



wwPDB EM Validation Summary Report ⓘ

Jul 14, 2024 – 06:27 pm BST

PDB ID : 8BHV
EMDB ID : EMD-16070
Title : DNA-PK XLF mediated dimer bound to PAXX
Authors : Hardwick, S.W.; Chaplin, A.K.
Deposited on : 2022-11-01
Resolution : 4.51 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
MolProbity : 4.02b-467
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

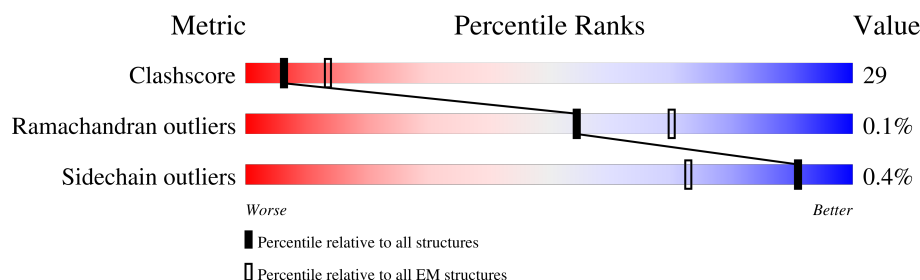
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.51 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	
1	F	4128	
2	K	336	
2	L	336	
2	N	336	
2	O	336	
3	M	911	
3	P	911	

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Mol	Chain	Length	Quality of chain
4	Q	299	
4	R	299	
5	a	609	
5	h	609	
6	b	732	
6	j	732	
7	c	204	
7	i	204	
8	D	27	
9	E	28	
10	I	24	
11	J	24	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 91357 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	3549	Total	C	N	O	S	0	0
			28250	18146	4783	5134	187		
1	F	3543	Total	C	N	O	S	0	0
			28263	18162	4780	5132	189		

- Molecule 2 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
2	L	195	Total	C	N	O	S	0	0
			1589	1009	271	302	7		
2	N	201	Total	C	N	O	S	0	0
			1625	1030	278	310	7		
2	O	194	Total	C	N	O	S	0	0
			1589	1009	271	302	7		

- Molecule 3 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	258	Total	C	N	O	S	0	0
			2085	1327	349	396	13		
3	P	246	Total	C	N	O	S	0	0
			1983	1261	339	371	12		

- Molecule 4 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	218	Total	C	N	O	S	0	0
			1745	1119	294	319	13		
4	R	225	Total	C	N	O	S	0	0
			1796	1150	301	330	15		

- Molecule 5 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	505	Total	C	N	O	S	0	0
			4038	2583	691	747	17		
5	h	505	Total	C	N	O	S	0	0
			4026	2578	681	750	17		

- Molecule 6 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	650	Total	C	N	O	S	0	0
			5214	3328	876	985	25		
6	j	636	Total	C	N	O	S	0	0
			5082	3252	854	951	25		

- Molecule 7 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	23	Total	C	N	O	S	0	0
			165	105	27	32	1		
7	i	23	Total	C	N	O	S	0	0
			162	102	27	32	1		

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	27	Total	C	N	O	P	0	0
			556	268	95	166	27		

- Molecule 9 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	28	Total	C	N	O	P	0	0
			576	277	107	164	28		

- Molecule 10 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	24	Total	C	N	O	P	0	0
			494	238	92	140	24		

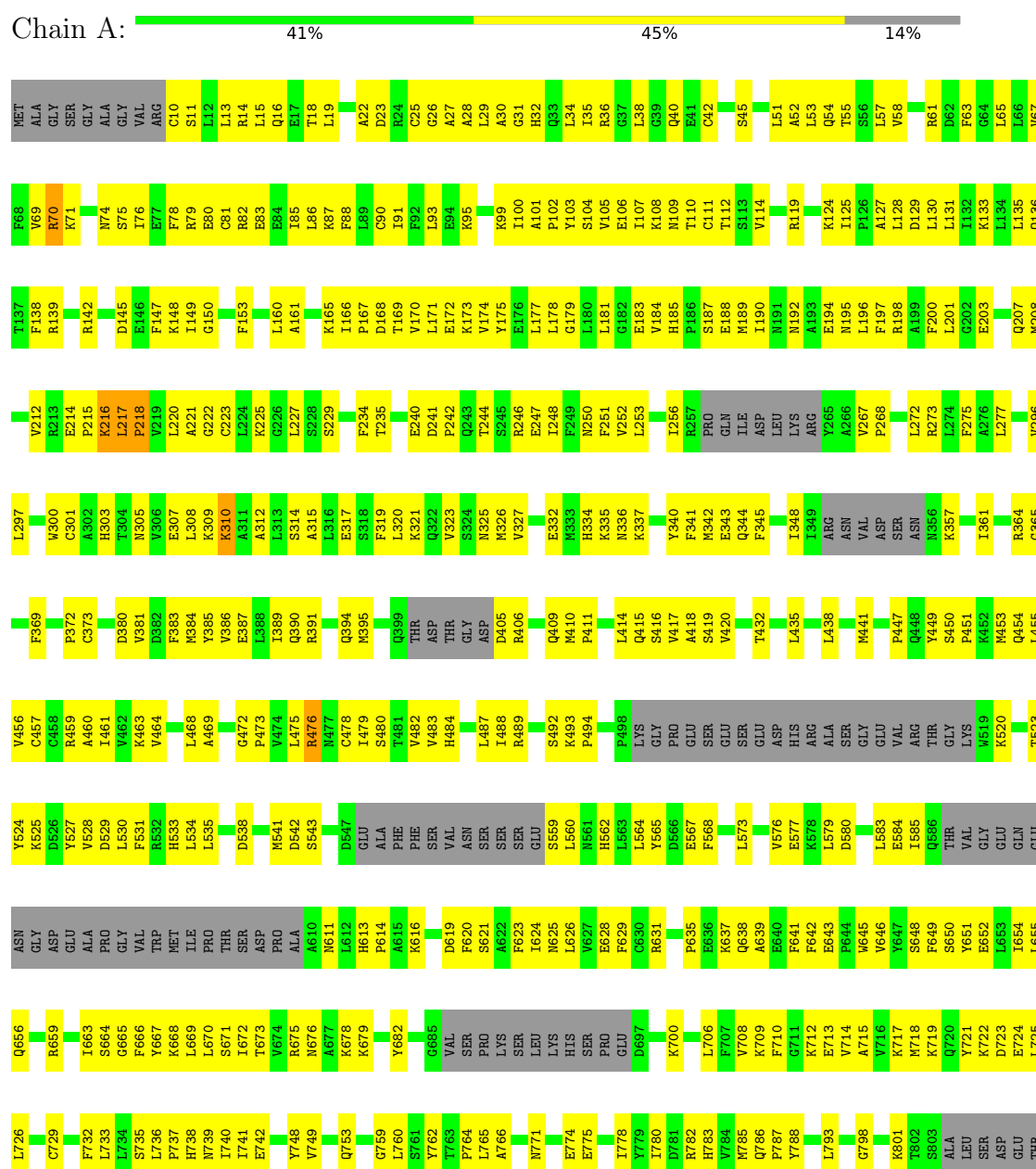
- Molecule 11 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	24	Total 491	C 239	N 79	O 149	P 24	0	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

