



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 04:07 pm BST

PDB ID : 7Z88
EMDB ID : EMD-14546
Title : DNA-PK in the intermediate state
Authors : Liang, S.; Blundell, T.L.
Deposited on : 2022-03-16
Resolution : 3.33 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

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.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

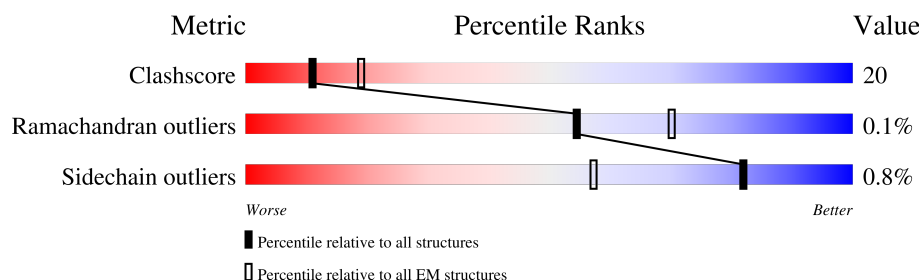
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4128	<div> <div>15%</div> <div>50%</div> <div>36%</div> <div>13%</div> </div>
2	B	609	<div> <div>10%</div> <div>46%</div> <div>33%</div> <div>20%</div> </div>
3	C	732	<div> <div>43%</div> <div>53%</div> <div>37%</div> <div>10%</div> </div>
4	D	26	<div> <div>12%</div> <div>50%</div> <div>50%</div> </div>
5	E	26	<div> <div>15%</div> <div>46%</div> <div>54%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 38754 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3599	Total	C	N	O	S	0	0
			28443	18257	4823	5179	184		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	490	Total	C	N	O	S	0	0
			3937	2525	667	728	17		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	661	Total	C	N	O	S	0	0
			5274	3372	882	994	26		

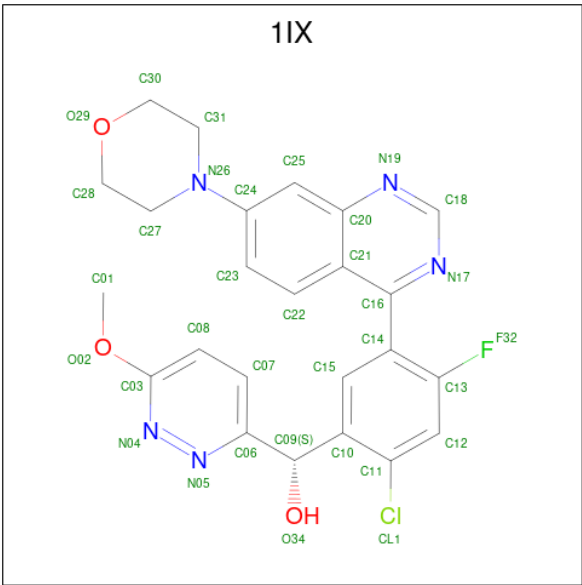
- Molecule 4 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	26	Total	C	N	O	P	0	0
			526	250	92	158	26		

- Molecule 5 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	26	Total	C	N	O	P	0	0
			540	254	106	154	26		

- Molecule 6 is ({S})-[2-chloranyl-4-fluoranyl-5-(7-morpholin-4-ylquinazolin-4-yl)phenyl]-(6-methoxypyridazin-3-yl)methanol (three-letter code: 1IX) (formula: C₂₄H₂₁ClFN₅O₃) (labeled as "Ligand of Interest" by depositor).

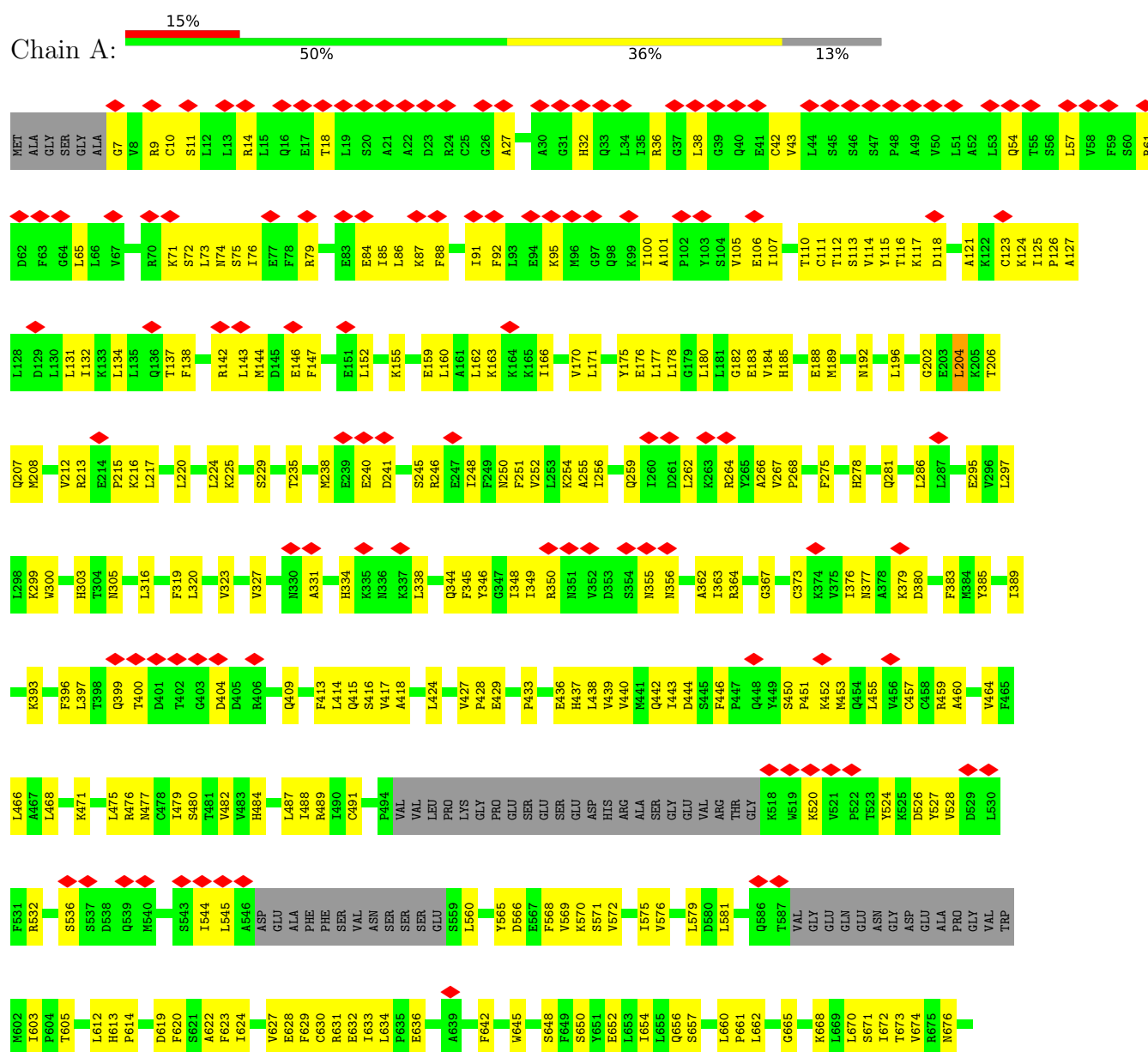


Mol	Chain	Residues	Atoms						AltConf
			Total	C	Cl	F	N	O	
6	A	1	34	24	1	1	5	3	0

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.

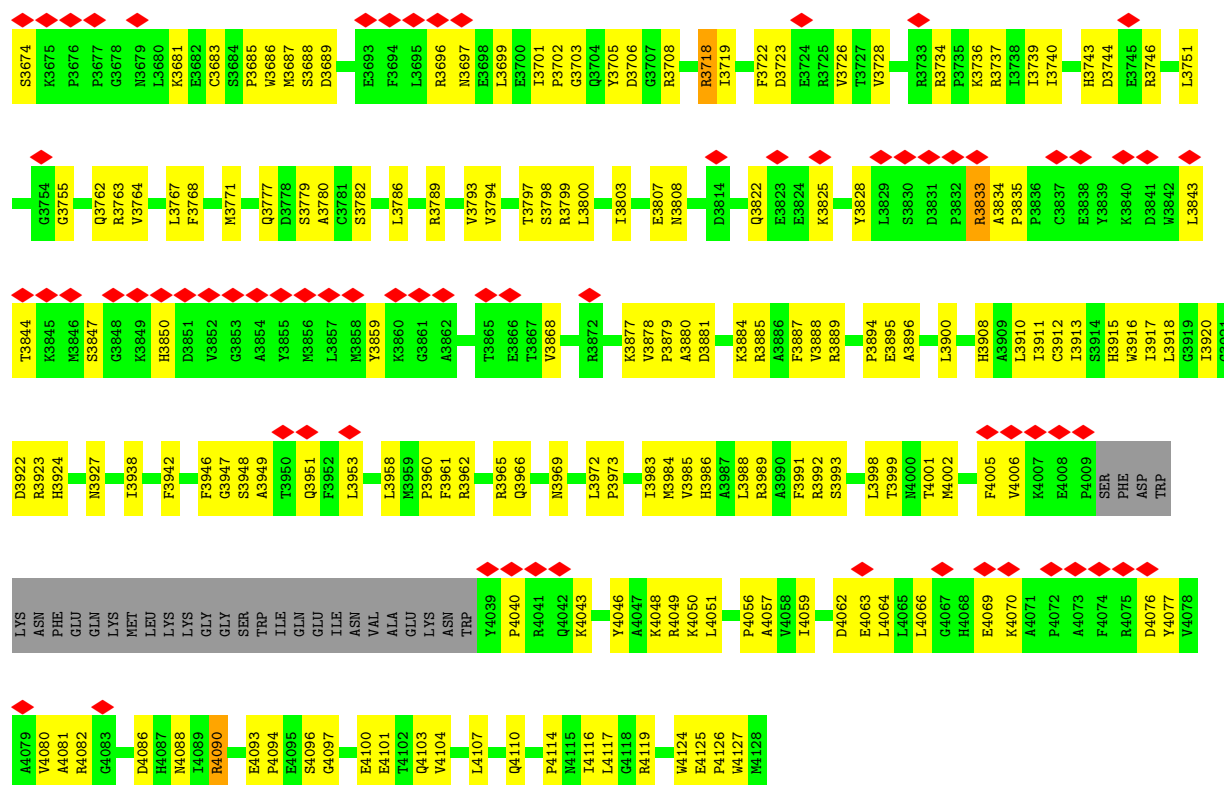
- Molecule 1: DNA-dependent protein kinase catalytic subunit



