129	E1130	K1131	Y1132	L1137	L1138	R1139	Q1140	R1143	V1144	K1145	H1146	L1147	V1150	D1151	F1152	I1155	L1168					
L1175	PRO	ASN	SER	SER	S1180	H1186	L1189	D1192	L1193	R1194	E1195	S1198	K1199	L1200	D1201	S1202	L1203	K1204	D1205	S1206	H1207	Q1210	D1211	F1212	W1213	T1216	N1221	THR	LEU	ASP	LYS	ARG	E1229	L1230	K1231	V1232	S1233	L1234	P1235	L1238	E1239	M1243	P1244	G1245	F1249								
L1252	Y1253	E1254	A1255	L1256	L1261	T1262	E1265	V1266	D1267	A1268	L1269	F1270	K1271	D1272	D1275	K1276	Y1277	D1278	E1279	K1281	L1284	K1285	F1286	M1287	C1288	T1289	M1290	N1291	L1292	Q1293	D1294	Q1295	K1296	I1299	V1303	I1306	T1311	L1312	H1313	Q1314	V1316	S1317	A1319	L1320	V1321	L1322	L1323	Q1324					
V1325	R1326	R1327	A1328	L1329	T1332	G1333	D1334	F1335	S1336	L1341	F1344	E1349	D1350	F1351	E1354	L1358	LEU	ASP	GLN	ILE	P1360	Q1362	F1363	I1364	K1365	Q1368	L1369	L1370	Q1371	D1372	I1373	S1374	P1375	P1376	R1377	Q1378	A1379	C1380	L1381	E1382	E1383	R1386	L1390	W1393	L1394	V1398	V1510	H1511	E1512	H1517			
G1416	E1417	N1418	D1419	H1429	Q1433	G1434	Y1435	R1445	D1450	H1454	L1455	Q1456	E1457	L1458	W1459	R1460	L1468	P1469	D1470	K1471	D1474	S1475	A1476	R1477	N1478	W1481	L1482	K1483	T1484	H1489	G1490	S1491	V1492	E1493	L1494	S1495	S1498	L1499	T1503	V1508	Y1509	V1510	H1511	E1512	G1517								
I1520	R1527	L1528	L1529	L1530	P1531	D1532	GLY	HIS	GLY	TYR	P1537	E1538	A1539	L1540	Y1543	L1548	K1549	E1550	L1551	L1552	M1553	K1554	L1555	M1556	L1557	M1558	S1559	G1560	K1561	H1564	S1565	N1566	T1567	L1568	E1569	V1570	E1571	E1575	M1580	Q1581	R1582	H1585	I1588	K1589	L1590	H1591	M1596	L1597	F1598				
R1599	T1600	W1601	T1602	N1616	F1617	G1618	L1619	E1620	L1621	S1622	Q1623	L1624	E1625	D1630	V1631	T1632	Q1633	C1639	R1640	E1643	D1644	L1645	L1646	E1649	V1650	V1652	K1656	R1657	A1658	E1659	H1660	F1661	Y1662	L1663	N1664	Y1666	L1667	A1668	E1669	Q1670	L1671	V1672	Y1673	L1674	S1675	E1676	S1677	L1678	R1679	K1680	S1684		
E1685	A1686	A1687	L1688	M1689	M1690	L1691	S1692	K1697	K1698	T1699	V1700	V1704	Q1705	A1706	T1707	C1710	K1713	A1714	D1715	Y1717	C1718	L1719	L1720	E1721	V1722	M1723	K1724	K1725	Q1729	L1730	E1733	L1736	M1737	G1738	K1739	L1740	V1742	A1743	M1744	S1747	L1748	V1749	Y1750	M1751	S1752	A1753	L1754	L1755	P1756				