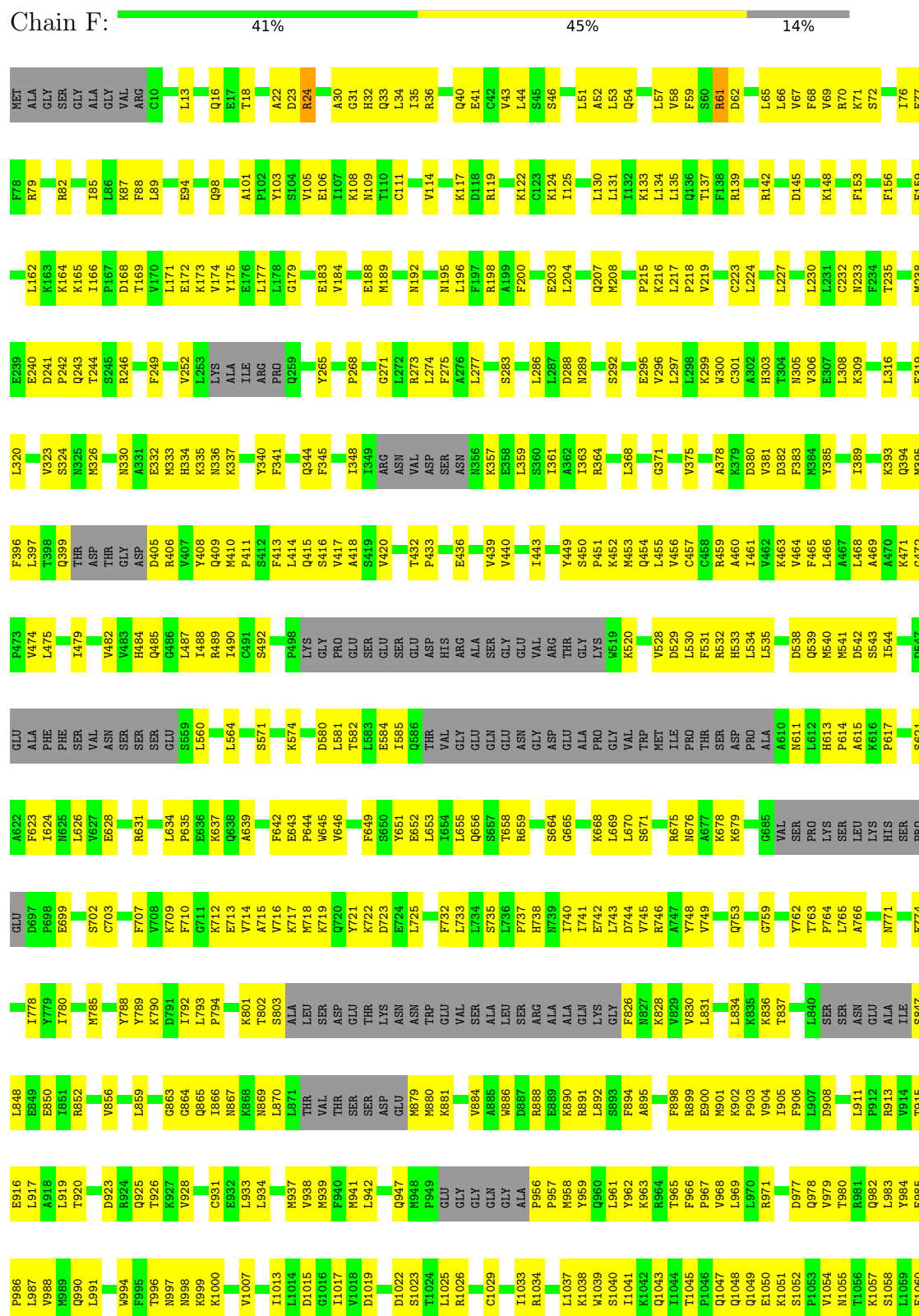






G4083	H4013	G3939	LYS	L3775	I3701	F3632	R3557	T3472	CYS	T3333	K3260	E3195	H3122	L3051
D4086	K4014	L3940	HIS	D3778	P3702	I3633	R3558	T3479	GLY	T3334	E3261	K3196	Q3123	L3054
H4087	PHE	H3944	D3851	T3778	G3707	Q3634	K3559	T3480	ALA	R3355	L3262	THR	R3125	
N4088	GLU	G3947	M3856	C3781	R3708	S3481	S3560	S3482	G3407	T3336	K3264	LEU	K3126	D3058
I4089	GLN	S3782	G3709	S3782	G3709	K3638	K3561	L3482	G3408	T3337	K3265	PRO	T3127	Q3059
R4090	LYS	A3785	Y3859	C3781	G3710	E3639	L3562	K3483	V3409	K3338	S3266	PRO	K3128	S3060
A4091	MET	A3786	K3860	A3785	P3711		D3663	V3490	L3416	A3340	K3267	GLU	L3061	L3061
Q4092	LEU	L3786		L3786	E3714	K3642	V3567	V3491	F3419	C3347	T3268	ASP	S3131	L3062
E4095	LYS	Q3787	R3864	Q3787	E3715	H3643	F3571	C3492	C3420	K3348	R3269	ASN	A3134	T3063
	GLY	R3788	E3865	R3788	H3716	K3646		C3493	K3438	L3348	D3270	SER	F3064	F3064
E4100	GLY	R3789	E3866	R3789	H3717	G3647		Q3494	A3349	L3346	D3271	MET	L3135	L3065
E4101	SER	V3793	V3868	V3793	R3718	GLY	A3874	F3495	E3850	E3337	W3272	VAL	E3137	K3067
T4102	TRP	P3956	T3869	P3956	I3719	SER	L3575	L3496	Q3422	I3351		ASP	I3138	
Q4103	ILE	M3796	K3873	M3796	F3722	LYS	D3576	S3497	Q3423	E3352		GLN	I3142	E3072
V4104	GLN	T3797	L3878	T3797	F3723	LEU	Q3577	W3498	L3424	D3353		ASP	I3145	L3073
V4105	GLU	S3798	R3879	S3798	I3724	ARG	K3578	I3499	R3425	D3354		GLY	I3145	Q3074
C4106	ILE	R3799	V3878	R3799	E3724	MET	S3879	S3500	K3426	D3354		ASP	I3145	K3075
L4107	ASN	L3800	P3879	L3800	R3725	LYS	N3880	H3501	E3429	R3357		PRO	A3076	A3076
M4108	VAL	G3801	A3880	G3801	V3728	LYS	N3881	K3502	ASN	R3358		SER	Q3148	L3077
	ALA	L3802	D3881	L3802	M3729	LEU	E3882	V3503	ALA	L3359		ASP	G3149	L3078
A4111	GLU	I3803	E3885	I3803	S3657	LEU	L3583	A3504	SER	L3360		ARG	N3150	E3079
T4112	GLY	E3804	A3730	E3804	D3658	GLN	L3584	L3505	VAL	E3361		MET	L3151	L3080
D4113	LYS	V3805	F3659	V3805	F3659	ILE	F3585	L3362	ILE	L3362		GLU	S3152	H3081
P4114	ASN	L3806	N3660	L3806	N3660	ASP	K3586	D3509	ASP	S3363		VAL		Y3082
M4115		M3971	D3661	M3971	Q3510	SER	D3887	Q3510	SER	K3364		GLN	P3156	S3083
T4116		L3972	R3733	L3972	A3511	ALA	W3588	A3511	ALA	C3293		GLU	L3157	L3074
L4117		P3973	R3734	P3973	V3512	LEU	S3589	V3512	LEU	S3294		GLN	K3158	E3085
		M3974	K3736	M3974	A3513	GLU	K3589	A3513	GLU	E3295		GLU	R3159	L3086
N4121		T3977	R3737	T3977	V3514	GLN	V3592	V3514	GLN	E3368		GLU	L3160	S3087
		G3978	I3738	G3978	Q3515		R3593	Q3515	A3443	D3369		D3226	L3161	L3088
N4124		L3815	L3739	L3815	H3516		A3594	H3516	Y3443	S3370		L3227	N3162	L3089
		M3820	I3740	M3820	S3517		E3595	S3517	P3443	E3371		S3228	T3163	L3090
N4127		S3821	R3741	S3821	V3518		L3596	V3518	A3444	K3372		S3229	W3164	L3091
M4128		Q3822	G3742	Q3822	V3670		A3597	V3670	L3445	V3373		L3230	T3165	L3092
		K3825	H3743	K3825	N3670		LYS	I3521	V3446	I3374		I3231	N3166	Q3093
		A3826	D3744	A3826			THR	V3525	V3447			R3232	R3167	D3094
		L3910	E3745	L3910	P3675		PRO	Y3525	E3448	R3380		K3235	Y3168	D3097
		I3911	P3677	I3911	P3677		N3602	V3530	K3449	A3381		F3236	D3170	R3098
		L3829	G3678	L3829	G3678		K3603	V3530	M3450	F3382		S3237	A3171	
		S3830	R3749	S3830	R3749		K3604	S3536	L3461	Q3383		M3238	K3172	Y3101
		D3831	F3750	D3831	F3750		N3605		K3452	R3384		K3239	M3173	Y3102
		P3832	L3751	P3832	L3751		K3606	S3539		E3386		M3240		I3103
		R3833	V3752	R3833	V3752		I3606	T3539	K3455	E3387		K3241	I3178	
		A3834	E3682	A3834	E3682		E3607	THR	L3456			N3242	W3179	Q3108
		P3835	C3683	P3835	C3683		K3608	SER	S3458	Q3390		I3243	D3180	S3109
		P3836	V3685	P3836	V3685		M3609	PHE	N3457	A3391			D3181	F3110
		Y3839	K3686	Y3839	K3686		Y3610	LYS	N3459	A3391			I3182	K3111
		K3840	R3759	K3840	R3759		E3611	ASP		E3393			I3183	Q3112
		D3841	Q3760	D3841	Q3760		R3612	T3545	R3462	E3394			N3113	Q3113
		W3842	D3761	W3842	D3761		L3617	S3546	L3463	E3395			R3186	Y3114
		L3843	Q3762	L3843	Q3762			G3548	F3465	ALA				S3115
		THR	V3764	THR	V3764		A3622	R3549	P3466	GLN			F3189	S3116
		LYS	K3771	LYS	K3771			K3550	R3467	PRO			D3190	T3117
		MET	G3772	MET	G3772		F3628	H3551	L3468	PRO			S3191	D3118
		SER	K3773	SER	K3773		R3629	H3552	L3469	SER			K3192	V3119
		GLY	I3774	GLY	I3774		K3631	E3553	Q3470	TRP			L3120	L3120
								F3554	I3471	SER			E3194	L3121