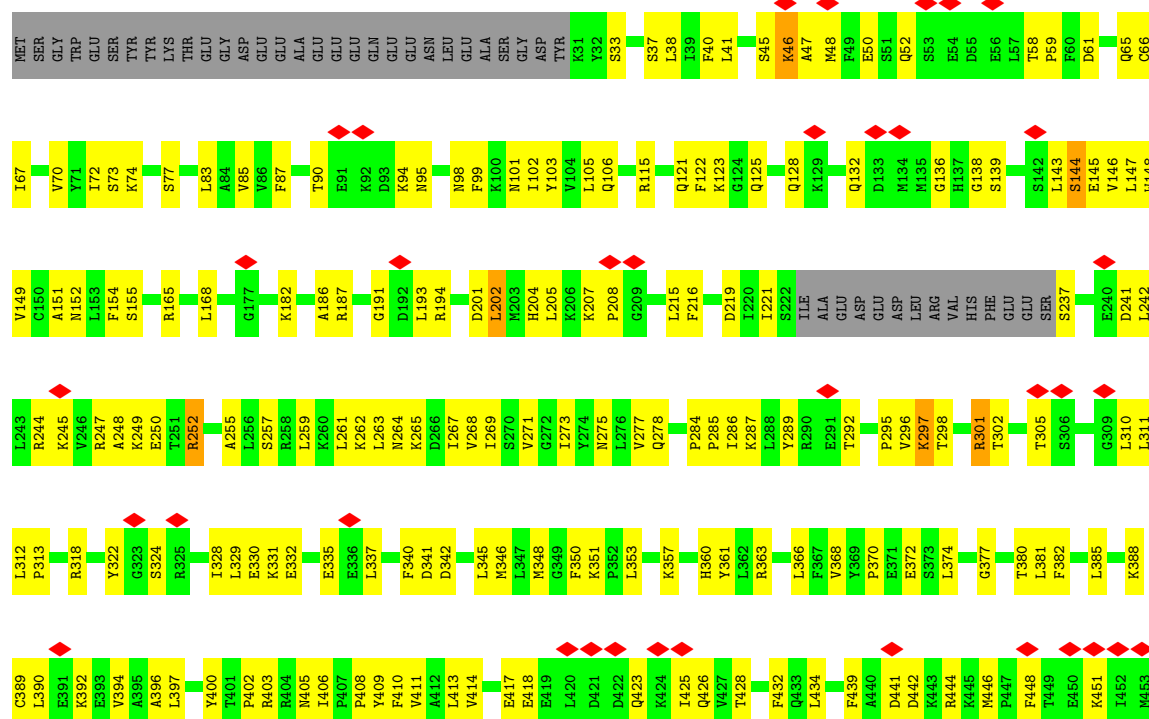
K679	G885	VAL	SER	PRO	LYS	SER	LEU	ASP	LYS	HIS	SER	PRO	GLU	ASN	PRO	TRP	ASP	GLU	K700	K712	V716	D723	P737	H738	N739	V749	P750	L751	L752	Q753	F756	G759	L760	S761	Y762	T763	P764	L765	A766	E767	V768	G769	L770	V784	P787	Y788	Y789	I792	L793	P794					
D797	G798	K801	THR	SER	ALA	LEU	SER	ASP	LYS	GLU	THR	LYS	ASN	ASN	TRP	E814	V815	S816	A817	L818	S819	R820	A821	A822	Q823	K824	G825	F826	N827	K828	V829	V830	L831	K832	H833	L834	K835	R836	T837	LYS	ASN	SER	SER	E844	A845	E849	E850	I851	R852	I853	R854	V855	M858	L859	G860
S861	L862	G863	G864	Q865	I866	N867	L870	V873	T874	S875	S876	D877	E878	M879	M880	S881	S882	Y883	W886	D887	R888	Q889	A895	V896	R899	E900	M901	K902	P903	V909	F910	L911	P912	R913	V914	T915	E916	L917	A918	L919	T920	A921	R924	K927	V928	C931	E932	L933	R934	V935					
S936	M937	V938	M939	F940	M941	L942	G943	K944	Q947	MET	PRO	GLU	GLY	GLN	GLY	ALA	P956	Y959	G960	L961	Y962	K963	R964	T965	V968	L969	A973	D977	Q978	Y979	T980	R981	Q982	L983	Y984	E985	P986	L987	V988	M989	N997	K1000	F1001	E1002	S1003	Q1004	V1007	E1011	A1012						
I1013	L1014	I1017	V1018	D1019	P1020	V1021	D1022	S1023	R1026	D1027	F1028	C1029	G1030	R1031	G1032	I1033	R1034	I1041	K1042	Q1043	I1044	T1045	P1046	Q1047	Q1048	Q1049	I1050	K1051	S1052	P1053	K1057	S1058	L1059	F1060	K1061	R1062	L1063	Y1064	S1065	L1066	A1067	L1068	R1075	L1076	G1077	W1083	R1084	I1085	E1088	F1089	R1090				
E1093	S1094	L1095	V1096	E1097	Q1098	F1099	V1100	F1101	E1102	V1105	I1106	Y1107	W1108	E1109	D1117	E1118	L1121	I1124	Q1125	Q1126	C1127	C1128	D1129	A1130	I1131	D1132	G1135	R1136	I1137	I1138	E1139	K1140	K1141	H1142	V1143	S1144	L1145	N1146	K1147	A1148	K1149	K1150	R1151	R1152	L1153	P1154	R1155	G1156	F1157	P1158	P1159	S1160	A1161	S1162	
L1163	C1164	L1165	L1166	D1167	K1170	W1171	A1174	H1175	R1178	P1179	Q1180	C1183	R1184	H1185	S1187	I1188	L1190	F1194	V1195	P1196	L1197	L1198	P1199	G1200	P1204	N1205	L1206	W1207	L1208	K1209	V1210	L1211	L1212	K1213	G1216	V1217	S1218	F1219	L1220	I1221	N1222	T1223	F1224	E1225	G1228	C1229	G1230	GLN	PRO						
SER	GLY	ILE	LEU	ALA	GLN	PRO	THR	L1241	L1244	F1248	S1249	L1257	D1258	L1261	C1266	Y1267	N1268	T1269	F1270	I1271	R1274	T1275	V1276	L1279	L1282	G1283	T1284	E1285	A1286	Q1287	S1288	L1290	L1291	V1294	F1297	L1298	E1299	S1300	I1301	A1302	M1303	HIS	ASP	ILE	ILE	ALA	ALA	GLU							
LYS	CYS	PHE	GLY	THR	GLY	ALA	ALA	GLY	ASN	ARG	THR	S1323	P1324	Q1325	E1326	Y1330	K1334	C1335	T1336	V1337	V1338	V1339	R1340	I1341	M1342	E1343	F1344	T1347	S1352	G1355	W1356	K1357	L1358	L1359	K1360	K1361	D1362	L1363	C1364	N1365	T1366	H1367	L1368	M1369	R1370	Y1371	L1372	C1377	E1378	P1379	T1382	G1383			
F1384	V1389	Q1390	D1397	V1398	C1399	V1400	N1401	L1402	L1406	K1407	M1408	S1409	P1410	T1414	L1415	H1418	L1419	R1420	E1421	K1422	I1423	T1424	A1425	Q1426	N1427	I1428	E1429	L1431	C1432	A1433	V1434	N1435	L1436	Y1437	A1441	Q1442	B1445	S1446	R1447	L1448	V1451	L1458	H1459	GLN	R1460	L1463	L1464	I1467							
L1468	P1469	Q1470	S1471	T1472	T1473	D1474	L1475	H1476	H1477	V1478	S1479	E1482	L1483	L1484	S1485	L1486	V1487	K1488	K1489	G1490	I1491	A1492	P1493	G1494	ASP	GLU	ARG	GLN	CYS	LEU	P1501	D1504	L1505	S1506	C1507	L1515	C1525	L1531	L1538	S1539	T1540	A1541	SER	LEU	GLY	SER	GLN	R1552							
F1553	S1554	H1555	Y1558	L1562	F1563	S1564	E1565	T1566	I1567	N1568	T1569	L1572	K1573	N1574	V1579	L1582	M1583	N1589	T1590	K1591	M1592	V1593	V1596	L1597	S1604	F1605	R1606	A1609	H1613	L1616	K1617	L1618	A1619	T1620	T1621	T1622	W1626	P1638	L1639	E1640	L1641	V1645	L1649	A1650	R1711	R1712	V1713	L1714	E1715	Q1716					