E3910	E3911	D3912	B3919	P3920	K3932	D3933	K3937	S3940	T3941	P3942	H3961	A3964	D3965	D3966	P3961	C3962	D3963	C3967	L3968	R3969	C3970	I3971	Q3972	T3973	K3974	L3975	P3977	G3978	Q3979	K3980	P3983	T3984	C3985	L3986	T3987	D3988	L3989	P3990	D3991	K3992	F3993	S3994	P3995	S3998	Q3999	D4000	H4001	R4002																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
L3824	L3825	K3826	W3832	L3833	Q3834	L3835	W3836	K3837	L3838	S3839	S3840	T3841	P3842	L3843	E3844	W3845	V3846	C3847	Y3851	W3763	W3764	H3765	S3855	T3859	R3860	I3863	Q3864	S3865	W3866	R3867	A3868	L3869	R3872	L3873	T3876	A3877	L3878	P3879	V3880	E3881	V3882	L3883	L3884	L3885	T3887	E3888	I3891	L3905	L3909	S3998	Q3999	D4000	H4001	R4002																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
L3720	S3726	R3727	E3728	A3736	R3742	E3743	L3744	Q3745	E3746	D3752	E3753	P3758	S3760	L3761	P3762	W3763	W3764	H3765	S3855	R3772	T3773	F3778	S3779	R3780	I3781	H3785	P3786	Q3787	V3788	L3789	L3792	A3795	A3796	E3797	K3798	L3801	E3805	L3808	D3809	A3810	F3811	C3816	K3821																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L3824	L3825	K3826	W3832	L3833	Q3834	L3835	W3836	K3837	L3838	S3839	S3840	T3841	P3842	L3843	E3844	W3845	V3846	C3847	Y3851	W3763	W3764	H3765	S3855	T3859	R3860	I3863	Q3864	S3865	W3866	R3867	A3868	L3869	R3872	L3873	T3876	A3877	L3878	P3879	V3880	E3881	V3882	L3883	L3884	L3885	T3887	E3888	I3891	L3905	L3909	S3998	Q3999	D4000	H4001	R4002																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
ARG	SER	ASN	GLU	MET	S3837	Q3842	M3845	R3846	L3847	Y3852	N3853	P3856	F3857	S3858	W3859	Y3864	L3865	E3866	E3867	L3868	W3669	Q3873	G3880	I3881	S3882	F3889	T3692	V3696	Q3700	F3701	P3702	V3703	A3704	Q3705	Q3706	Q3707	R3708	L3709	L3710	Q3711	S3712	L3713	L3714	K3715	D3716	F3717																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
E3540	R3544	K3547	F3548	W3549	E3553	A3559	L3560	Q3561	E3562	T3565	F3566	R3567	H3568	K3572	R3573	V3574	Q3575	V3576	L3582	I3586	T3589	G3680	I3681	S3682	H3785	P3786	Q3787	V3788	L3789	L3792	A3795	A3796	E3797	K3798	L3801	E3805	L3808	D3809	A3810	F3811	C3816	K3821																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
GLU	GLU	MET	LYS	ALA	SER	ASP	PRO	ARG	SER	CYS	ASP	CYS	S3472	Q3473	F3474	L3475	D3476	T3477	T3478	R3479	L3480	V3481	Q3482	S3483	C3484	V3485	Q3486	V3489	R3493	D3494	S3498	R3501	N3502	K3503	R3504	R3505	V3506	T3507	L3508	L3509	L3512	D3516	R3519	R3525	K3529	H3532	N3536																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L3379	S3380	R3381	M3382	E3383	S3384	F3391	Q3310	Y3311	L3395	R3396	R3397	H3400	D3401	D3402	D3403	L3404	I3409	M3410	D3413	T3414	T3415	K3416	S3423	K3427	E3428	ASP	LYS	PRO	GLU	GLN	GLU	GLU	ILE	GLU	THR	SER	GLN	SER	LYS	GLU	LEU	ALA	GLU	GLU	GLN	MET	GLU	VAL	ASN	ASP	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
E3295	L3296	R3297	A3300	P3303	Q3310	Y3311	D3312	E3313	F3314	Y3315	S3316	F3317	L3318	V3324	L3325	T3326	N3327	G3328	S3329	F3330	V3331	Q3332	V3333	Q3337	F3340	D3341	Y3342	H3352	R3353	S3354	F3355	S3356	H3357	L3358	Q3359	S3360	T3361	T3362	G3363	S3364	G3365	T3367	K3368	D3369	F3370	V3371	F3372	L3373	M3374	F3375	V3376	K3377	L3378																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
R3199	D3200	L3201	T3202	E3203	E3204	L3205	K3208	L3217	L3218	D3219	P3223	D3224	A3225	V3226	S3230	L3234	G3235	S3236	F3237	K3240	Q3241	Y3246	H3252	R3253	S3254	F3255	V3256	R3257	F3258	L3259	Q3260	A3261	H3262	H3267	H3268	R3271	I3277	T3278	T3279	F3280	S3281	R3282	L3283	L3284	L3292	L3293	L3294	L3295	L3296	L3297	L3298	L3299	L3300	L3301	L3302	L3303	L3304	L3305	L3306	L3307	L3308	L3309	L3310	L3311	L3312	L3313	L3314	L3315	L3316	L3317	L3318	L3319	L3320	L3321	L3322	L3323	L3324	L3325	L3326	L3327	L3328	L3329	L3330	L3331	L3332	L3333	L3334	L3335	L3336	L3337	L3338	L3339	L3340	L3341	L3342	L3343	L3344	L3345	L3346	L3347	L3348	L3349	L3350	L3351	L3352	L3353	L3354	L3355	L3356	L3357	L3358	L3359	L3360	L3361	L3362	L3363	L3364	L3365	L3366	L3367	L3368	L3369	L3370	L3371	L3372	L3373	L3374	L3375	L3376	L3377	L3378	L3379	L3380	L3381	L3382	L3383	L3384	L3385	L3386	L3387	L3388	L3389	L3390	L3391	L3392	L3393	L3394	L3395	L3396	L3397	L3398	L3399	L3400	L3401	L3402	L3403	L3404	L3405	L3406	L3407	L3408	L3409	L3410	L3411	L3412	L3413	L3414	L3415	L3416	L3417	L3418	L3419	L3420	L3421	L3422	L3423	L3424	L3425	L3426	L3427	L3428	L3429	L3430	L3431	L3432	L3433	L3434	L3435	L3436	L3437	L3438	L3439	L3440	L3441	L3442	L3443	L3444	L3445	L3446	L3447	L3448	L3449	L3450	L3451	L3452	L3453	L3454	L3455	L3456	L3457	L3458	L3459	L3460	L3461	L3462	L3463	L3464	L3465	L3466	L3467	L3468	L3469	L3470	L3471	L3472	L3473	L3474	L3475	L3476	L3477	L3478	L3479	L3480	L3481	L3482	L3483	L3484	L3485	L3486	L3487	L3488	L3489	L3490	L3491	L3492	L3493	L3494	L3495	L3496	L3497	L3498	L3499	L3500	L3501	L3502	L3503	L3504	L3505	L3506	L3507	L3508	L3509	L3510	L3511	L3512	L3513	L3514	L3515	L3516	L3517	L3518	L3519	L3520	L3521	L3522	L3523	L3524	L3525	L3526	L3527	L3528	L3529	L3530	L3531	L3532	L3533	L3534	L3535	L3536	L3537	L3538	L3539	L3540	L3541	L3542	L3543	L3544	L3545	L3546	L3547	L3548	L3549	L3550	L3551	L3552	L3553	L3554	L3555	L3556	L3557	L3558	L3559	L3560	L3561	L3562	L3563	L3564	L3565	L3566	L3567	L3568	L3569	L3570	L3571	L3572	L3573	L3574	L3575	L3576	L3577	L3578	L3579	L3580	L3581	L3582	L3583	L3584	L3585	L3586	L3587	L3588	L3589	L3590	L3591	L3592	L3593	L3594	L3595	L3596	L3597	L3598	L3599	L3600	L3601	L3602	L3603	L3604	L3605	L3606	L3607	L3608	L3609	L3610	L3611	L3612	L3613	L3614	L3615	L3616	L3617	L3618	L3619	L3620	L3621	L3622	L3623	L3624	L3625	L3626	L3627	L3628	L3629	L3630	L3631	L3632	L3633	L3634	L3635	L3636	L3637	L3638	L3639	L3640	L3641	L3642	L3643	L3644	L3645	L3646	L3647	L3648	L3649	L3650	L3651	L3652	L3653	L3654	L3655	L3656	L3657	L3658	L3659	L3660	L3661	L3662	L3663	L3664	L3665	L3666	L3667	L3668	L3669	L3670	L3671	L3672	L3673	L3674	L3675	L3676	L3677	L3678	L3679	L3680	L3681	L3682	L3683	L3684	L3685	L3686	L3687	L3688	L3689	L3690	L3691	L3692	L3693	L3694	L3695	L3696	L3697	L3698	L3699	L3700	L3701	L3702	L3703	L3704	L3705	L3706	L3707	L3708	L3709	L3710	L3711	L3712	L3713	L3714	L3715	L3716	L3717	L3718	L3719	L3720	L3721	L3722	L3723	L3724	L3725	L3726	L3727	L3728	L3729	L3730	L3731	L3732	L3733	L3734	L3735	L3736	L3737	L3738	L3739	L3740	L3741	L3742	L3743	L3744	L3745	L3746	L3747	L3748	L3749	L3750	L3751	L3752	L3753	L3754	L3755	L3756	L3757	L3758	L3759	L3760	L3761	L3762	L3763	L3764	L3765	L3766	L3767	L3768	L3769	L3770	L3771	L3772	L3773	L3774	L3775	L3776	L3777	L3778	L3779	L3780	L3781	L3782	L3783	L3784	L3785	L3786	L3787	L3788	L3789	L3790	L3791	L3792	L3793	L3794	L3795	L3796	L3797	L3798	L3799	L3800	L3801	L3802	L3803	L3804	L3805	L3806	L3807	L3808	L3809	L3810	L3811	L3812	L3813	L3814	L3815	L3816	L3817	L3818	L3819	L3820	L3821	L3822	L3823	L3824	L3825	L3826	L3827	L3828	L3829	L3830	L3831	L3832	L3833	L3834	L3835	L3836	L3837	L3838	L3839	L3840	L3841	L3842	L3843	L3844	L3845	L3846	L3847	L3848	L3849	L3850	L3851	L3852	L3853	L3854	L3855	L3856	L3857	L3858	L3859	L3860	L3861	L3862	L3863	L3864	L3865	L3866	L3867	L3868	L3869	L3870	L3871	L3872	L3873	L3874	L3875	L3876	L3877	L3878	L3879	L3880	L3881	L3882	L3883	L3884	L3885	L3886	L3887	L3888	L3889	L3890	L3891	L3892	L3893	L3894	L3895	L3896	L3897	L3898	L3899	L3900	L3901	L3902	L3903	L3904	L3905	L3906	L3907	L3908	L3909	L3910	L3911	L3912	L3913	L3914	L3915	L3916	L3917	L3918	L3919	L3920	L3921	L3922	L3923	L3924	L3925	L3926	L3927	L3928	L3929	L3930	L3931	L3932	L3933	L3934	L3935	L3936	L3937	L3938	L3939	L3940	L3941	L3942	L3943	L3944	L3945	L3946	L3947	L3948	L3949	L3950	L3951	L3952	L3953	L3954	L3955	L3956	L3957	L3958	L3959	L3960	L3961	L3962	L3963	L3964	L3965	L3966	L3967	L3968	L3969	L3970	L3971	L3972	L3973	L3974	L3975	L3976	L3977	L3978	L3979	L3980	L3981	L3982	L3983	L3984	L3985	L3986	L3987	L3988	L3989	L3990	L3991	L3992	L3993	L3994	L3995	L3996	L3997	L3998	L3999	L4000	L4001	L4002
E2937	K2938	K2939	G2940	L2941	D2942	E2943	L2944	L2945	L2946	L2947	L2948	L2949	L2950	L2951	L2952	L2953	L2954	L2955	L2956	L2957	L2958	L2959	L2960	L2961	L2962	L2963	L2964	L2965	L2966	L2967	L2968	L2969	L2970	L2971	L2972	L2973	L2974	L2975	L2976	L2977	L2978	L2979	L2980	L2981	L2982	L2983	L2984	L2985	L2986	L2987	L2988	L2989	L2990	L2991	L2992	L2993	L2994	L2995	L2996	L2997	L2998	L2999	L3000	L3001	L3002	L3003	L3004	L3005	L3006	L3007	L3008	L3009	L3010	L3011	L3012	L3013	L3014	L3015	L3016	L3017	L3018	L3019	L3020	L3021	L3022	L3023	L3024	L3025	L3026	L3027	L3028	L3029	L3030	L3031	L3032	L3033	L3034	L3035	L3036	L3037	L3038	L3039	L3040	L3041	L3042	L3043	L3044	L3045	L3046	L3047	L3048	L3049	L3050	L3051	L3052	L3053	L3054	L3055	L3056	L3057	L3058	L3059	L3060	L3061	L3062	L3063	L3064	L3065	L3066	L3067	L3068	L3069	L3070	L3071	L3072	L3073	L3074	L3075	L3076	L3077	L3078	L3079	L3080	L3081	L3082	L3083	L3084	L308																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	33242	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.021	Depositor
Minimum map value	-0.007	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00484	Depositor
Map size (Å)	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, ATP

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	0.17	0/37557	0.40	2/50804 (0.0%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2051	ARG	CA-C-N	-5.71	105.81	122.38
1	A	2051	ARG	C-N-CA	-5.71	105.81	122.38

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4165	GLU	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	36787	0	36880	1338	0
2	A	62	0	24	11	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
All	All	36852	0	36904	1338	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 18.