● Molecule 1: DNA-dependent protein kinase catalytic subunit

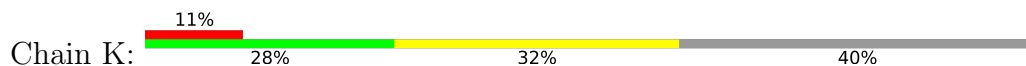


GLU	L1939	L1872	E1803	P1730	K1651	L1572	CYS	K1422	W1356	L1282	L1212	K1061
ILE	Y1940	Y1873	M1804		L1652	K1573	LEU	I1423			K1213	R1062
ARG	H1941	K1874	F1805	T1733	L1653	K1573	PRO	T1424	L1357	S1289	K1146	L1063
LYS	K1875	K1875	R1806		D1576	D1576	SER	A1425	L1358		E1215	Y1064
GLU	C1947	I1876	ASP	F1736	F1661	V1579	D1504	S1427	K1360	K1292	F1219	A1067
ALA	A1948	L1877	LYS	M1737	M1662	L1580	L1505	I1428	D1362	LEU	L1220	
ARG	I1949	D1878	ASP	W1738	T1663	E1581	S1506					P1070
GLU	S1950	V1879	PRO	Y1739	S1664	L1582	C1507	L1431	H1367	T1223	F1224	N1071
ALA	V1951	M1880	ARG	V1740	H1665	M1583	S1508			F1296		R1155
ASN	I1952	Y1881	LEU	M1743	G1666	Q1584	Q1509	L1440	M1368	L1298		F1072
ASN	C1953	R1882	SER	M1743	S1667	Q1584	Q1508	A1441	M1369	E1299		K1074
GLY		R1883	PHE	K1744	E1670	D1588	L1510	Q1442	R1370	P1232		R1075
ASP	F1956	L1884	T1815	K1745		M1589	A1511	Q1443	V1371	S1233		L1076
SER		P1885	R1816	F1746		M1589	S1512					G1077
ASP		LYS	Q1817	F1746	T1674	M1590	G1513	D1444	L1372	Q1231		
GLY	K1960	ASP	S1818	L1747	Y1675	K1591	L1514	D1445	V1373	I1235		A1081
PRO	F1961	ASP	F1819	D1748		M1592	L1515	R1446	Q1374	L1236		F1082
PRO	Y1962	VAL	W1820	A1749	L1678	V1593	E1516	R1447	T1375	I1237		N1083
Q1963	GLY	VAL	D1821	L1750	L1679	S1594	L1517	L1448	L1376	I1238		N1084
TYR		HIS	D1822	E1751		A1595	A1518		C1377	P1239		
ALA		ALA		L1762				V1452	C1378	T1240		I1085
LYS	T1815	LYS	S1823	S1753	K1683	V1596	F1521	S1453	P1379	LEU		N1086
LYS	R1816	GLU	L1824	Q1754	D1685	L1597		A1454	A1380	LEU		R1087
SER	Q1817	SER		S1755	D1685			C1455		TVR		
SER	Q1754	SER		S1755	L1686	M1600	R1527	K1456	I1382	ARG		R1090
LYS	L1828	LYS	W1829	M1757	H1687	L1601	L1528	K1457	G1383	GLY		E1091
ASN	H1830	ASN	H1830	L1758	L1688	D1602	V1529	Q1457	F1384	PRO		E1092
GLN		GLN			K1689	Q1603	S1530	L1458	M1385	ALA		S1094
ASN	D1834	PHE	A1835	M1762	Q1691	S1604	L1531	H1459		ALA		L1095
GLY	L1836	GLY	L1836	L1766	A1692	F1605		A1461	D1388	ASN		V1096
HIS	R1837	GLY	R1837	C1767	V1693	R1608	M1534		V1389	ARG		Q1097
GLY	E1838	SER		R1768	T1694	A1609	L1538	H1465	M1392			E1098
ILE		ILE		E1769		M1610	S1539	H1466				Q1098
CYS		CYS	T1843	Q1770	F1697	Q1611	T1540	L1467	L1395	S1323	L1254	R1184
THR		THR		Q1771	F1698	ALA		L1468		P1324	C1255	H1185
GLN	D1846	GLU		H1772	F1699	Q1614	ALA		D1397	E1326	W1256	V1100
GLY		GLY		V1773			SER	Q1471	V1398	E1327	D1258	F1101
ASP		ASP	D1849		THR		LEU			E1328	L1259	
PRO	ASP	PRO	V1850	M1774	SER	K1617	GLY	D1474	V1399	R1329	L1260	L1104
ARG	LEU	LEU	L1851	E1775	LEU		SER	L1475			L1261	
ALA	ARG	ALA	K1852	E1776	THR	T1620	SER	H1476	N1401	M1331	A1262	M1108
THR	ARG	THR		L1777	GLY		GLN	H1477	L1402	Y1330	A1263	L1111
GLY	THR	GLY	SER	F1779	GLY	Q1624	SER	H1478	M1403	E1332	L1264	H1115
ARG	PHE	ARG	PHE	Q1779	SER	H1625	V1550	V1479	K1404	S1333	L1265	
ASN	THR	ASN	THR	S1780	L1707	W1626	I1551	G1480	A1405	K1334	C1266	K1119
ASN	ASN	ASN	LYS	S1781	E1708	K1628	H1552	T1481	L1406	C1336	Y1267	
PHE	PHE	PHE	LYS	F1782	E1709		F1553		V1337	V1337	T1268	I1124
PRO	PRO	PRO	LEU	R1783	L1710	W1633		L1483	W1338	W1338	T1269	Q1125
VAL	VAL	VAL	GLU	R1784	R1711	A1634	G1556	E1482	V1407		G1200	
GLU	GLU	GLU	GLU	I1785	R1712			L1484			F1270	
GLN	GLU	ALA	SER	A1786	V1713	K1635	E1557		P1410	W1201		
ARG	VAL	GLY	T1862	R1787	L1714		Y1558	V1487	K1412	R1202	I1271	I1131
ASP	PRO	GLU	F1863	R1788	E1715	L1639	F1559		D1413	S1203	G1272	D1132
PRO	PRO	ASN	T1864	G1789		E1640	Y1560	A1491	I1414	M1204	E1273	L1133
THR	GLU	GLN	T1865		P1723	K1642	S1561	A1492	L1415	N1205	R1274	L1134
VAL	ARG	LEU		Q1794	M1724		L1562	PRO	F1416	F1344	T1275	
GLY	LYS	LYS	Q1866	V1795	S1726	L1646		GLY	T1417	T1345	V1276	T1138
ALA	LYS	LYS	I1867				M1568	ASP	H1418	L1208	G1277	
HIS	LYS	LYS	T1868		S1800	L1649	E1569	GLU	L1419	L1209	A1278	H1142
ASP	LYS	LYS	K1869		V1801		T1570	ARG	R1420	D1210		V1143
ASP	TYR	VAL	K1870	S1800	V1801	L1649	E1570	ARG		G1209		S1144
VAL	TYR	VAL		V1801	V1801							
LEU	ILE	R1938	M1871	Y1802	F1729	A1650	L1571	GLN		T1351	V1281	
GLU												
LEU												
MET												
ASP												
GLU												
ALA												
GLU												
ASN												
R2090												
C2093												
P2096												
L2097												
L2100												
V2101												
K2102												
H2103												
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L2108												
GLY												
PRO												
PRO												
ALA												
GLN												
GLY												
GLU												
ASP												
TYR												
VAL												
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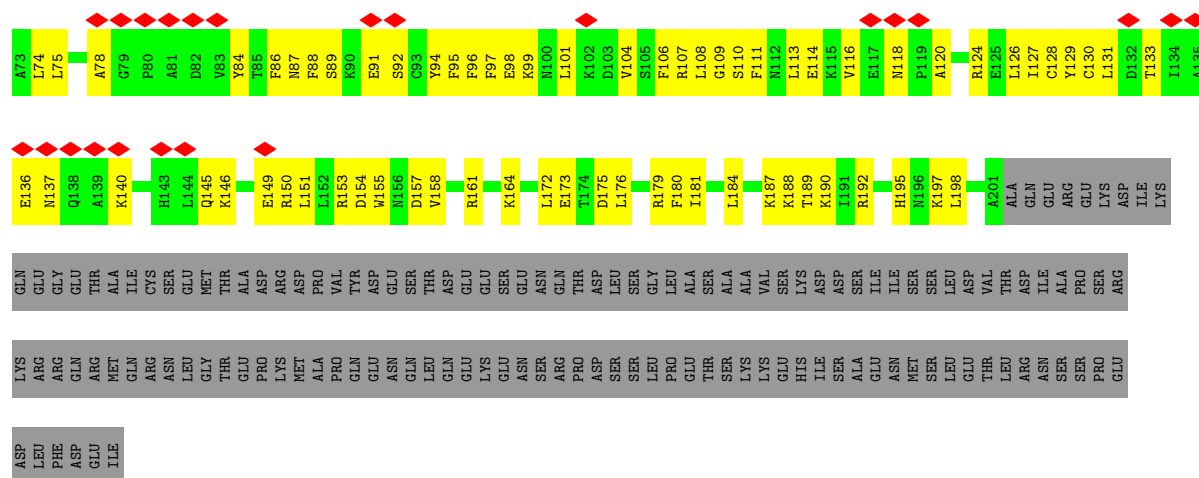
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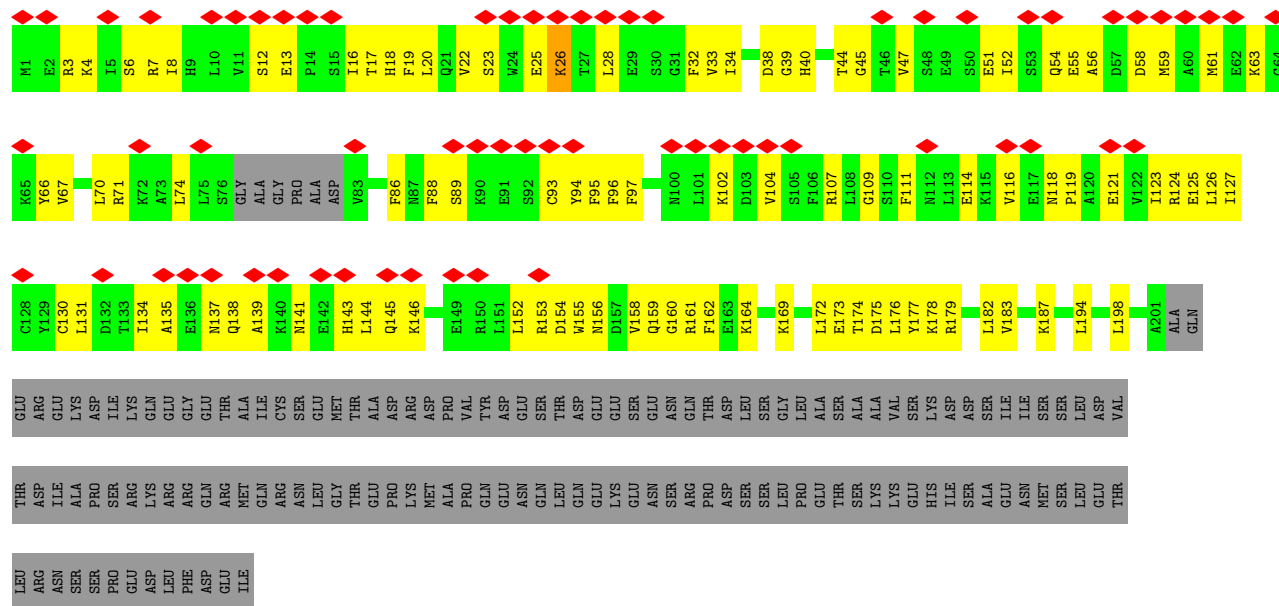
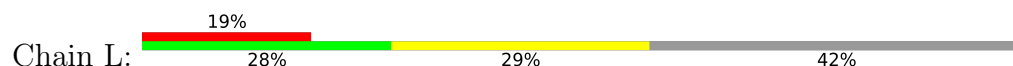
• Molecule 2: DNA repair protein XRCC4