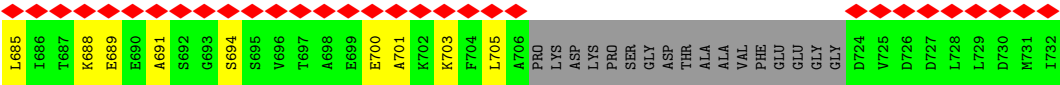
Y3614	E3553	T3484	A3417	E3353	R3287	ARG	K3147	E3079	E3007	V2920	F2840	LYS
A3615	F3554	T3487	D3418	D3354	S3288	MET	Q3148	Y3082	W3008	W2923	N2841	GLU
A3616	V3555	S3488	F3419	K3355	R3289	GLU	G3149	L3086	K3009	V2924	L2844	LYS
L3617	A3556	S3489	C3420	A3356	S3290	VAL	N3150	L3086	S3010	L2844	L2844	SER
G3618	R3557	V3490	D3421	R3357	Q3296	GLU	L3151	L3086	L3011	A2927	T2846	GLU
D3619	K3558	F3495	Q3422	R3358	V3297	GLN	S3152	L3089	E3013	R2831	L2846	LEU
P3620	S3559	I3496	Q3423	I3359	I3298	GLN	S3153	L3090	Y3012	R2831	L2846	LYS
K3621	K3560	S3497	L3424	I3360	T3299	GLU	S3154	L3091	A3017	F2851	F2851	MET
A3622	W3498	W3498	K3426	E3361	V3300	GLU	Q3154	L3092	S3018	P2853	P2853	LYS
P3623	L3562	I3499	E3427	E3362	L3301	GLU	P3155	Q3093	S3019	F2854	F2854	ASP
G3624	D3563	S3500	E3428	SER	K3302	D3226	P3156	Q3093	I3019	C2857	C2857	ALA
L3625	Q3564	H3501	E3429	GLY	S3305	I3227	L3157	D3094	I3019	I2842	I2842	GLN
A3626	V3502	V3503	ASN	SER	L3306	S3228	S3157	D3094	S3021	Q2859	Q2859	VAL
G3627	K3504	A3504	ALA	SER	L3307	S3229	K3158	D3095	S3021	I2861	I2861	LEU
F3628	L3505	L3506	SER	GLU	I3308	S3230	R3159	D3096	N3028	D2861	D2861	TYR
R3629	L3507	D3507	ILE	GLU	E3309	S3231	K3160	D3097	N3028	Q2864	Q2864	ARG
K3630	F3571	K3508	ASP	D3369	N3310	S3232	L3161	D3097	P3025	L2868	L2868	SER
R3631	N3572	P3572	SER	E3370	N3311	S3233	R3167	D3097	D3026	L2958	L2958	TYR
K3632	N3573	K3509	ALA	E3371	V3312	C3234	D3170	D3098	N3028	R2962	R2962	HIS
L3633	A3574	D3509	GLU	E3372	S3313	S3235	K3171	A3099	N3028	S2963	S2963	GLY
F3634	L3575	Q3510	LEU	I3373	M3240	S3236	K3172	K3100	K3029	L2871	L2871	ASP
G3635	D3576	A3511	GLU	I3374	K3241	S3237	K3173	K3100	I3030	D2872	D2872	LEU
T3636	Y3378	V3512	Q3440	Y3378	K3242	S3238	M3176	K3100	W3031	A2875	A2875	PRO
A3637	A3381	A3513	A3441	A3381	M3242	S3239	W3179	K3100	S3032	V2876	V2876	ASP
K3638	H3384	V3514	P3443	H3384	I3243	S3240	K3182	K3100	E2967	Q2879	Q2879	ILE
F3639	S3587	V3514	F3444	S3386	D3244	S3241	I3182	K3100	A2968	C2880	C2880	GLY
L3640	E3588	K3519	L3446	S3387	R3247	K3242	I3183	K3100	E2974	S2883	S2883	ASP
P3641	L3588	E3520	V3447	E3387	K3248	S3243	K3186	K3100	E2975	L2884	L2884	LEU
K3642	L3588	T3522	K3448	E3387	Q3249	S3244	C3187	K3100	E2976	Q2885	Q2885	LEU
H3643	P3526	P3526	K3452	A3388	L3259	S3245	F3188	K3100	E2977	Q2886	Q2886	LEU
F3644	T3529	V3530	A3453	V3389	L3262	S3246	F3189	K3100	E2978	V2888	V2888	PRO
G3645	V3531	V3531	L3454	Q3390	H3263	S3265	K3196	K3100	E2979	L2898	L2898	LEU
K3646	P3532	P3532	A3461	GLU	K3264	S3266	E3194	K3100	Q3046	L2899	L2899	LEU
L3647	F3533	F3533	K3462	GLU	S3267	S3267	E3195	K3100	S3047	LEU	LEU	LEU
G3648	I3534	I3534	F3465	ALA	T3268	S3268	K3196	K3100	K3048	ALA	ALA	ALA
S3649	T3535	T3535	P3466	PRO	R3269	S3269	L3126	K3100	L3049	GLU	GLU	GLU
K3650	S3536	S3536	R3467	TRP	D3270	S3270	L3127	K3100	L3049	PRO	PRO	PRO
L3651	S3537	S3537	L3468	SER	K3271	S3271	L3128	K3100	L3049	ALA	ALA	ALA
R3652	E3538	E3538	L3469	TRP	W3272	S3272	L3129	K3100	L3049	LYS	LYS	LYS
K3653	S3539	S3539	Q3470	CYS	L3273	S3273	L3130	K3100	L3049	ARG	ARG	ARG
L3654	S3539	S3539	I3471	GLY	V3274	S3274	L3131	K3100	L3049	VAL	VAL	VAL
K3655	V3540	V3540	F3472	PRO	S3275	S3275	L3132	K3100	L3049	ARG	ARG	ARG
L3656	S3541	S3541	E3473	A3406	W3276	S3276	L3133	K3100	L3049	GLY	GLY	GLY
S3657	F3542	F3542	R3474	A3407	V3277	S3277	L3134	K3100	L3049	LYS	LYS	LYS
D3658	P3544	P3544	Y3475	G3408	K3339	S3278	L3135	K3100	L3049	ALA	ALA	ALA
F3659	V3601	V3601	P3476	I3410	A3340	S3279	L3136	K3100	L3049	ARG	ARG	ARG
K3660	K3544	K3544	F3477	I3410	L3341	S3280	L3137	K3100	L3049	VAL	VAL	VAL
D3661	S3546	S3546	P3478	D3411	E3344	C3281	L3138	K3100	L3049	GLY	GLY	GLY
L3662	T3547	T3547	E3478	A3412	P3345	R3282	L3139	K3100	L3049	ALA	ALA	ALA
T3663	G3548	G3548	T3479	A3413	F3346	L3283	L3140	K3100	L3049	ARG	ARG	ARG
T3663	M3414	M3414	L3480	C3347	C3347	S3284	L3141	K3100	L3049	LYS	LYS	LYS
N3664	L3415	L3415	S3481	T3415	L3348	H3285	L3142	K3100	L3049	ALA	ALA	ALA
K3665	L3416	L3416	L3416	L3416	A3349	C3286	L3143	K3100	L3049	ARG	ARG	ARG
L3666	E3551	E3551	E3350	E3351	E3352	E3352	L3144	K3100	L3049	LEU	LEU	LEU
L3667	K3552	K3552	E3352	E3352	E3352	E3352	L3145	K3100	L3049	LEU	LEU	LEU
L3668	K3552	K3552	E3352	E3352	E3352	E3352	L3146	K3100	L3049	LEU	LEU	LEU
K3669	K3552	K3552	E3352	E3352	E3352	E3352	L3147	K3100	L3049	LEU	LEU	LEU
L3670	K3552	K3552	E3352	E3352	E3352	E3352	L3148	K3100	L3049	LEU	LEU	LEU
L3671	K3552	K3552	E3352	E3352	E3352	E3352	L3149	K3100	L3049	LEU	LEU	LEU
L3672	K3552	K3552	E3352	E3352	E3352	E3352	L3150	K3100	L3049	LEU	LEU	LEU
L3673	K3552	K3552	E3352	E3352	E3352	E3352	L3151	K3100	L3049	LEU	LEU	LEU



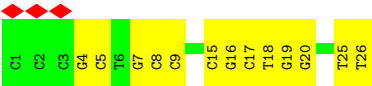
• Molecule 2: X-ray repair cross-complementing protein 6







• Molecule 4: DNA (26-MER)