The worst 5 of 1338 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:1619:LEU:HD21	1:A:1622:LEU:HB3	1.49	0.95
1:A:1216:THR:HG21	1:A:1245:CYS:HB2	1.53	0.90
1:A:3025:PRO:HB3	1:A:3058:MET:HB2	1.57	0.87
1:A:2114:ALA:O	2:A:5201:ATP:N6	2.09	0.86
1:A:3006:THR:HG21	1:A:3011:ALA:HB2	1.58	0.85

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	4552/5161 (88%)	4198 (92%)	353 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4166	PRO

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	ATP	A	5205	-	32,33,33	0.49	1 (3%)	48,52,52	0.38	0
2	ATP	A	5201	3	32,33,33	0.53	0	48,52,52	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	5205	-	-	6/22/38/38	0/3/3/3
2	ATP	A	5201	3	-	4/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5205	ATP	PA-O3A	-2.03	1.57	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

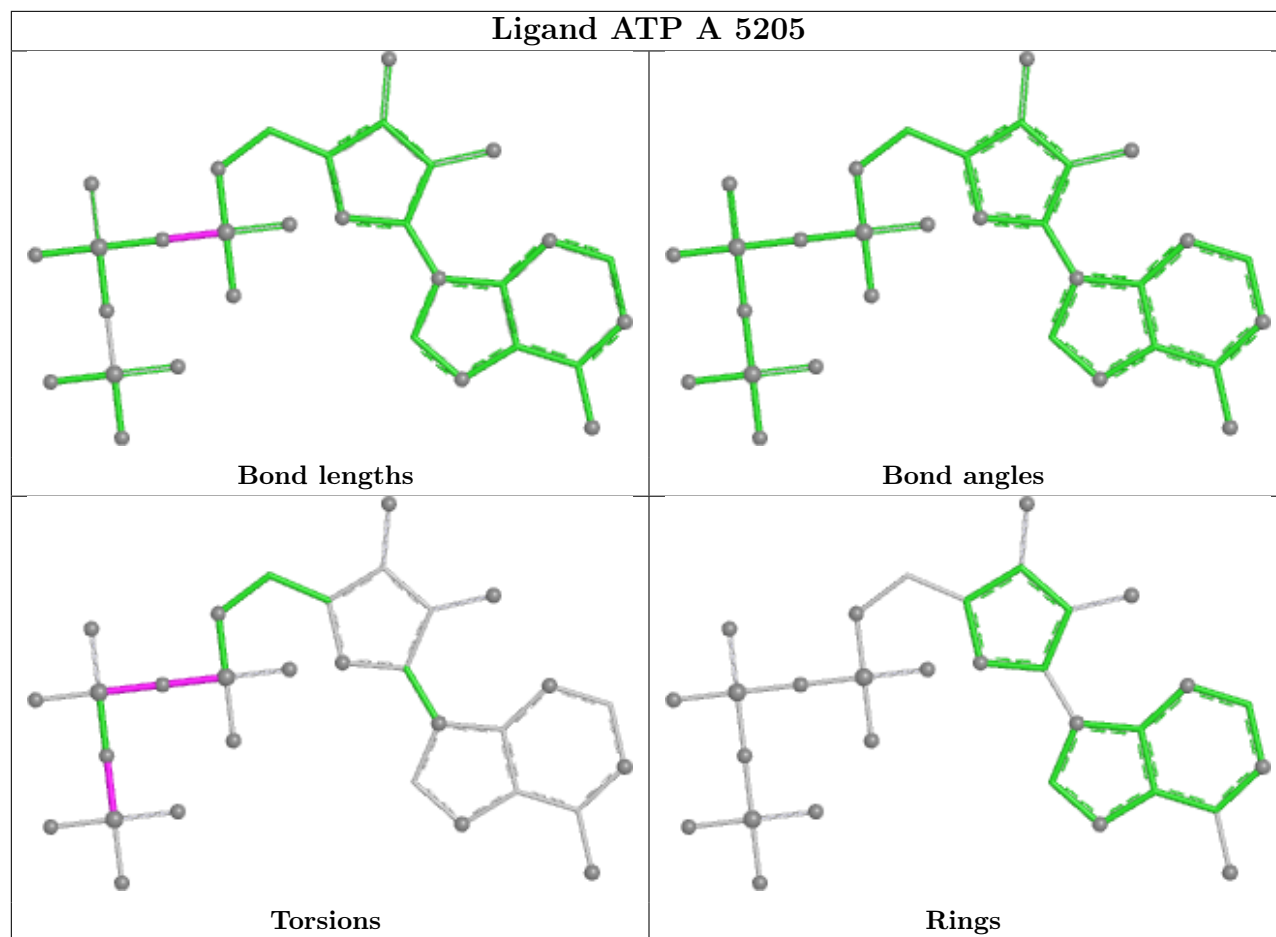
Mol	Chain	Res	Type	Atoms
2	A	5201	ATP	C5'-O5'-PA-O1A
2	A	5205	ATP	PB-O3B-PG-O1G
2	A	5205	ATP	PB-O3B-PG-O2G
2	A	5201	ATP	PA-O3A-PB-O2B
2	A	5205	ATP	PA-O3A-PB-O1B

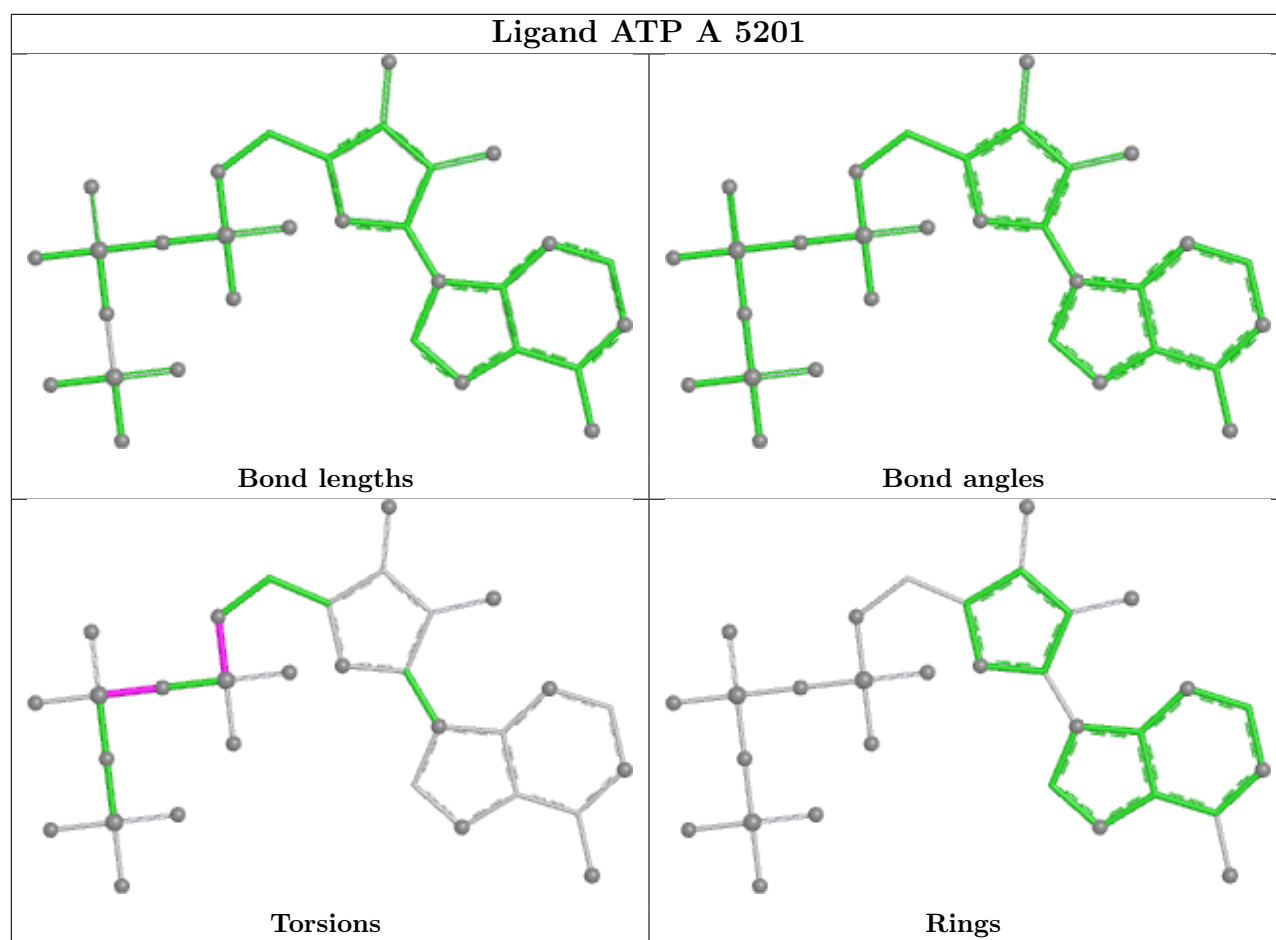
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5205	ATP	7	0
2	A	5201	ATP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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.