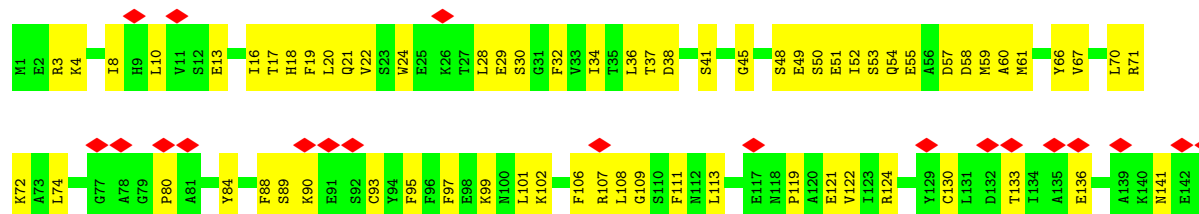
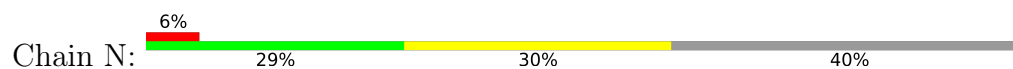
M1	R7	V11	P14	S15	I16	H18	F19	L20	Q21	V22	S23	W24	E25	K26	T27	L28	E29	S30	G31	F32	V33	I34	T35	H40	S41	A42	V43	T44	G45	T46	V47	S48	E49	S50	I51	I52	S53	Q54	E55	A56	M59	A60	M61	E62	K63	G64	R71	K72
----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