• Molecule 5: DNA (26-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	190498	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 ($e^-/\text{\AA}^2$)	47.22	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.648	Depositor
Minimum map value	-2.277	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	456.4, 456.4, 456.4	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IIX

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	0.30	0/29016	0.53	1/39251 (0.0%)
2	B	0.32	0/4014	0.60	3/5408 (0.1%)
3	C	0.27	0/5374	0.50	2/7246 (0.0%)
4	D	0.56	0/587	0.91	0/902
5	E	0.56	0/607	0.86	0/936
All	All	0.31	0/39598	0.55	6/53743 (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	4
2	B	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	424	LEU	CA-CB-CG	5.78	128.60	115.30
2	B	385	LEU	CA-CB-CG	5.65	128.29	115.30
1	A	204	LEU	CA-CB-CG	5.60	128.17	115.30
2	B	497	LEU	CA-CB-CG	5.34	127.57	115.30
2	B	202	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1020	PRO	Peptide
1	A	1175	HIS	Peptide
1	A	3025	PRO	Peptide
1	A	3462	ARG	Peptide
2	B	252	ARG	Peptide

5.2 Too-close contacts

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	28443	0	28622	1176	0
2	B	3937	0	4013	194	0
3	C	5274	0	5275	252	0
4	D	526	0	293	12	0
5	E	540	0	291	14	0
6	A	34	0	0	0	0
All	All	38754	0	38494	1577	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 20.

The worst 5 of 1577 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:322:TYR:CE2	3:C:274:LYS:HG3	1.64	1.32
3:C:323:PHE:CE1	3:C:328:GLU:HB3	1.82	1.13
2:B:322:TYR:HE2	3:C:274:LYS:CG	1.68	1.05
1:A:2225:HIS:ND1	1:A:2226:PRO:HD2	1.72	1.04
1:A:3190:LEU:HB3	1:A:3235:LYS:HZ2	1.27	0.98

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	3555/4128 (86%)	3157 (89%)	395 (11%)	3 (0%)	51	82
2	B	486/609 (80%)	418 (86%)	67 (14%)	1 (0%)	47	78
3	C	653/732 (89%)	585 (90%)	68 (10%)	0	100	100
All	All	4694/5469 (86%)	4160 (89%)	530 (11%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2548	PRO
1	A	1021	VAL
2	B	144	SER
1	A	1020	PRO

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	3121/3671 (85%)	3099 (99%)	22 (1%)	84	91
2	B	439/548 (80%)	435 (99%)	4 (1%)	78	88
3	C	585/649 (90%)	578 (99%)	7 (1%)	71	84
All	All	4145/4868 (85%)	4112 (99%)	33 (1%)	82	90

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	239	LYS
3	C	323	PHE
3	C	670	GLN
1	A	2899	ARG
1	A	2365	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	480	ASN
3	C	488	GLN
3	C	511	HIS
3	C	452	ASN
1	A	2807	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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
6	1IX	A	4201	-	37,38,38	2.25	10 (27%)	50,54,54	2.00	18 (36%)

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
6	1IX	A	4201	-	-	0/18/26/26	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4201	1IX	C14-C16	6.37	1.56	1.49
6	A	4201	1IX	C12-C13	5.77	1.47	1.37
6	A	4201	1IX	C11-CL1	4.25	1.83	1.73
6	A	4201	1IX	C21-C20	-3.50	1.36	1.42
6	A	4201	1IX	C24-N26	3.36	1.48	1.38

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4201	1IX	C21-C16-N17	-5.35	119.52	123.04
6	A	4201	1IX	C18-N19-C20	4.50	121.60	115.40
6	A	4201	1IX	C21-C20-N19	-4.21	118.34	122.83
6	A	4201	1IX	N19-C18-N17	-4.21	122.10	128.68
6	A	4201	1IX	C15-C10-C11	3.23	120.30	117.12

There are no chirality outliers.

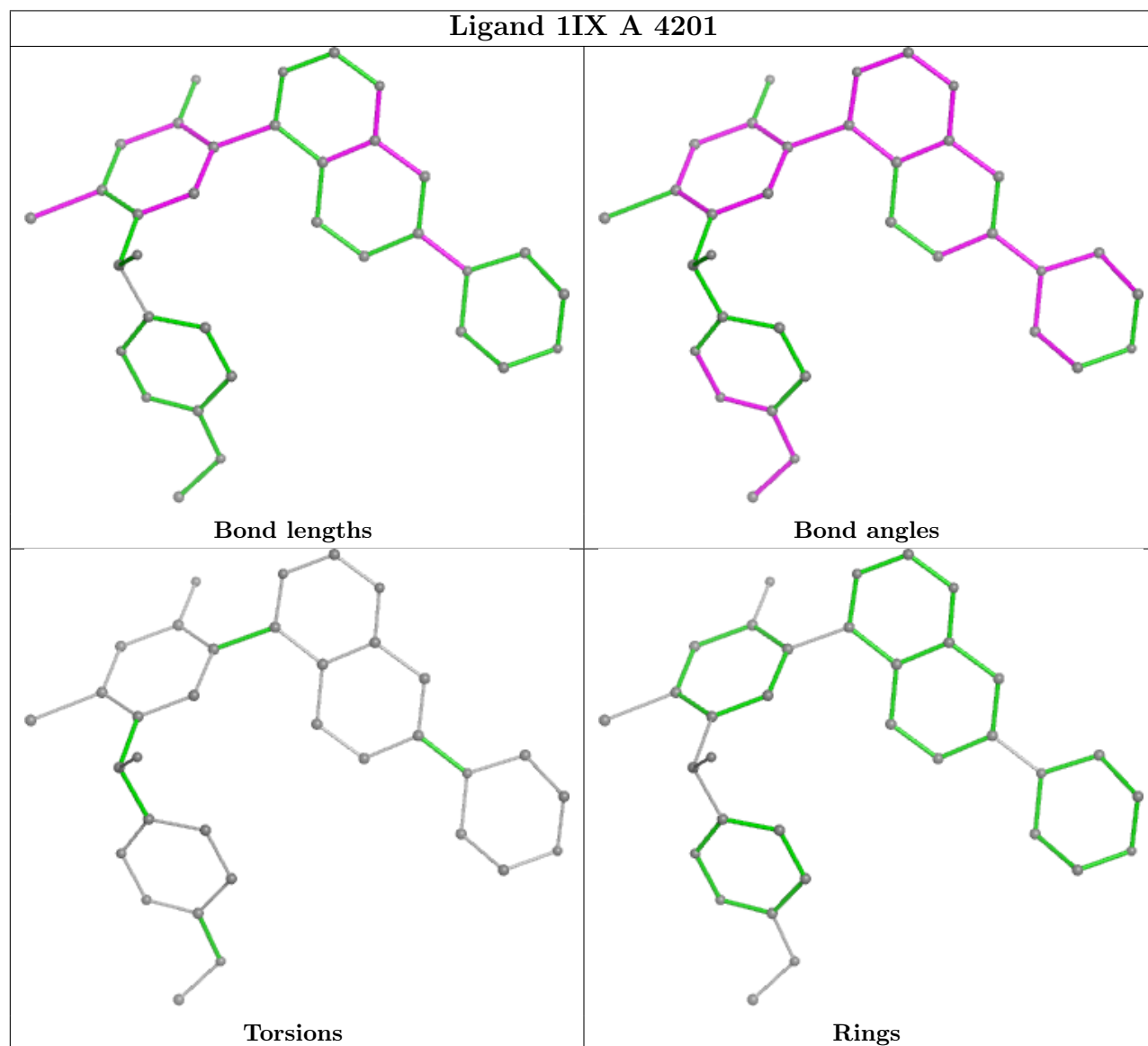
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

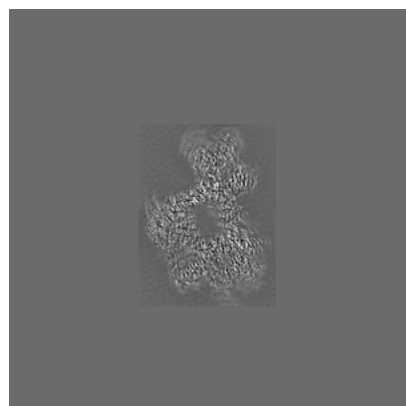
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14546. 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