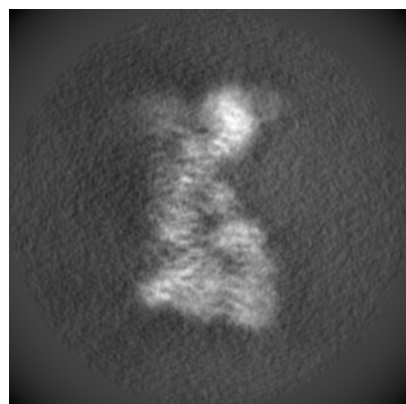
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52570. These allow visual inspection of the internal detail of the map and identification of artifacts.

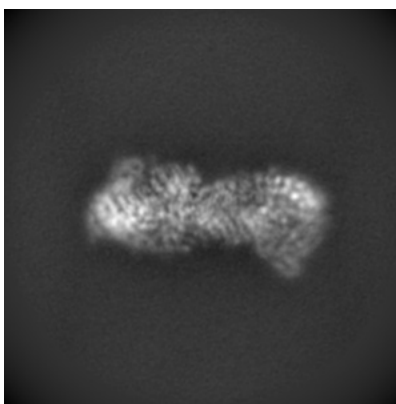
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

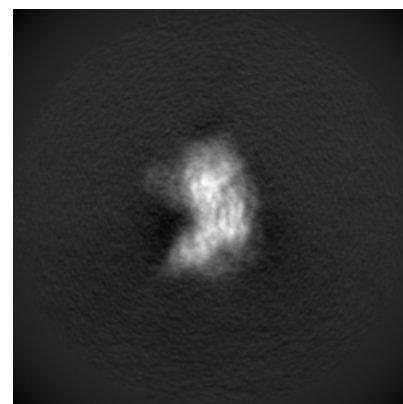
#### 6.1.1 Primary map



X

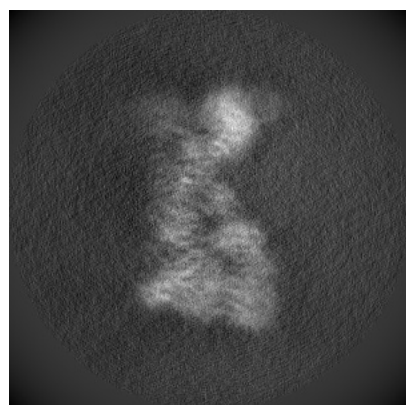


Y

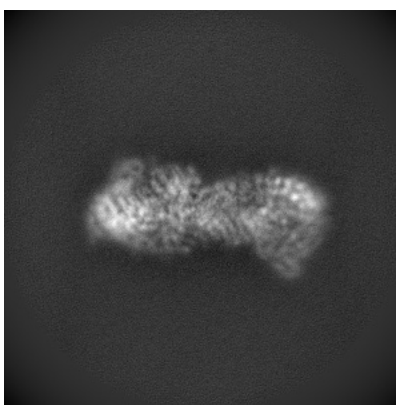


Z

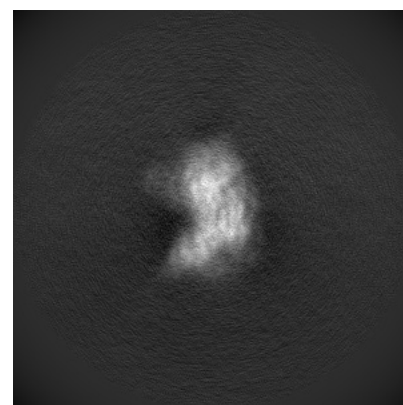
#### 6.1.2 Raw map



X



Y

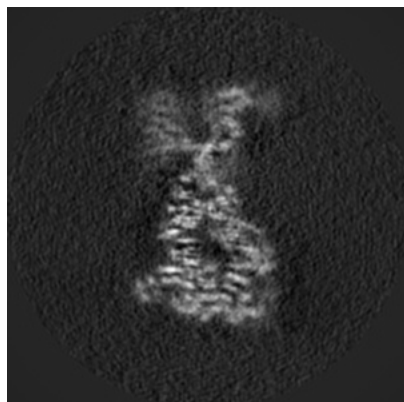


Z

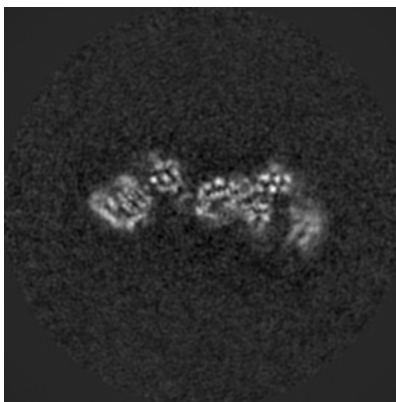
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

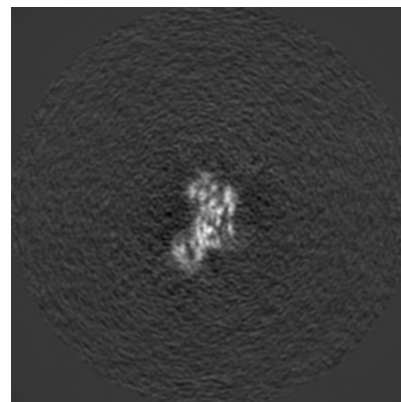
### 6.2.1 Primary map



X Index: 176

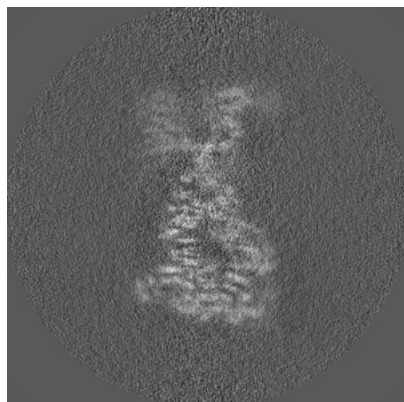


Y Index: 176

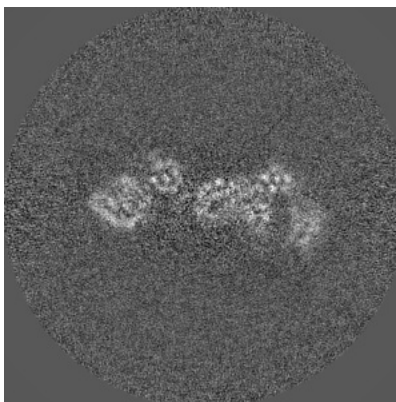


Z Index: 176

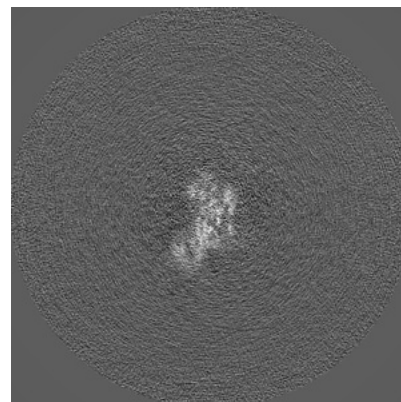
### 6.2.2 Raw map



X Index: 176



Y Index: 176

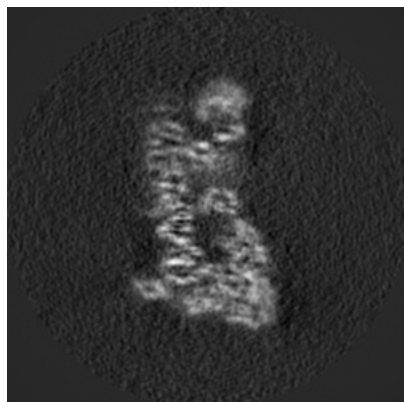


Z Index: 176

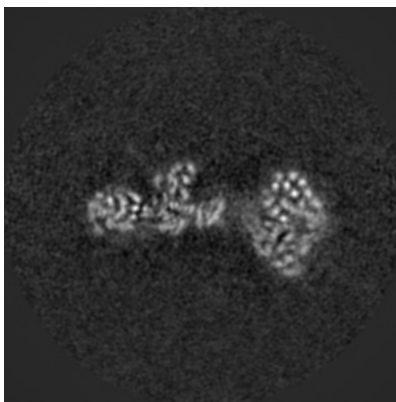
The images above show central slices of the map in three orthogonal directions.