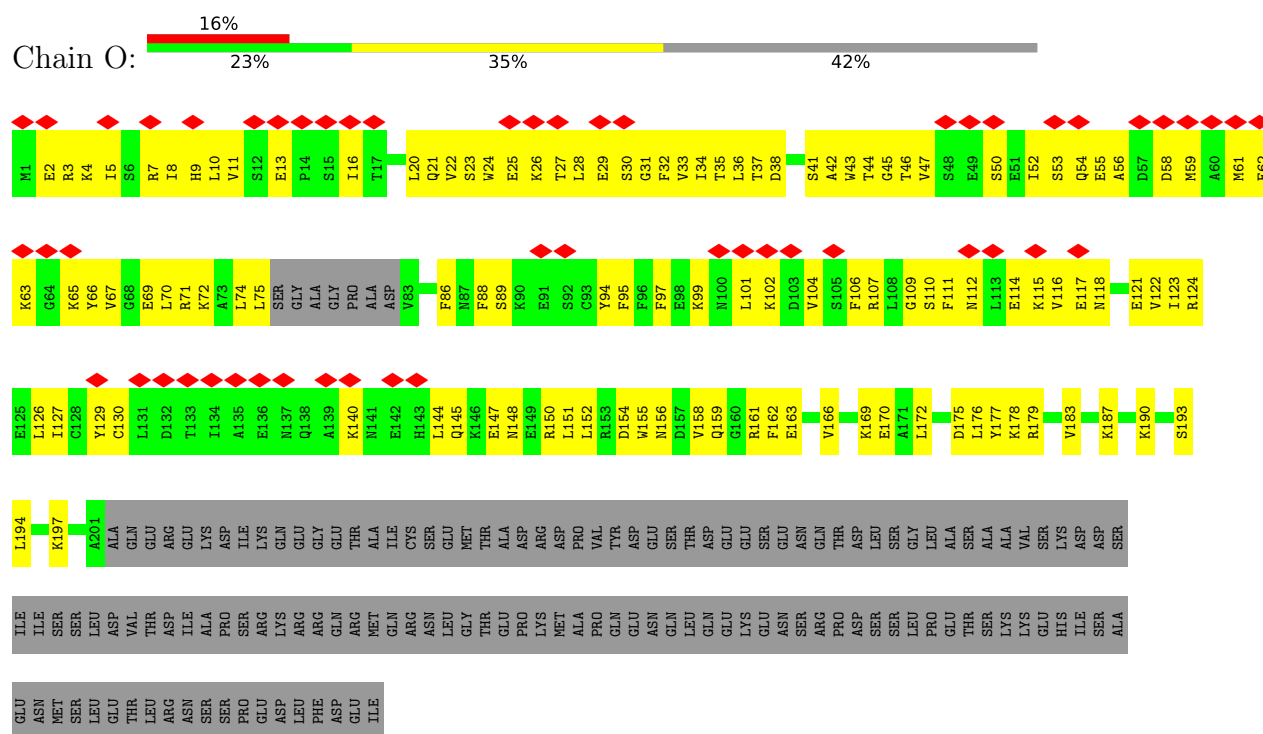
• Molecule 2: DNA repair protein XRCC4



• Molecule 2: DNA repair protein XRCC4



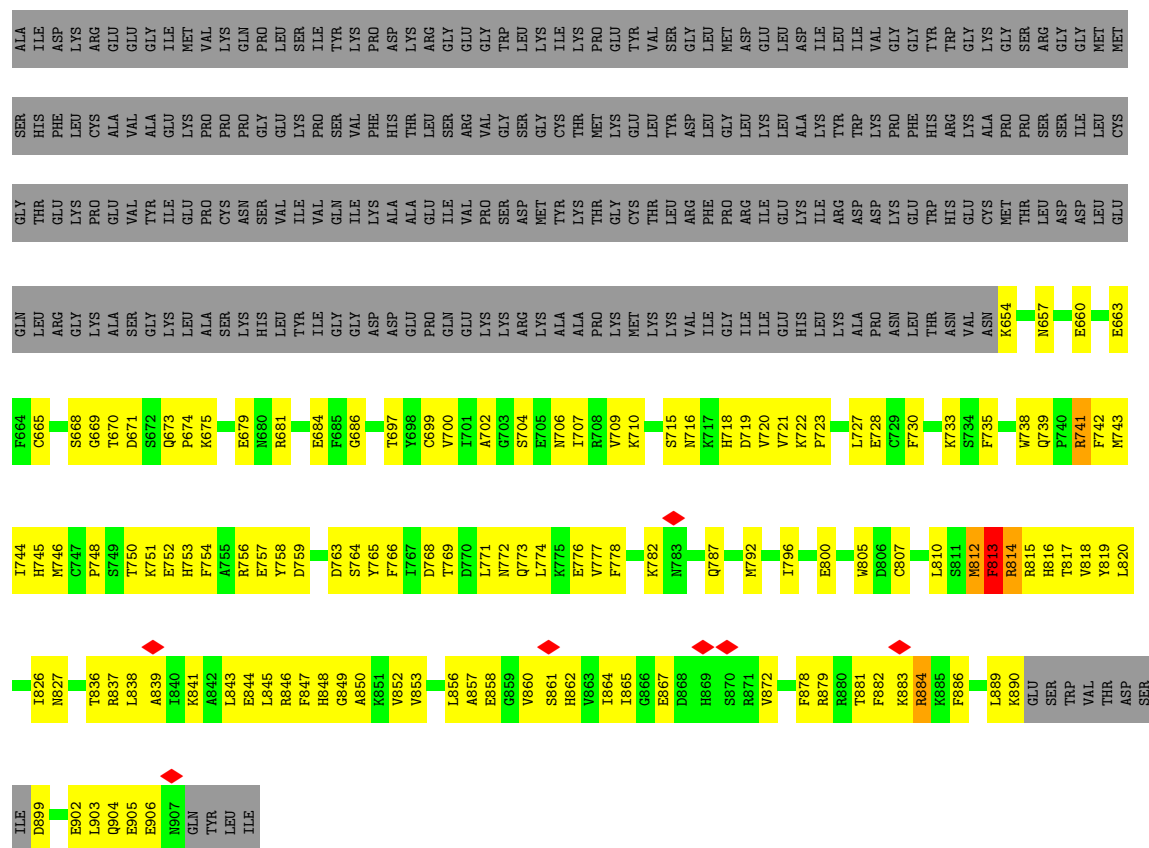
- Molecule 2: DNA repair protein XRCC4



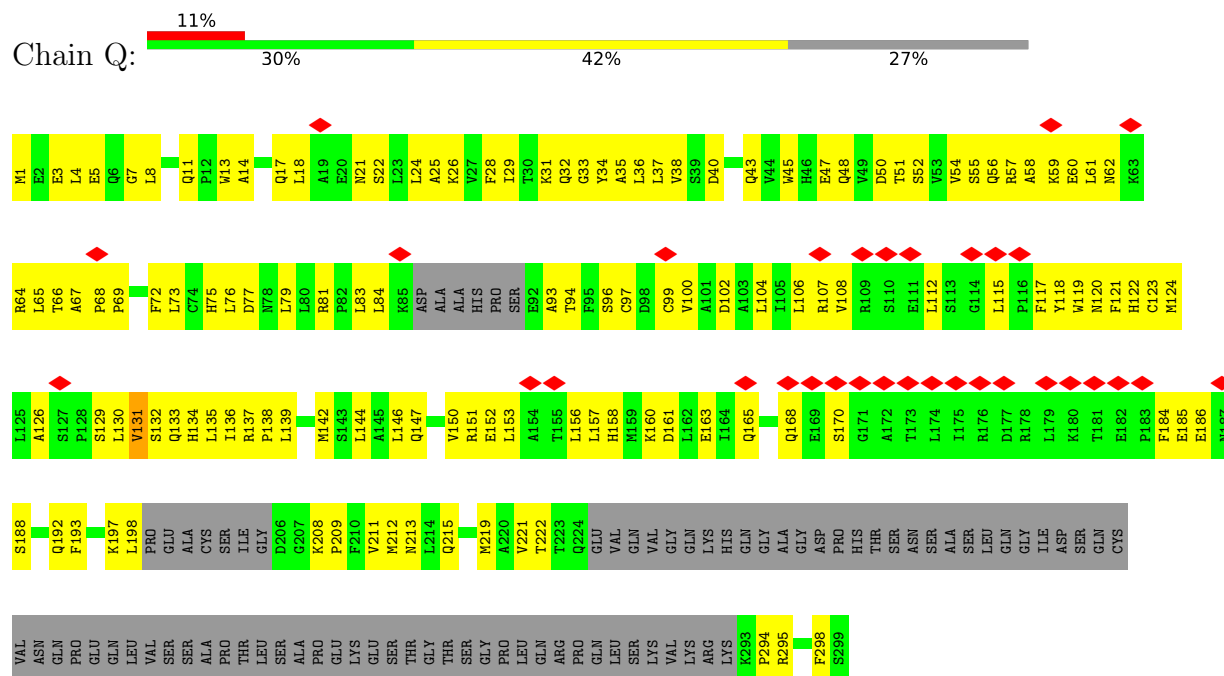
- Molecule 3: DNA ligase 4



[illegible]