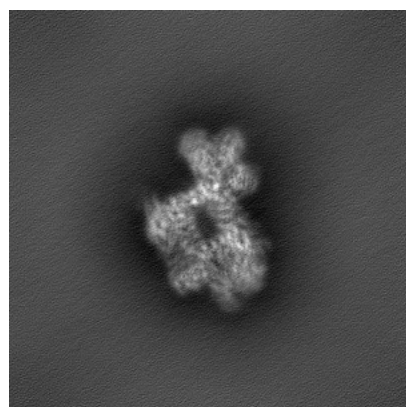


Y

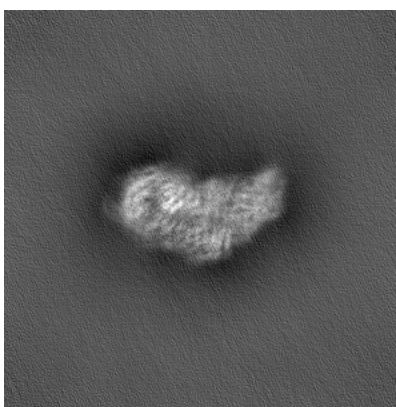


Z

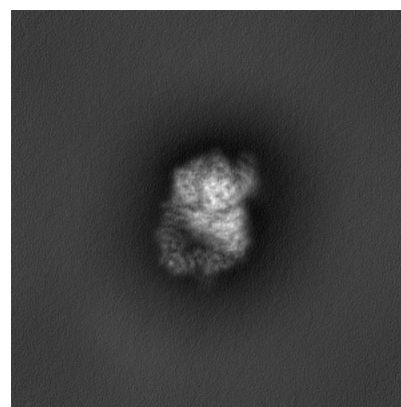
6.1.2 Raw map



X



Y

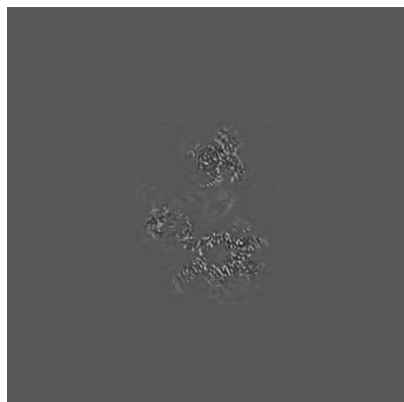


Z

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

6.2 Central slices [i](#)

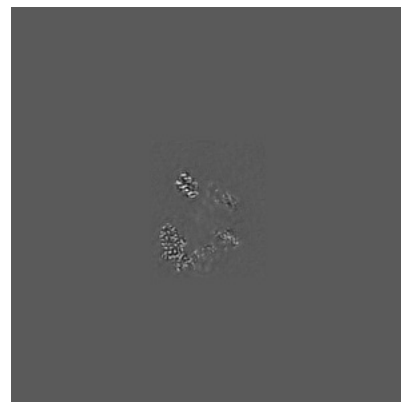
6.2.1 Primary map



X Index: 175

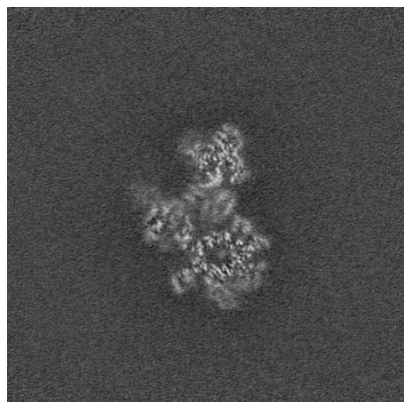


Y Index: 175

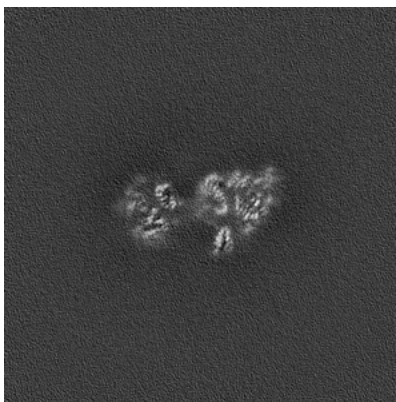


Z Index: 175

6.2.2 Raw map



X Index: 175



Y Index: 175

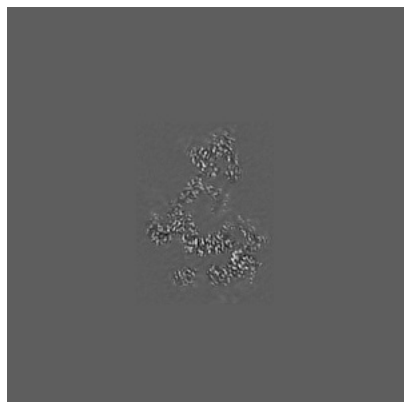


Z Index: 175

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

6.3 Largest variance slices [i](#)

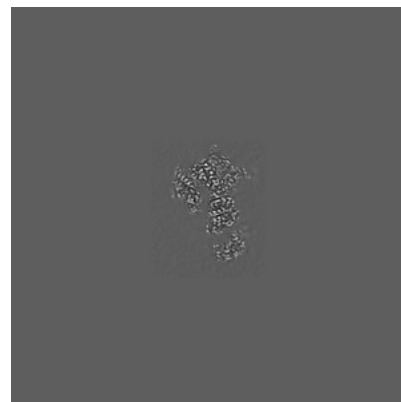
6.3.1 Primary map



X Index: 182

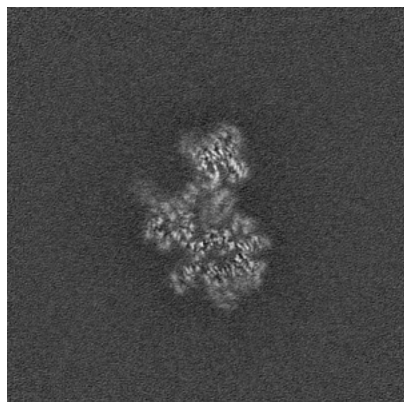


Y Index: 194

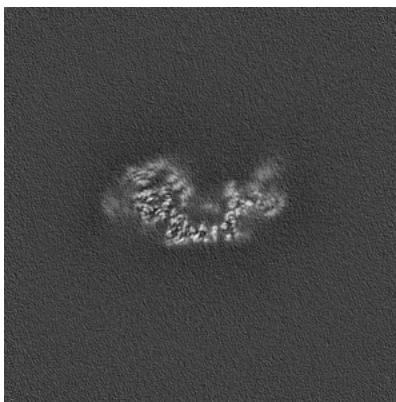


Z Index: 143

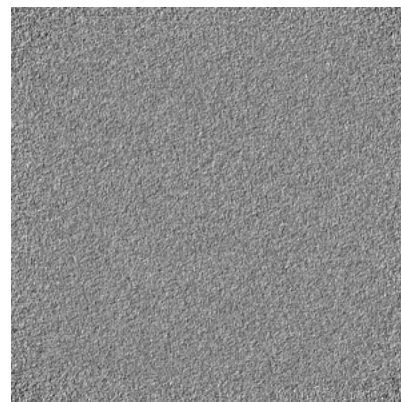
6.3.2 Raw map



X Index: 177



Y Index: 197

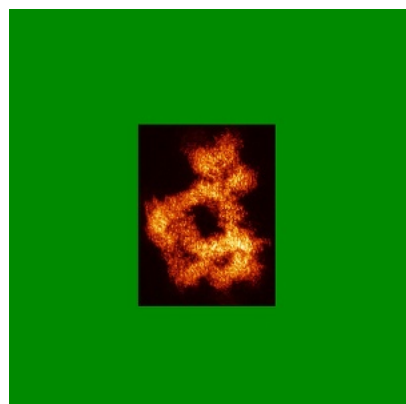


Z Index: 0

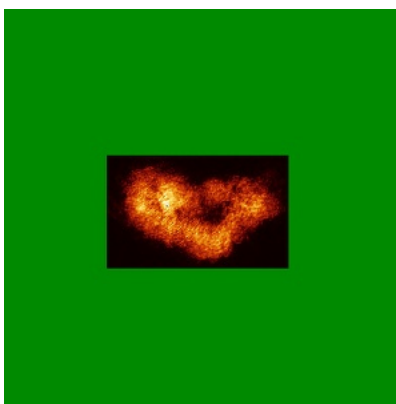
The images above show the largest variance slices of the map in three orthogonal directions.