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

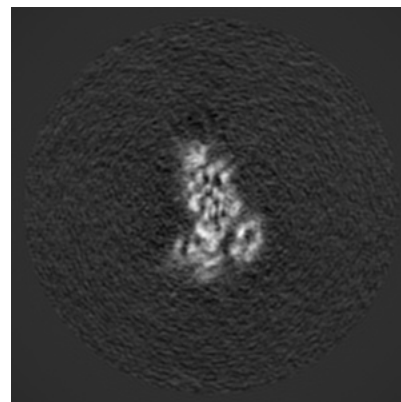
### 6.3.1 Primary map



X Index: 168

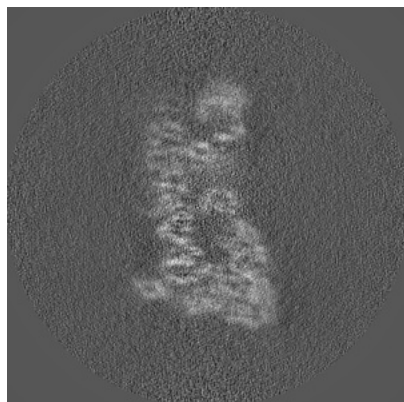


Y Index: 197

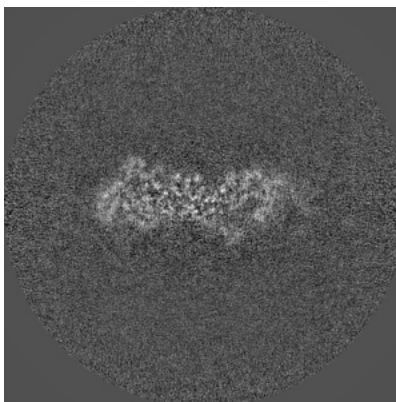


Z Index: 110

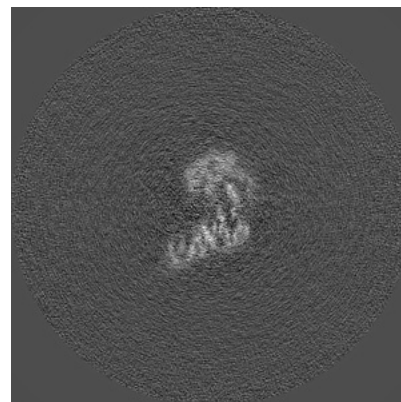
### 6.3.2 Raw map



X Index: 168



Y Index: 160



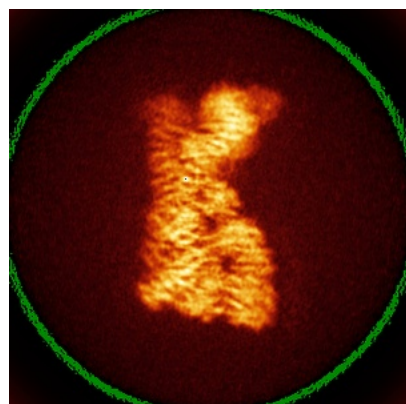
Z Index: 155

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

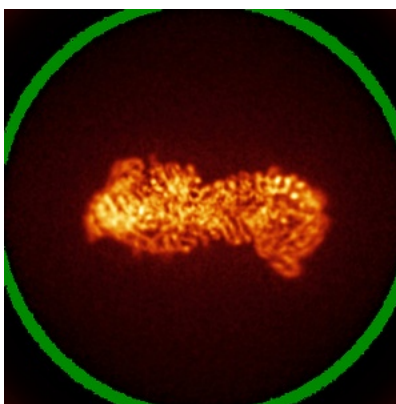


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

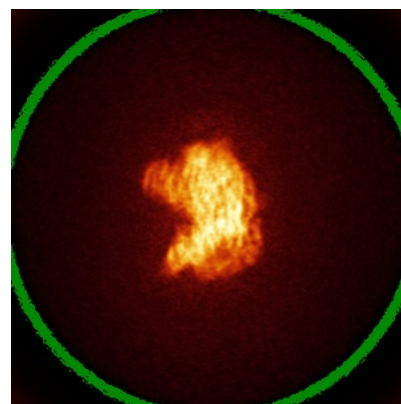
### 6.4.1 Primary map



X

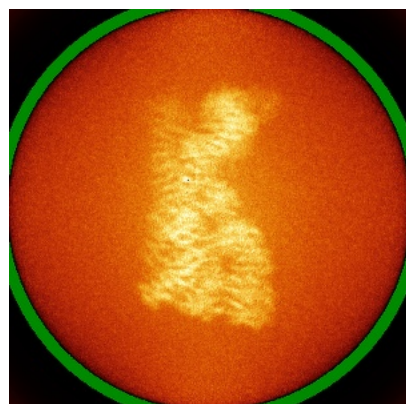


Y

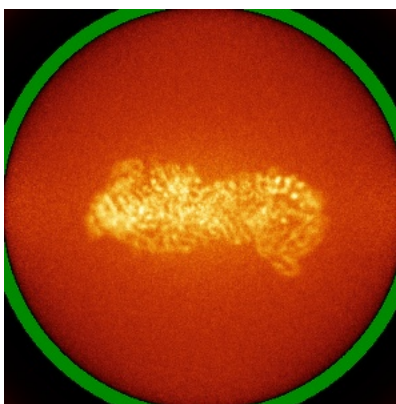


Z

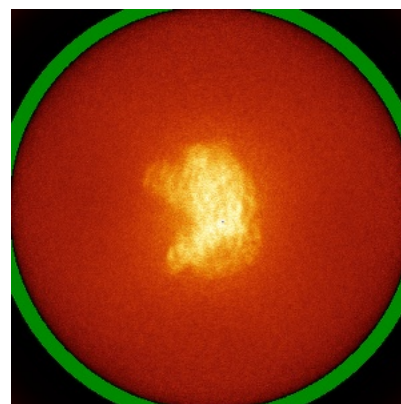
### 6.4.2 Raw map



X



Y



Z

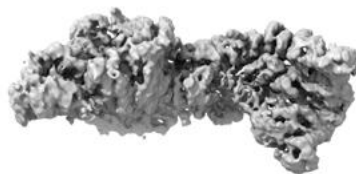
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



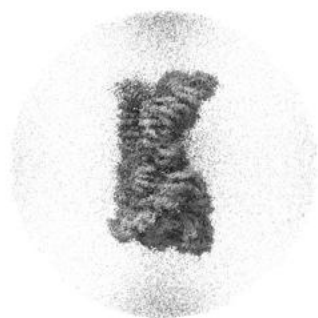
Y



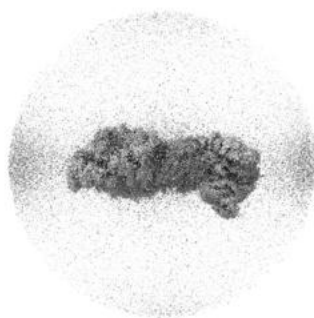
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00484. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

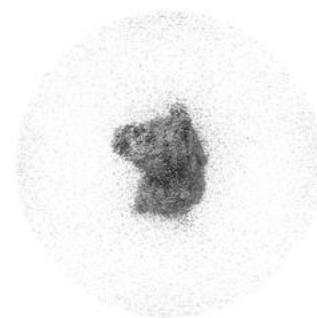
### 6.5.2 Raw map



X



Y



Z

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.