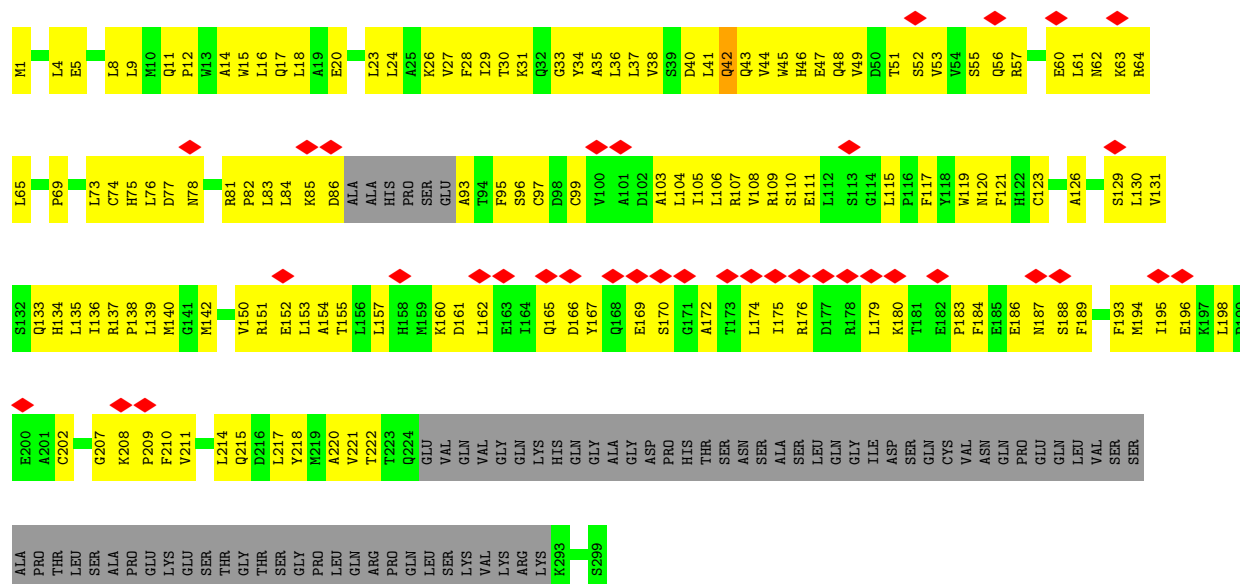


• Molecule 4: Non-homologous end-joining factor 1



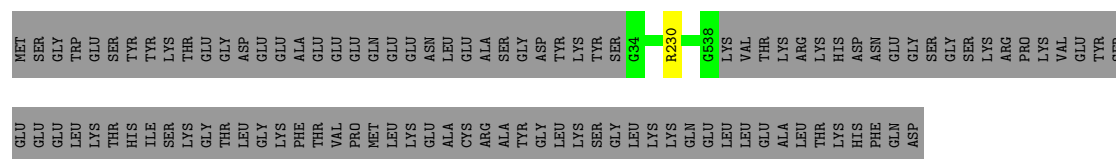
• Molecule 4: Non-homologous end-joining factor 1





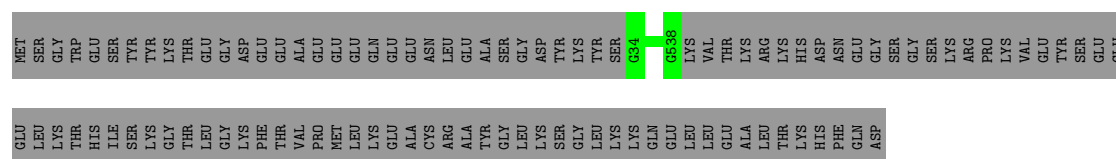
• Molecule 5: X-ray repair cross-complementing protein 6

Chain a: 83% 17%



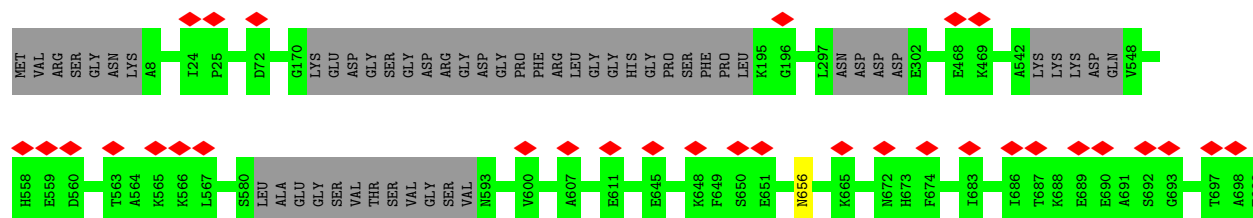
• Molecule 5: X-ray repair cross-complementing protein 6

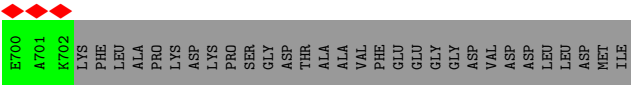
Chain h: 83% 17%



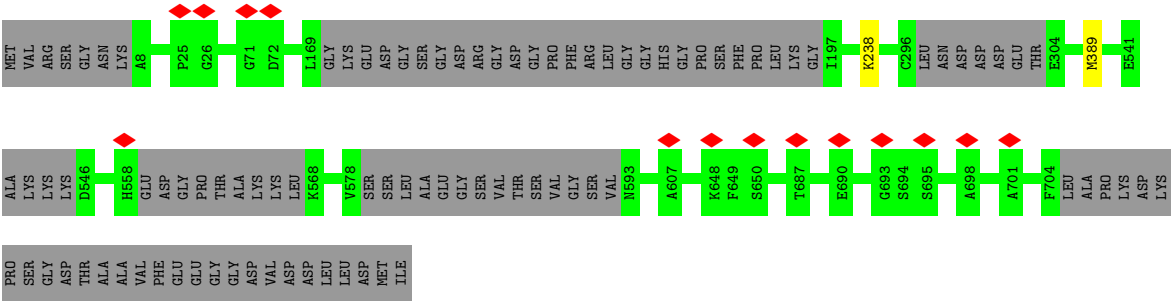
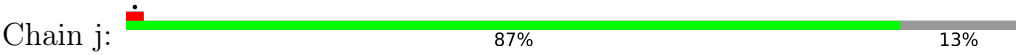
• Molecule 6: X-ray repair cross-complementing protein 5

Chain b: 5% 89% 11%

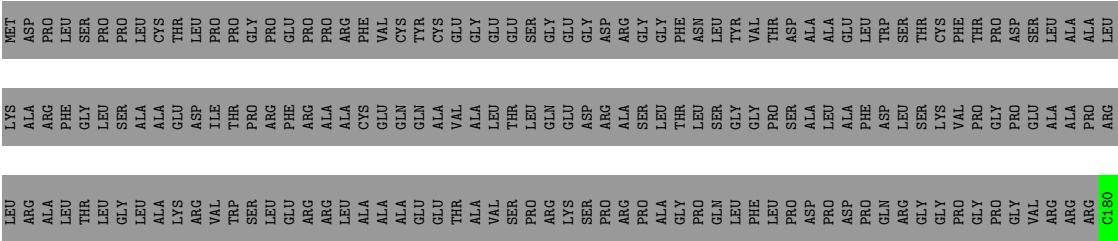




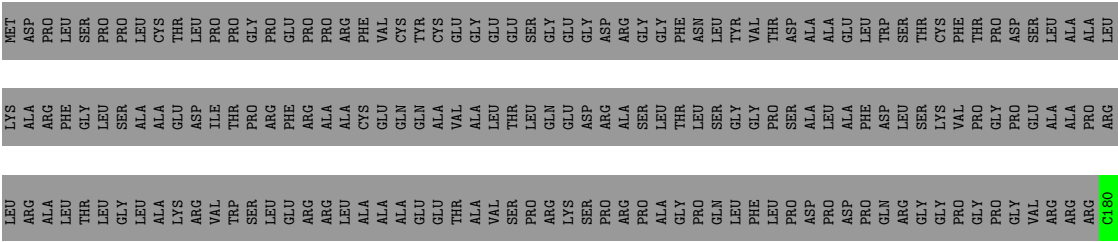
• Molecule 6: X-ray repair cross-complementing protein 5