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

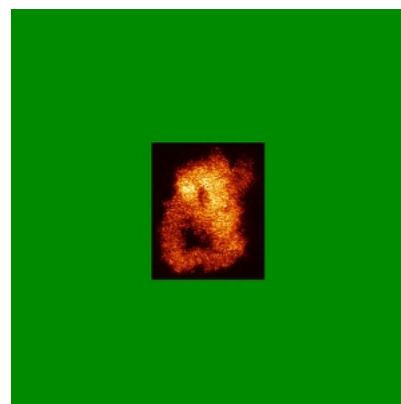
6.4.1 Primary map



X

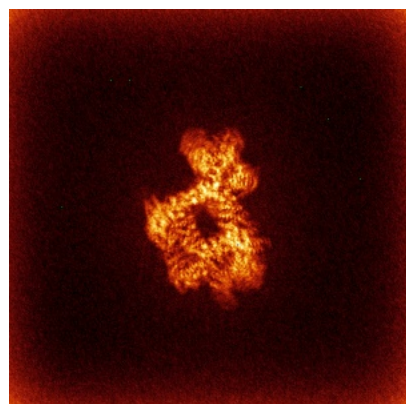


Y

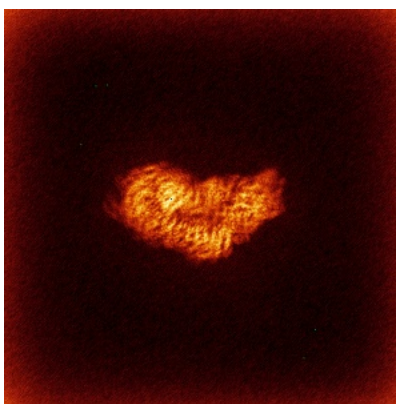


Z

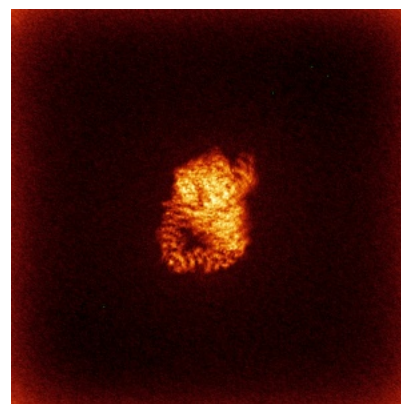
6.4.2 Raw map



X



Y



Z

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

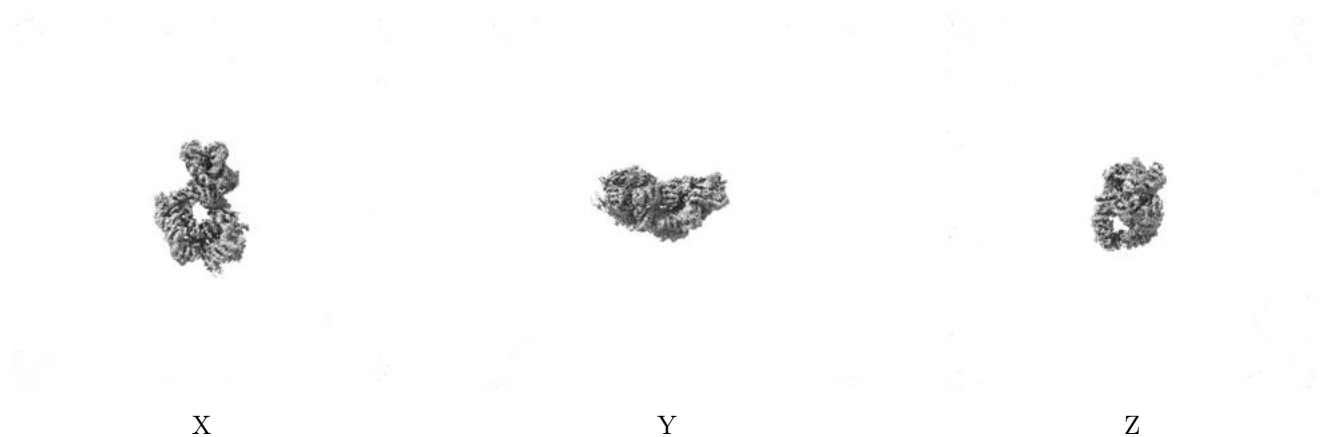
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

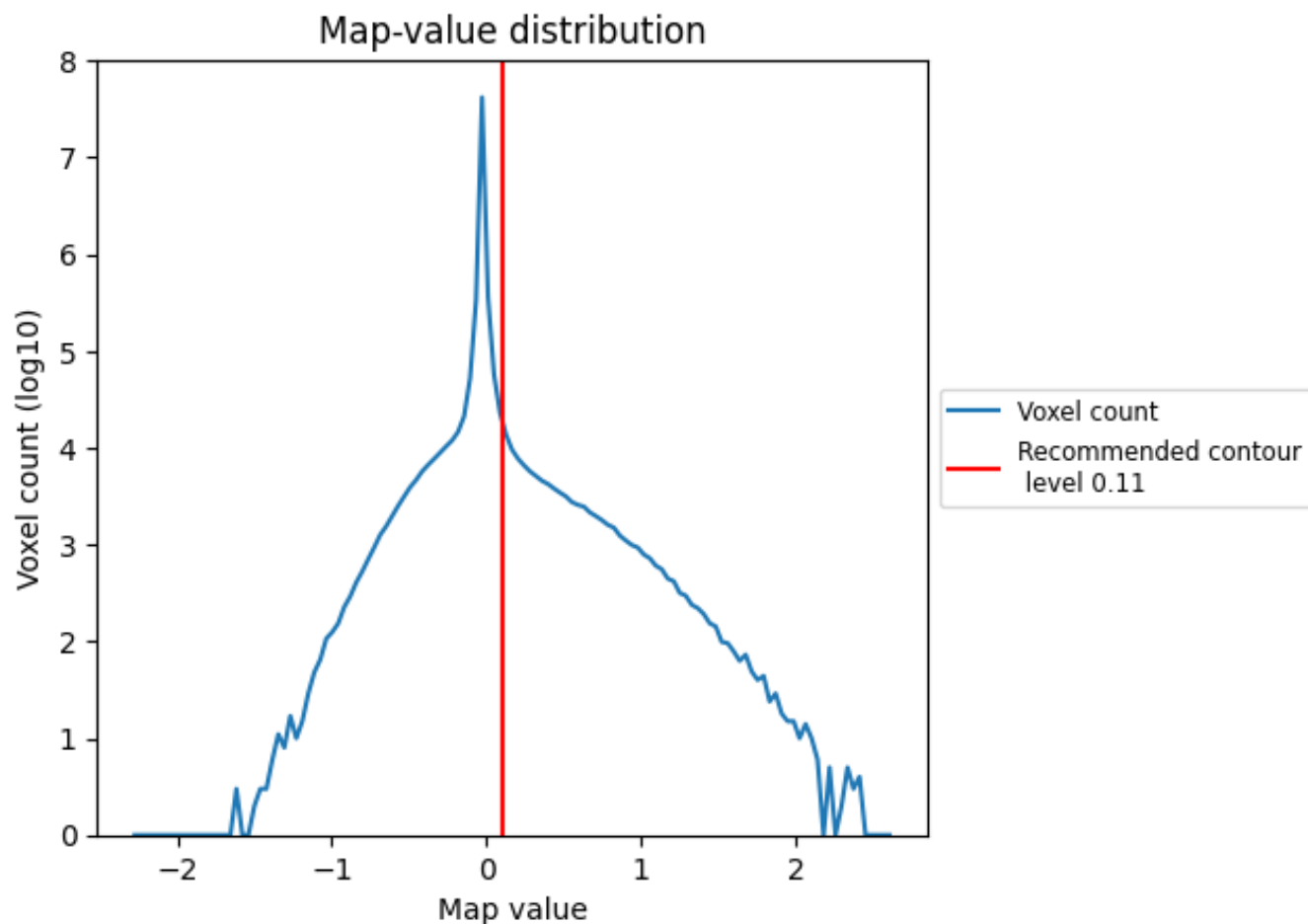
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

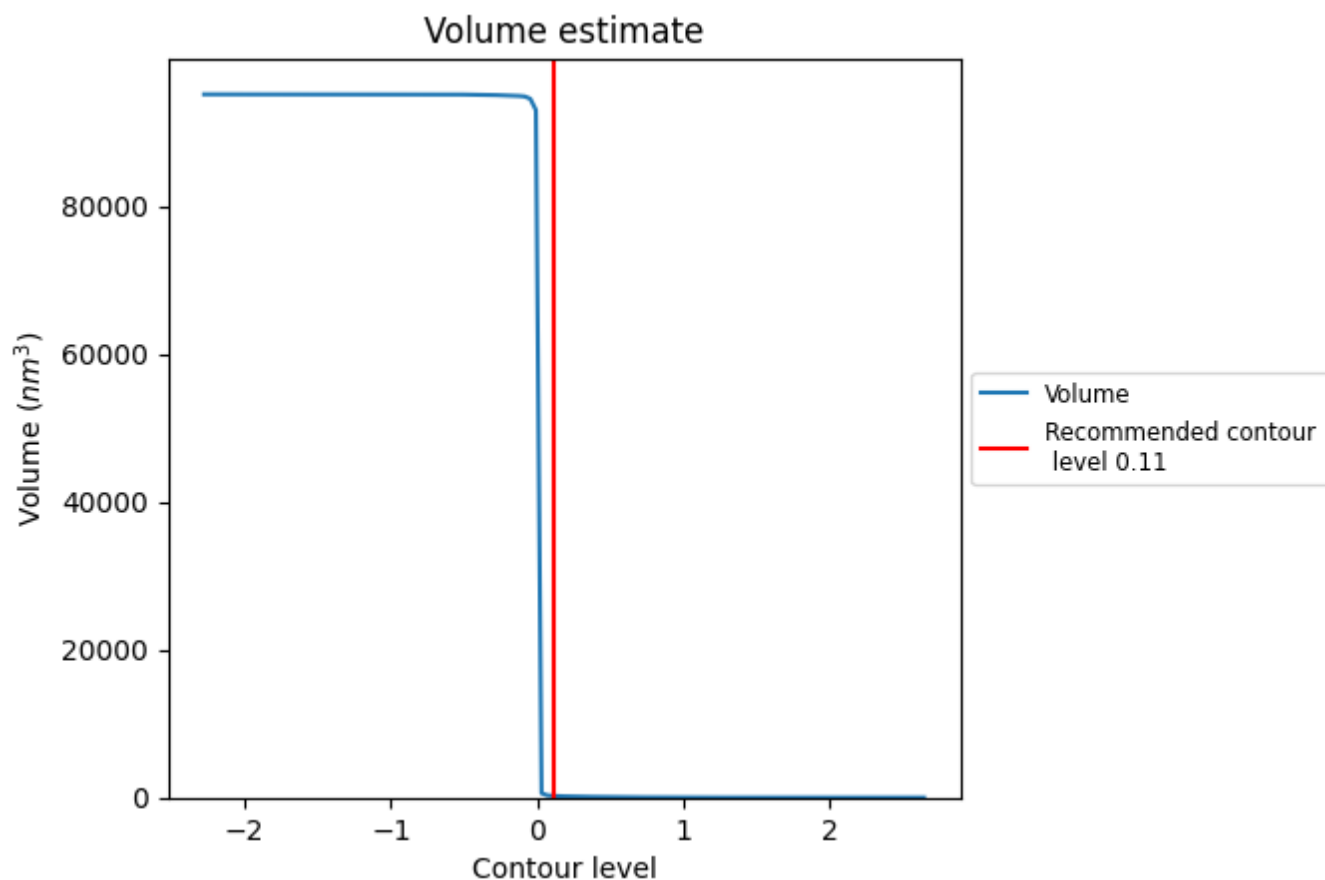
This section contains the results of statistical analysis of the map.