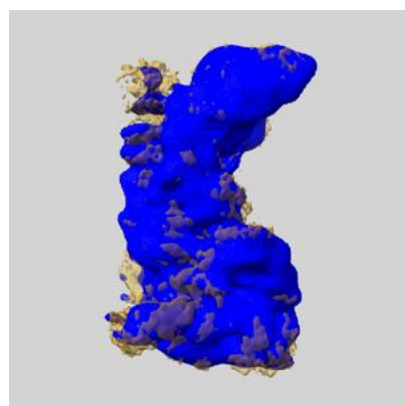
## 6.6 Mask visualisation [i](#)

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

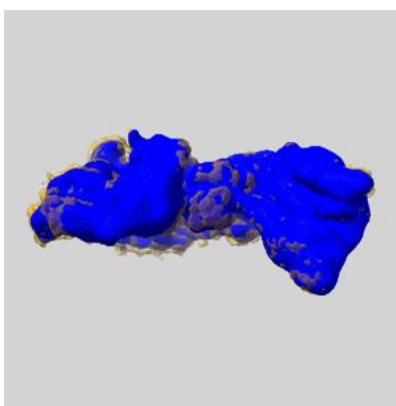
A mask typically either:

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

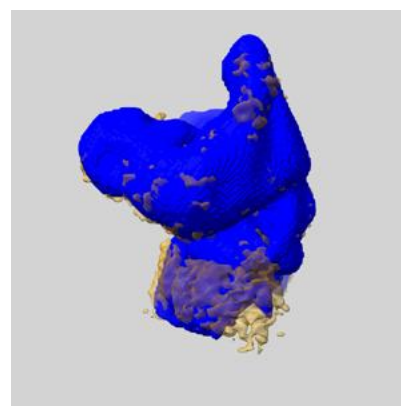
### 6.6.1 emd\_52570\_msk\_1.map [i](#)



X



Y

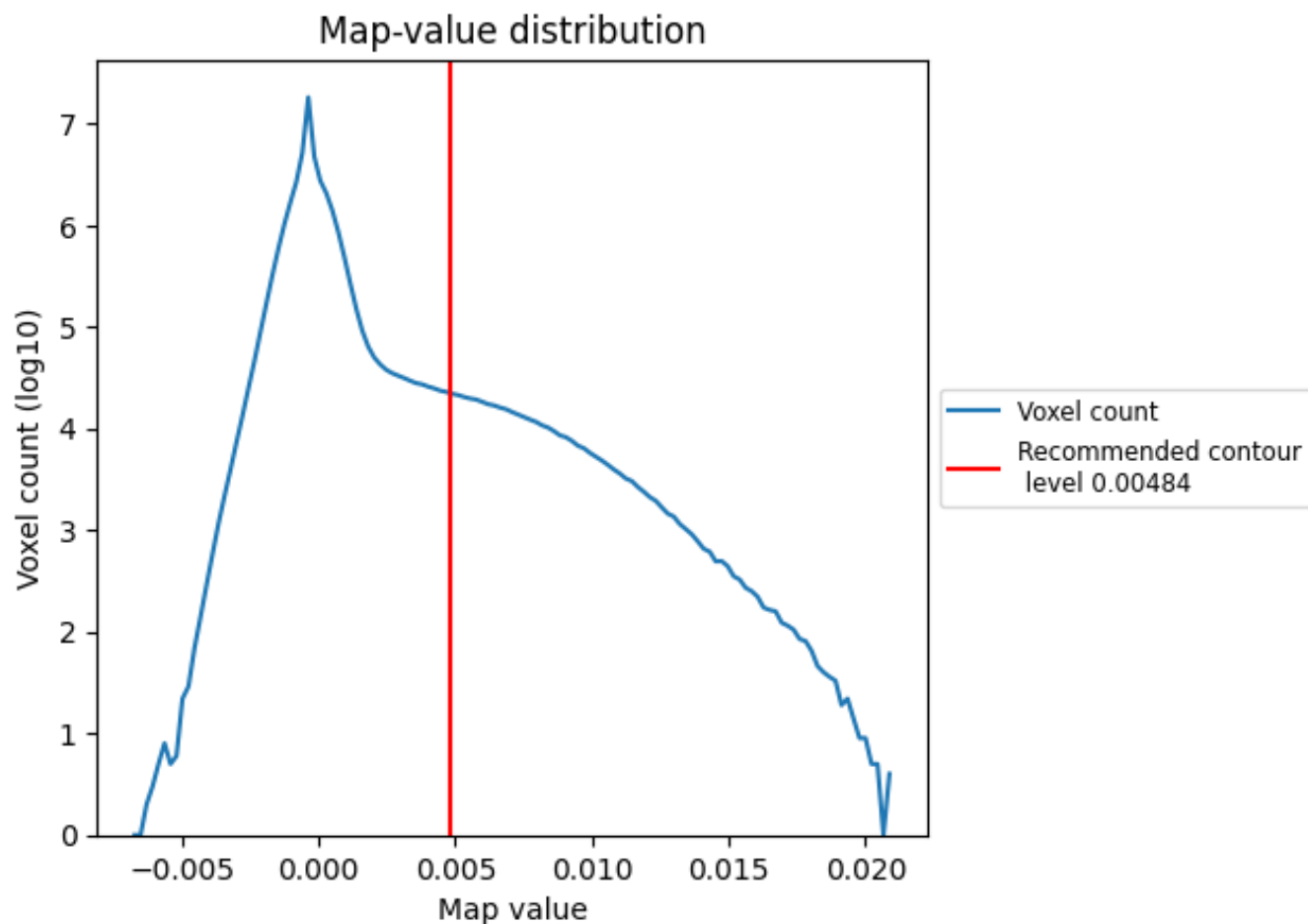


Z

## 7 Map analysis [i](#)

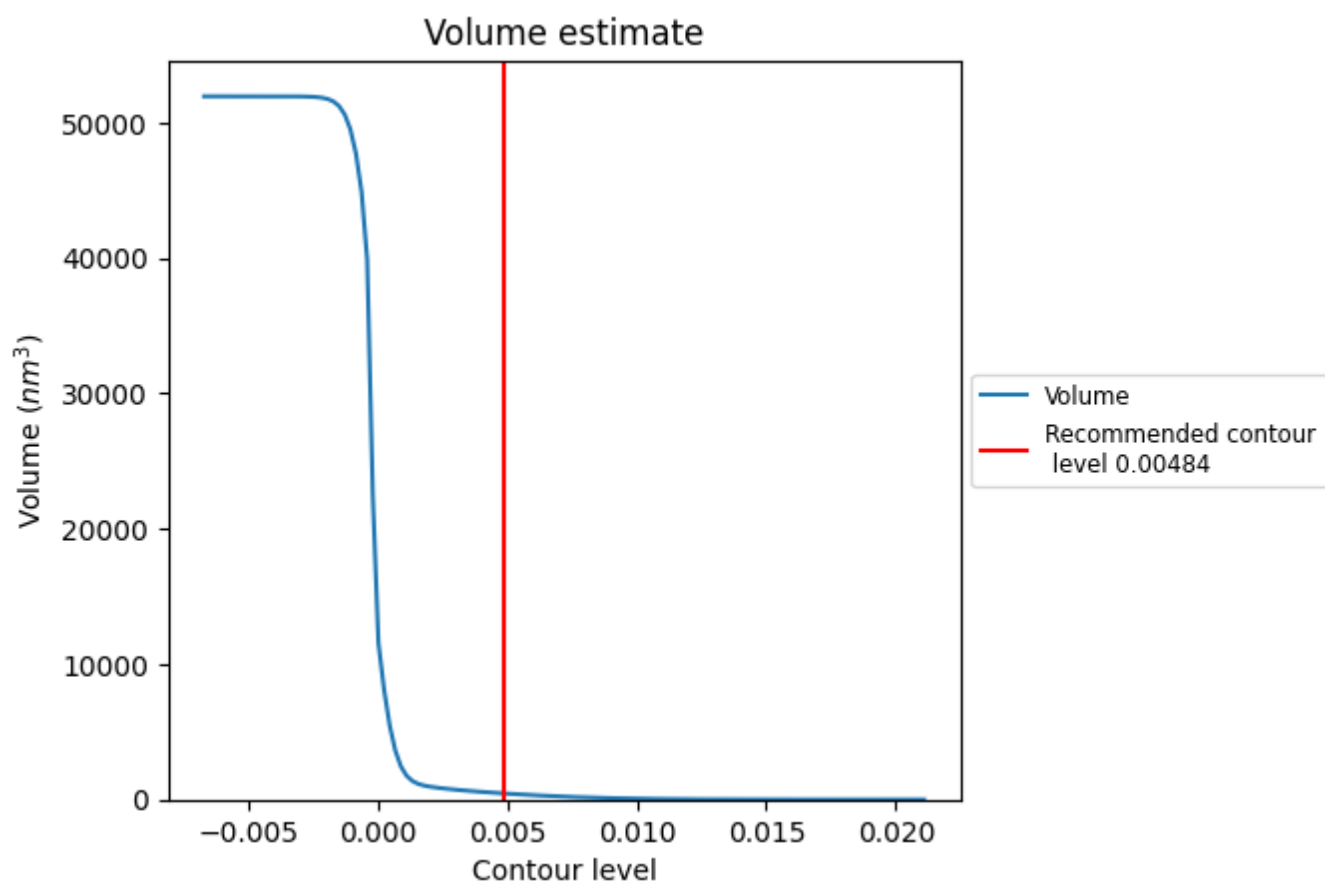
This section contains the results of statistical analysis of the map.