• Molecule 7: Protein PAXX

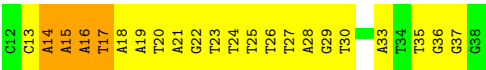


• Molecule 7: Protein PAXX

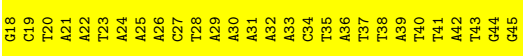


• Molecule 8: DNA (26-MER)

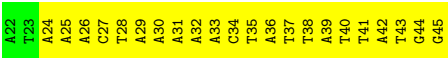
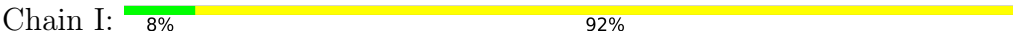




- Molecule 9: DNA (27-MER)



- Molecule 10: DNA (28-MER)



- Molecule 11: DNA (24-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	11019	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 ($e^-/\text{\AA}^2$)	48.03	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.720	Depositor
Minimum map value	-0.164	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.168	Depositor
Map size (Å)	678.08, 678.08, 678.08	wwPDB
Map dimensions	520, 520, 520	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

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	0/28804	0.50	0/38906
1	F	0.30	0/28820	0.50	1/38928 (0.0%)
2	K	0.26	0/1657	0.48	0/2228
2	L	0.26	0/1616	0.50	0/2170
2	N	0.27	0/1654	0.50	0/2224
2	O	0.27	0/1616	0.50	0/2170
3	M	0.28	0/2134	0.48	0/2884
3	P	0.28	0/2028	0.51	0/2737
4	Q	0.28	0/1778	0.55	0/2403
4	R	0.27	0/1831	0.56	0/2476
5	a	0.29	0/4116	0.51	0/5549
5	h	0.29	0/4105	0.50	0/5538
6	b	0.27	0/5313	0.48	0/7159
6	j	0.28	0/5178	0.49	1/6979 (0.0%)
7	c	0.29	0/169	0.38	0/226
7	i	0.28	0/166	0.38	0/222
8	D	0.70	0/622	1.16	4/959 (0.4%)
9	E	0.70	0/647	0.96	0/996
10	I	0.72	0/555	1.00	0/854
11	J	0.80	0/548	1.15	1/844 (0.1%)
All	All	0.31	0/93357	0.53	7/126452 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	14	DA	P-O3'-C3'	-8.45	109.56	119.70
8	D	17	DT	P-O3'-C3'	-8.05	110.04	119.70
8	D	16	DA	P-O3'-C3'	-7.49	110.71	119.70
1	F	956	PRO	N-CA-CB	6.07	110.58	103.30
11	J	31	DT	O4'-C4'-C3'	-5.70	102.22	104.50

There are no chirality outliers.

There are no planarity outliers.

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	28250	0	28465	1559	0
1	F	28263	0	28500	1573	0
2	K	1628	0	1620	123	0
2	L	1589	0	1581	99	0
2	N	1625	0	1612	120	0
2	O	1589	0	1587	120	0
3	M	2085	0	2024	144	0
3	P	1983	0	1924	130	0
4	Q	1745	0	1754	132	0
4	R	1796	0	1814	143	0
5	a	4038	0	4092	0	0
5	h	4026	0	4069	0	0
6	b	5214	0	5231	0	0
6	j	5082	0	5069	0	0
7	c	165	0	160	0	0
7	i	162	0	151	0	0
8	D	556	0	310	58	0
9	E	576	0	318	53	0
10	I	494	0	273	44	0
11	J	491	0	278	45	0
All	All	91357	0	90832	4131	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 29.

The worst 5 of 4131 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:F:2440:TYR:HA	1:F:2443:MET:HE3	1.39	1.01
1:F:1269:THR:O	1:F:1273:GLU:HB2	1.66	0.95
1:F:1268:ASN:HD21	1:F:1344:PHE:HA	1.34	0.92
1:F:2225:HIS:HB2	1:F:2231:PHE:HB2	1.51	0.91
4:Q:131:VAL:HG12	4:R:44:VAL:HG22	1.50	0.91

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	3477/4128 (84%)	3144 (90%)	328 (9%)	5 (0%)	51	85
1	F	3467/4128 (84%)	3148 (91%)	319 (9%)	0	100	100
2	K	199/336 (59%)	179 (90%)	20 (10%)	0	100	100
2	L	191/336 (57%)	182 (95%)	9 (5%)	0	100	100
2	N	199/336 (59%)	186 (94%)	13 (6%)	0	100	100
2	O	190/336 (56%)	183 (96%)	7 (4%)	0	100	100
3	M	256/911 (28%)	238 (93%)	18 (7%)	0	100	100
3	P	242/911 (27%)	218 (90%)	21 (9%)	3 (1%)	13	50
4	Q	210/299 (70%)	185 (88%)	24 (11%)	1 (0%)	29	68
4	R	219/299 (73%)	192 (88%)	26 (12%)	1 (0%)	29	68
5	a	503/609 (83%)	464 (92%)	39 (8%)	0	100	100
5	h	503/609 (83%)	471 (94%)	32 (6%)	0	100	100
6	b	640/732 (87%)	599 (94%)	41 (6%)	0	100	100
6	j	624/732 (85%)	597 (96%)	27 (4%)	0	100	100
7	c	21/204 (10%)	21 (100%)	0	0	100	100
7	i	21/204 (10%)	21 (100%)	0	0	100	100
All	All	10962/15110 (72%)	10028 (92%)	924 (8%)	10 (0%)	54	85

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	PRO
3	P	814	ARG
4	Q	131	VAL
1	A	216	LYS

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Mol	Chain	Res	Type
3	P	812	MET

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	3097/3671 (84%)	3082 (100%)	15 (0%)	88	93
1	F	3109/3671 (85%)	3095 (100%)	14 (0%)	88	93
2	K	180/303 (59%)	180 (100%)	0	100	100
2	L	176/303 (58%)	174 (99%)	2 (1%)	73	85
2	N	178/303 (59%)	177 (99%)	1 (1%)	86	92
2	O	177/303 (58%)	176 (99%)	1 (1%)	86	92
3	M	232/808 (29%)	231 (100%)	1 (0%)	91	94
3	P	217/808 (27%)	213 (98%)	4 (2%)	59	77
4	Q	192/262 (73%)	192 (100%)	0	100	100
4	R	200/262 (76%)	199 (100%)	1 (0%)	88	93
5	a	445/548 (81%)	444 (100%)	1 (0%)	93	96
5	h	445/548 (81%)	445 (100%)	0	100	100
6	b	583/649 (90%)	582 (100%)	1 (0%)	93	96
6	j	562/649 (87%)	561 (100%)	1 (0%)	93	96
7	c	18/160 (11%)	18 (100%)	0	100	100
7	i	17/160 (11%)	17 (100%)	0	100	100
All	All	9828/13408 (73%)	9786 (100%)	42 (0%)	91	94

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	4090	ARG
3	P	782	LYS
2	L	26	LYS
2	N	107	ARG

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Mol	Chain	Res	Type
3	P	884	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	141	ASN
6	b	551	GLN
2	N	18	HIS
4	R	62	ASN
6	j	614	ASN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

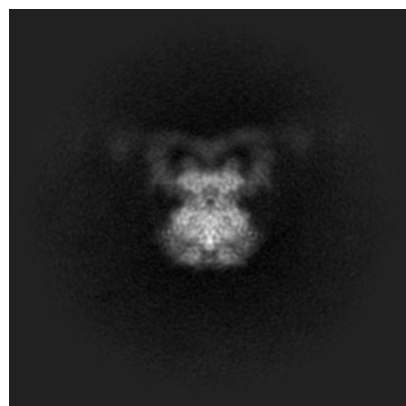
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16070. These allow visual inspection of the internal detail of the map and identification of artifacts.