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.

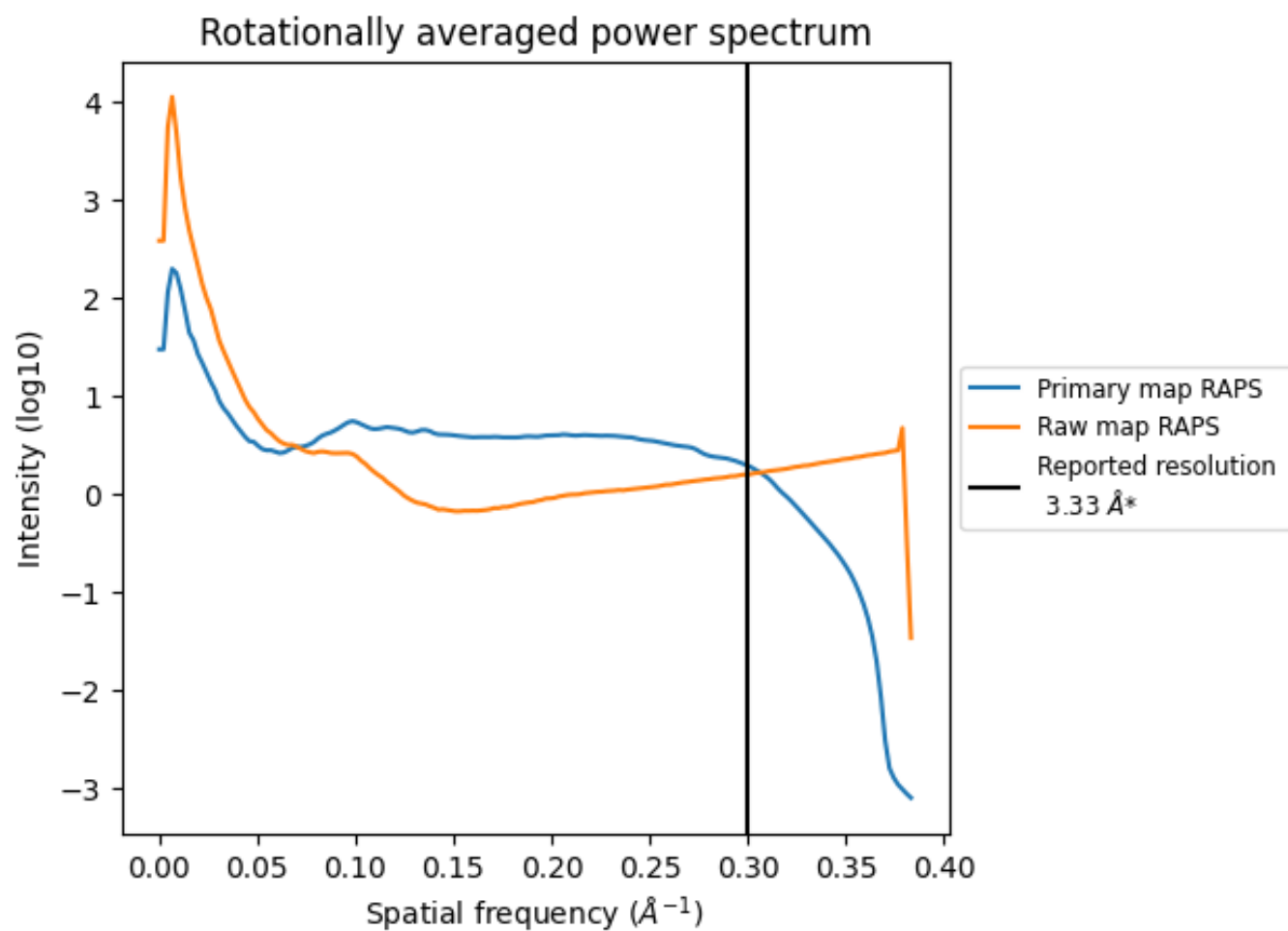
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 229 nm^3 ; this corresponds to an approximate mass of 207 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 ⓘ

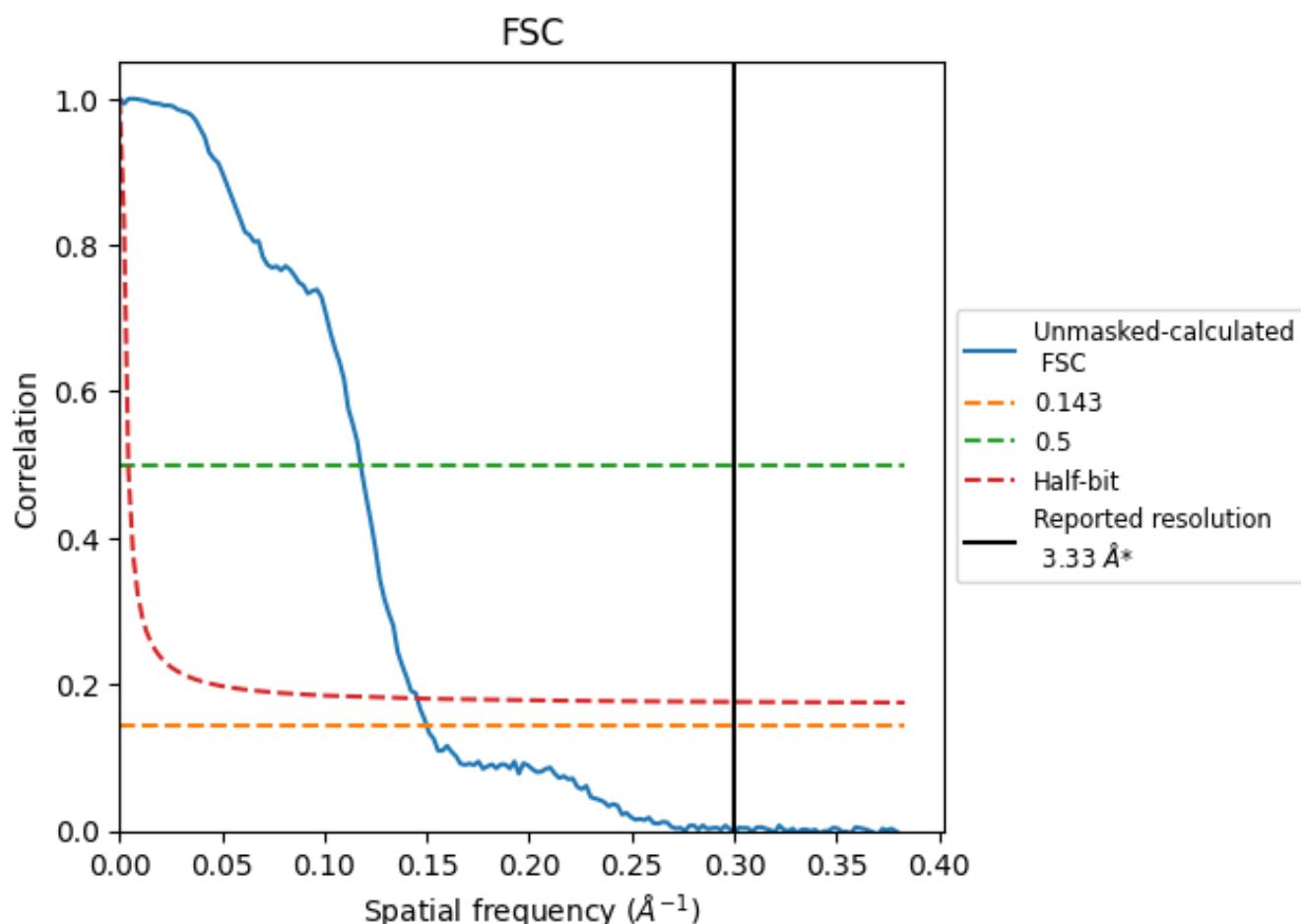


*Reported resolution corresponds to spatial frequency of 0.300 \AA^{-1}

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 0.300 Å⁻¹

8.2 Resolution estimates [i](#)

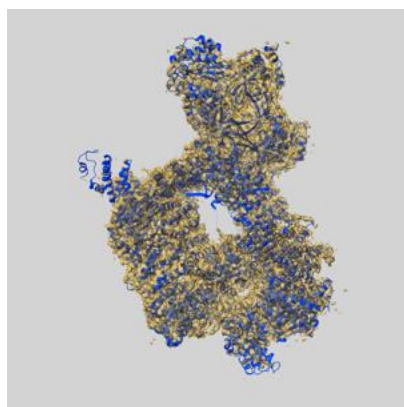
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.67	8.49	6.88

*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 6.67 differs from the reported value 3.33 by more than 10 %

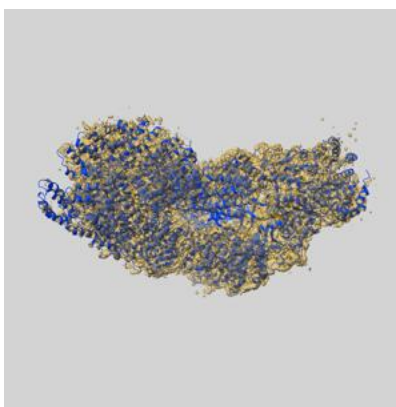
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14546 and PDB model 7Z88. Per-residue inclusion information can be found in section 3 on page 5.