### 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](#)

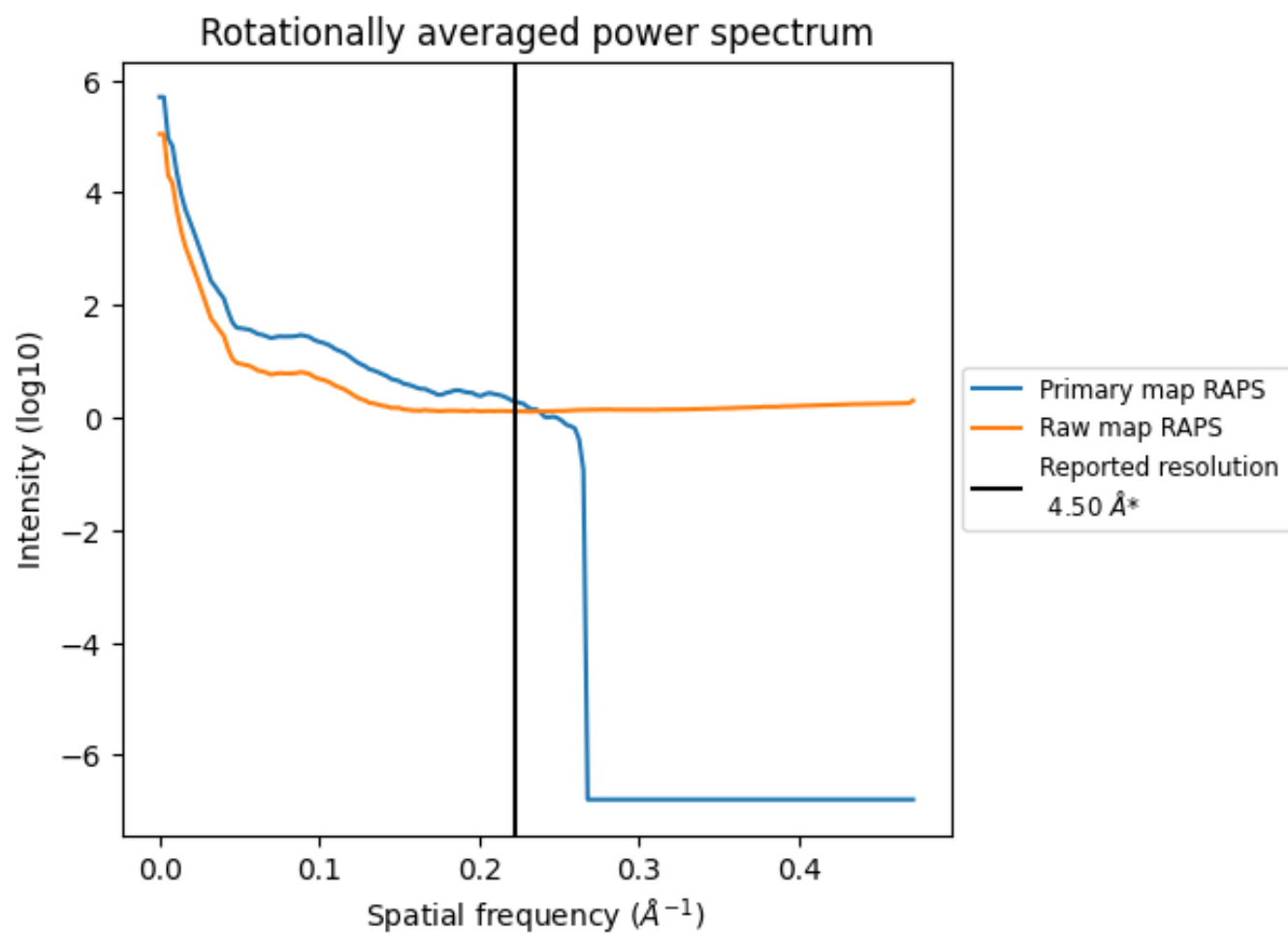


The volume at the recommended contour level is 455 nm<sup>3</sup>; this corresponds to an approximate mass of 411 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



### 7.3 Rotationally averaged power spectrum ⓘ

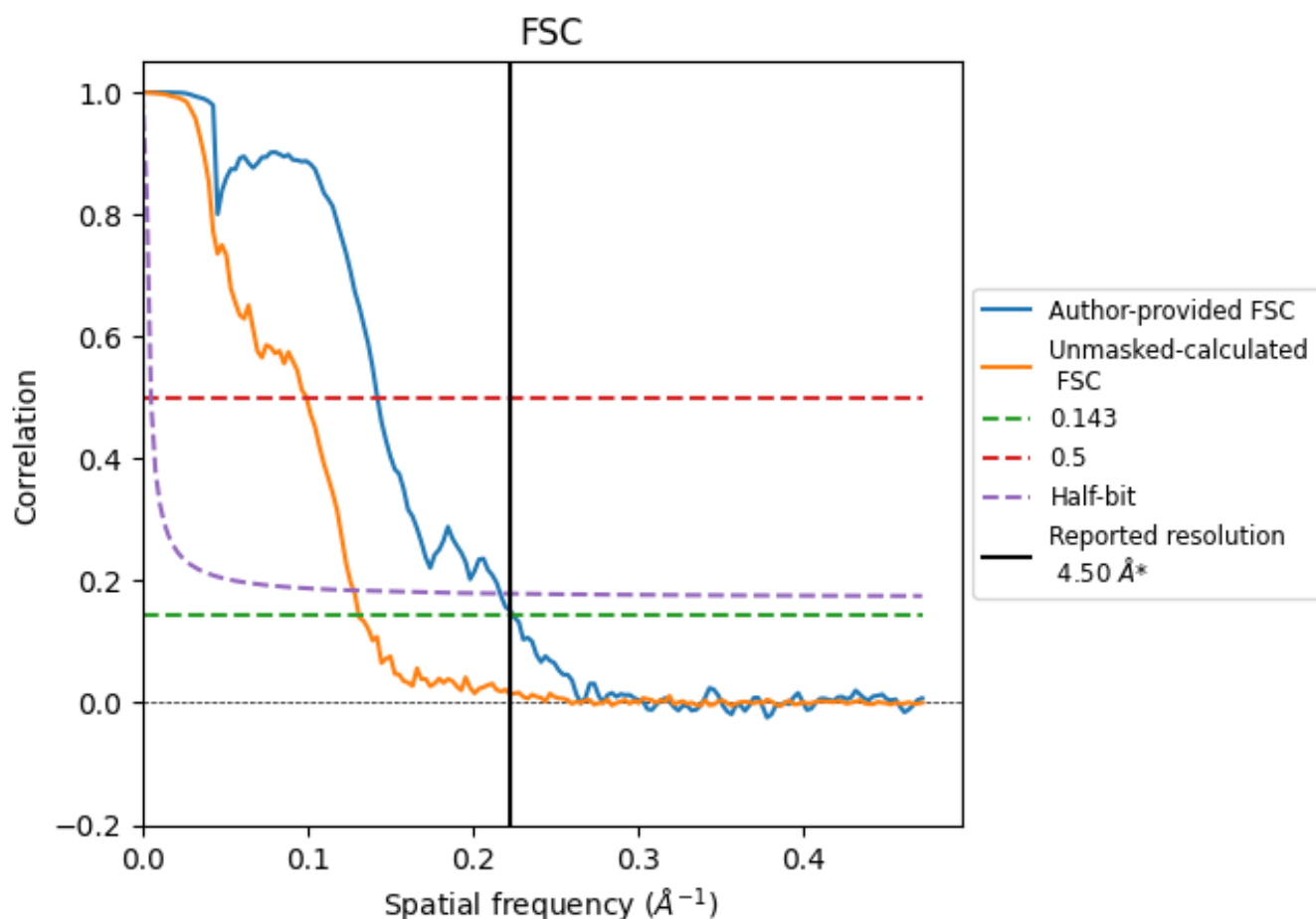


\*Reported resolution corresponds to spatial frequency of 0.222  $\text{\AA}^{-1}$

## 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  $0.222 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

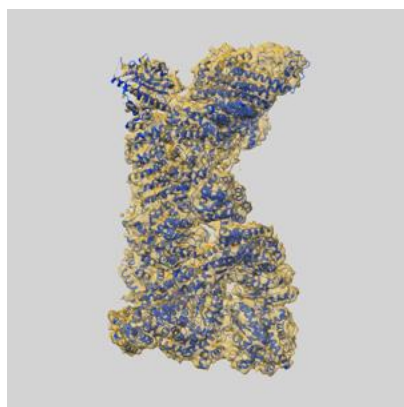
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.46	7.03	4.62
Unmasked-calculated*	7.63	10.07	7.82

\*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 7.63 differs from the reported value 4.5 by more than 10 %

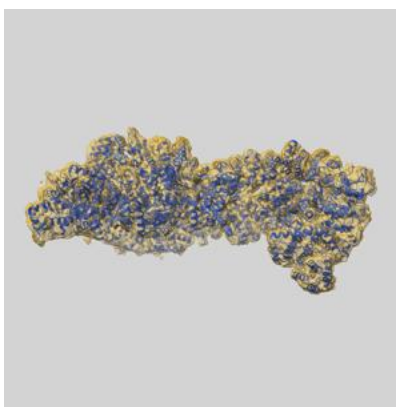
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52570 and PDB model 9I1I. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

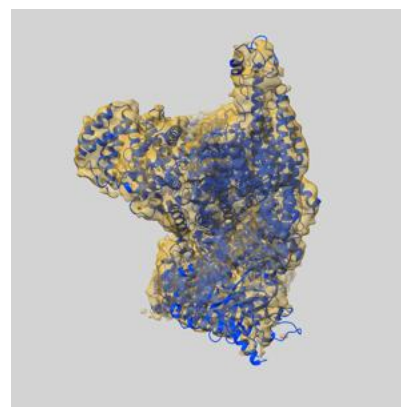
### 9.1 Map-model overlay [i](#)



X



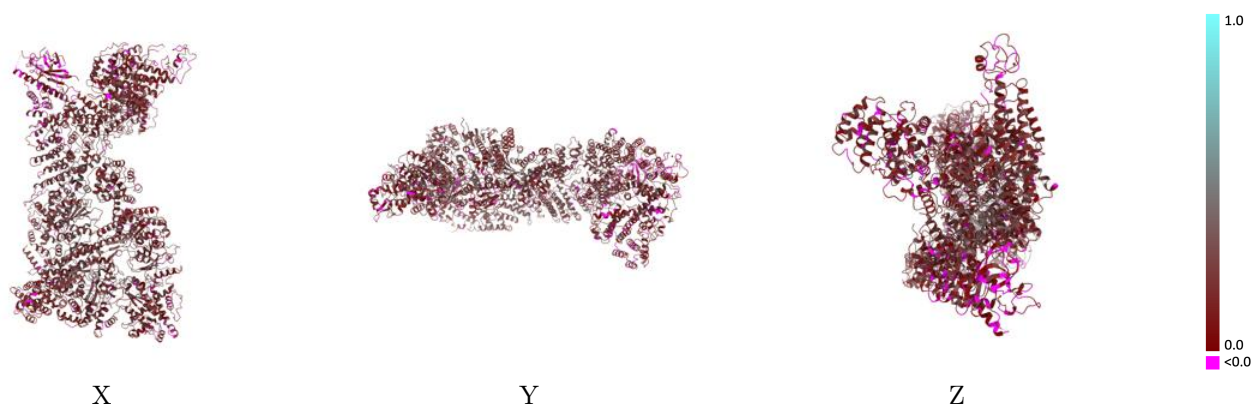
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00484 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](#)

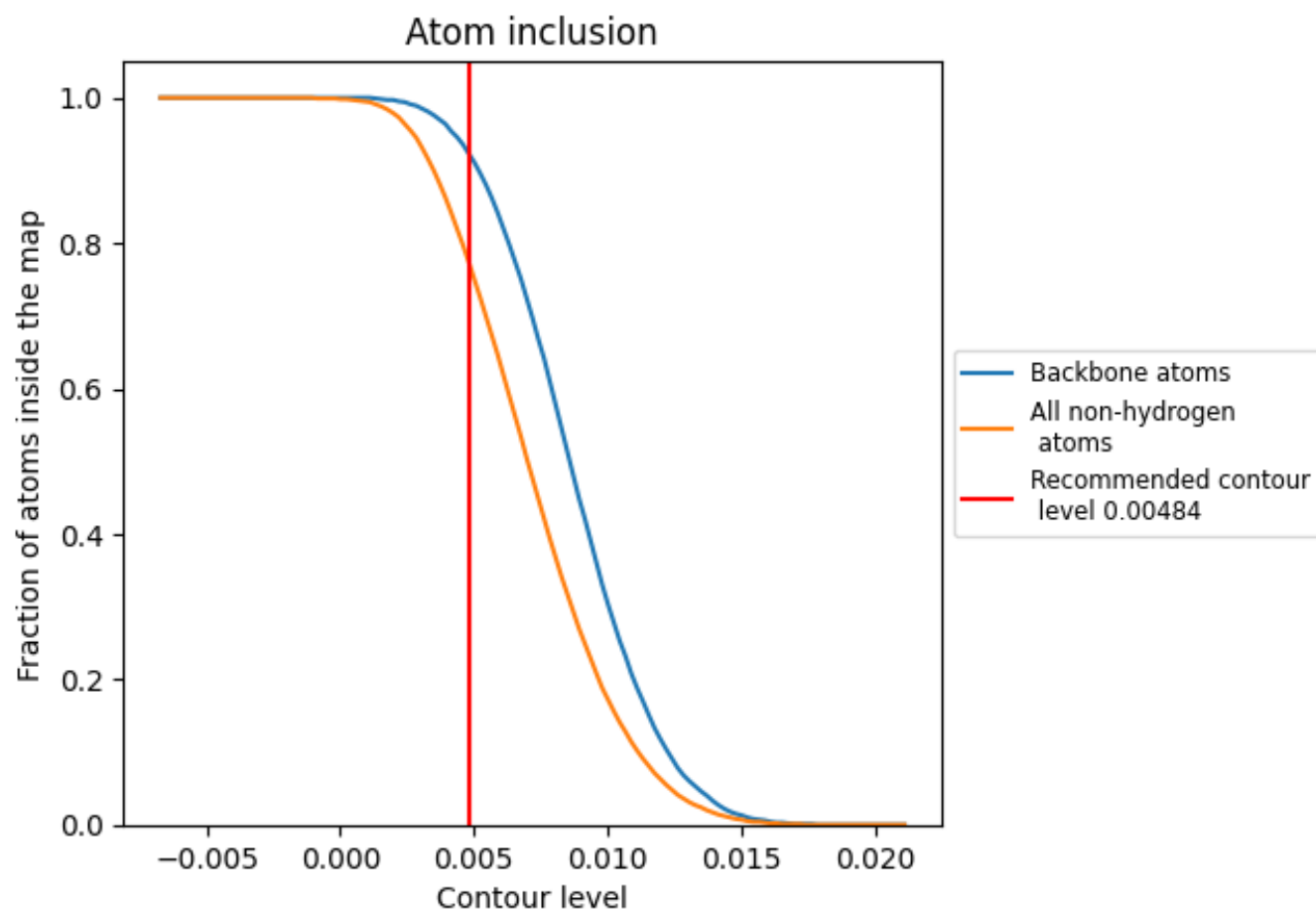


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 77% 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 (0.00484) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7700	<div></div> 0.2080
A	<div></div> 0.7700	<div></div> 0.2080