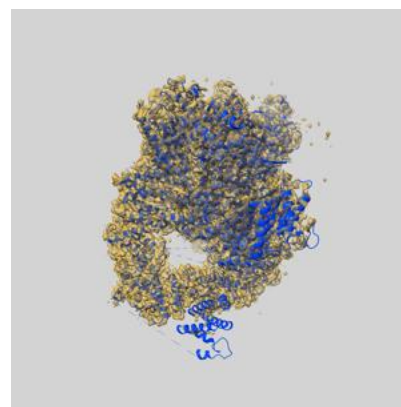
9.1 Map-model overlay [i](#)



X



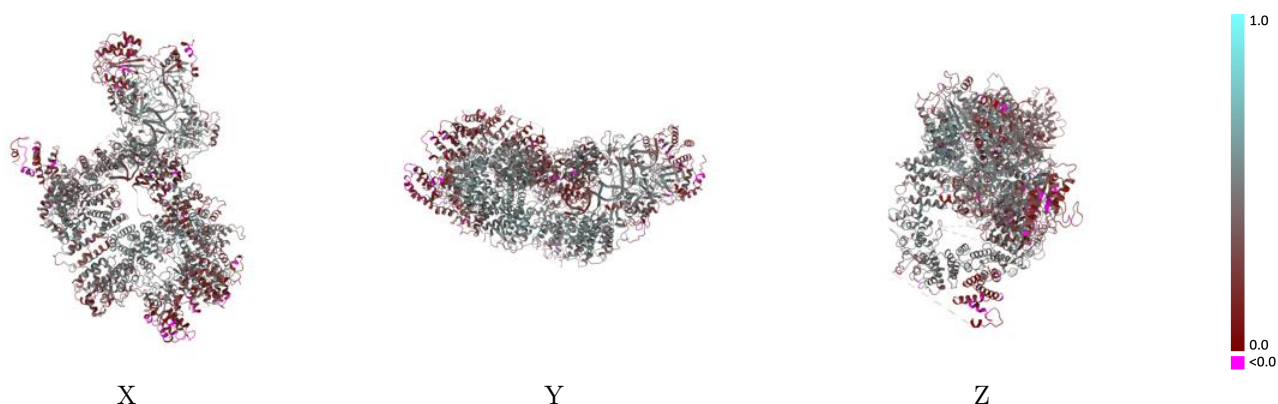
Y



Z

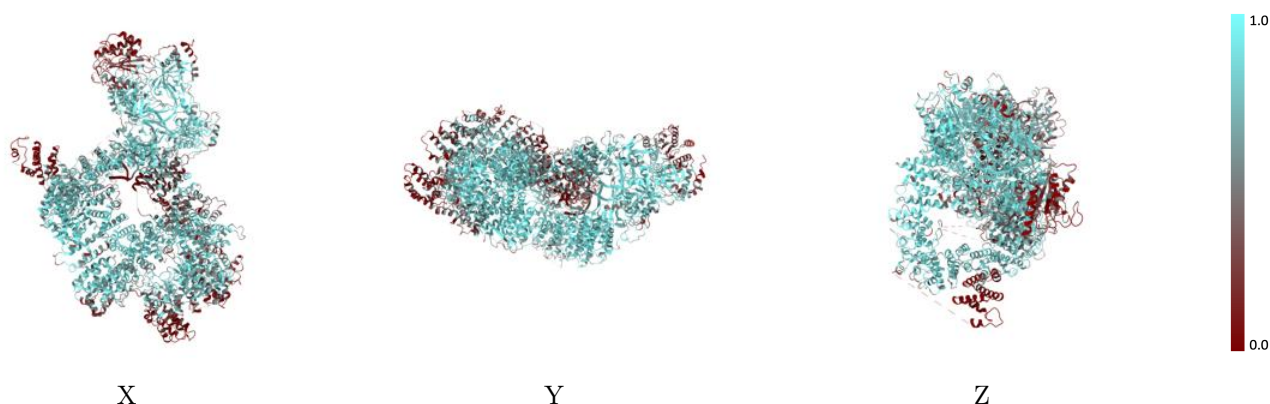
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



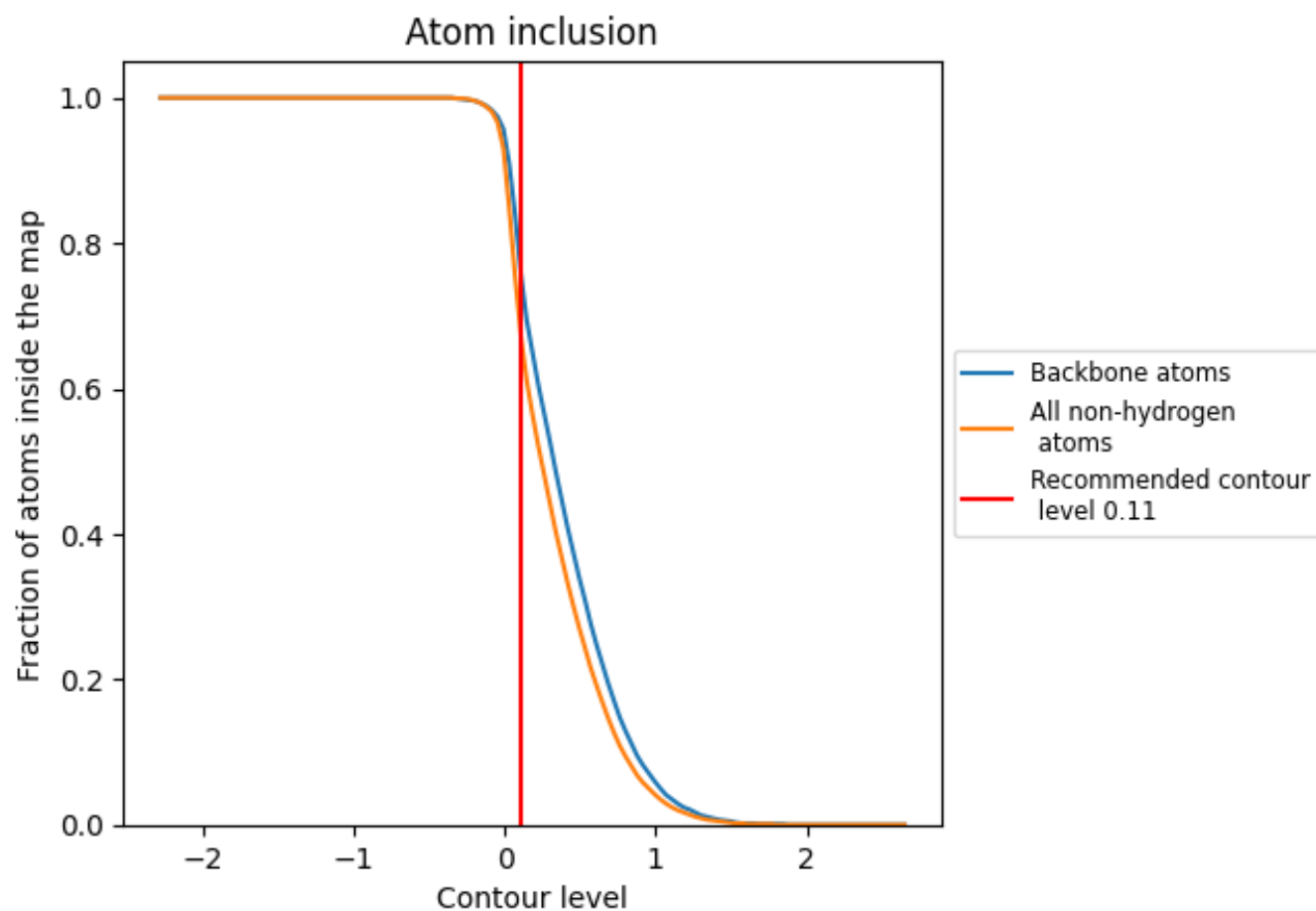
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6700	<div></div> 0.3890
A	<div></div> 0.7000	<div></div> 0.4010
B	<div></div> 0.7340	<div></div> 0.4110
C	<div></div> 0.4540	<div></div> 0.3040
D	<div></div> 0.7450	<div></div> 0.4420
E	<div></div> 0.6940	<div></div> 0.3990