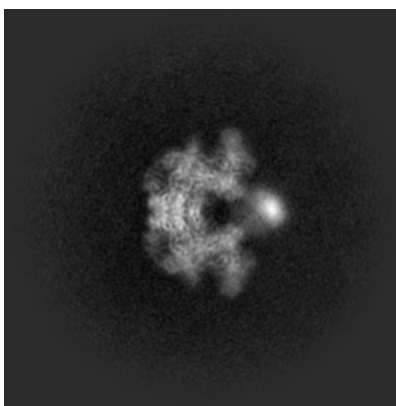
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

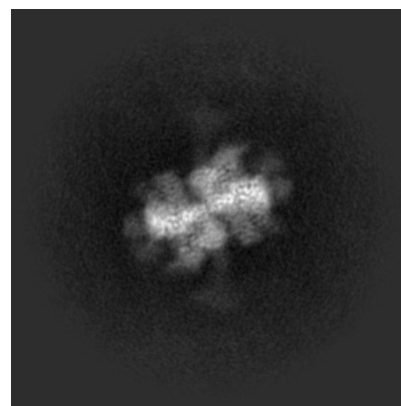
6.1.1 Primary map



X

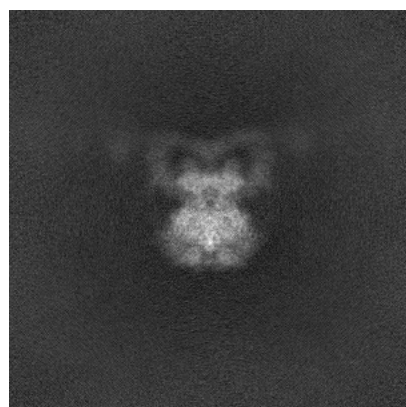


Y

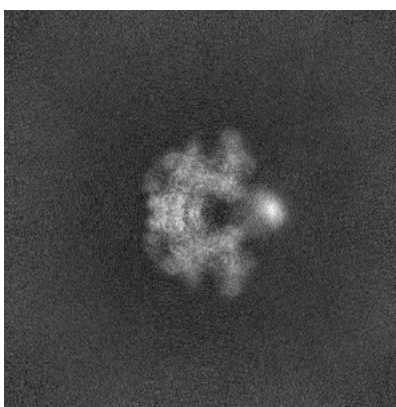


Z

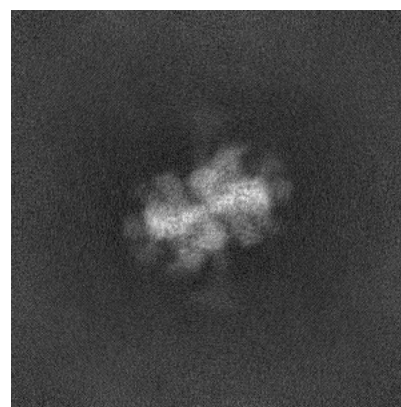
6.1.2 Raw map



X



Y

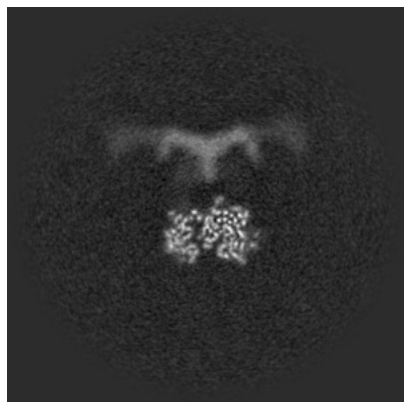


Z

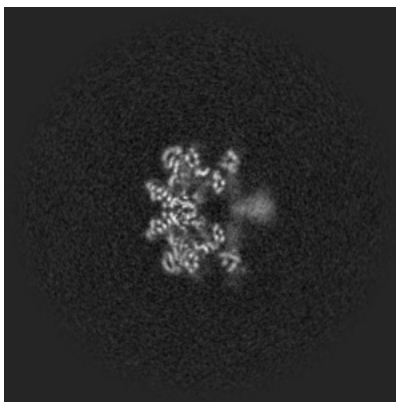
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

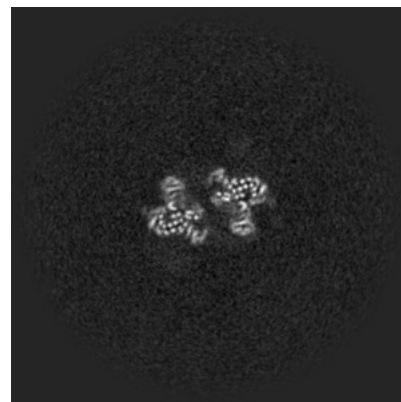
6.2.1 Primary map



X Index: 260

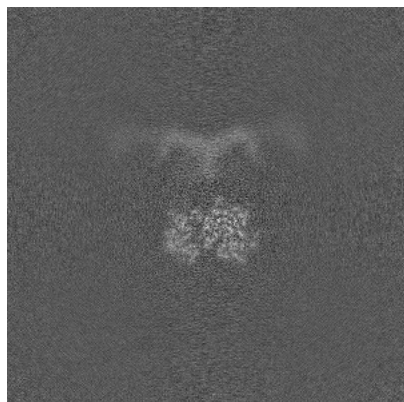


Y Index: 260

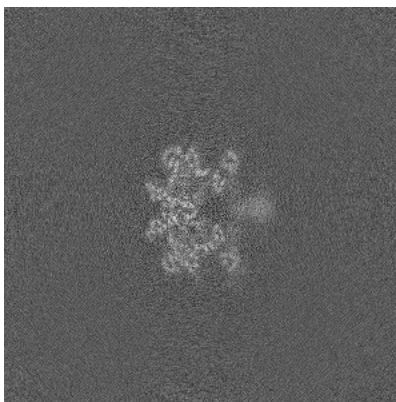


Z Index: 260

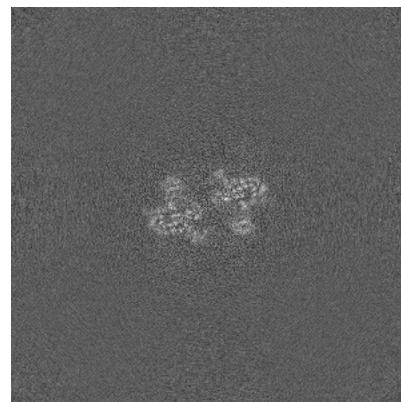
6.2.2 Raw map



X Index: 260



Y Index: 260

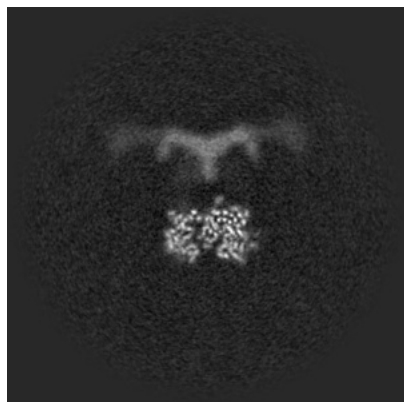


Z Index: 260

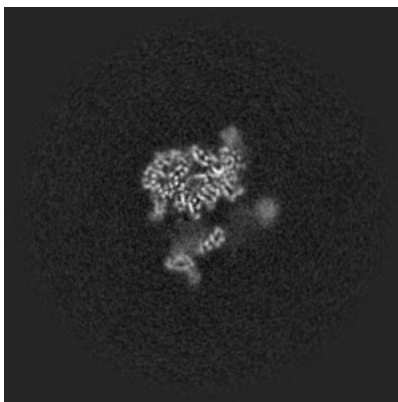
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

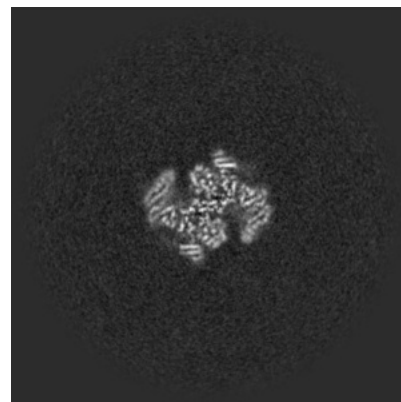
6.3.1 Primary map



X Index: 259

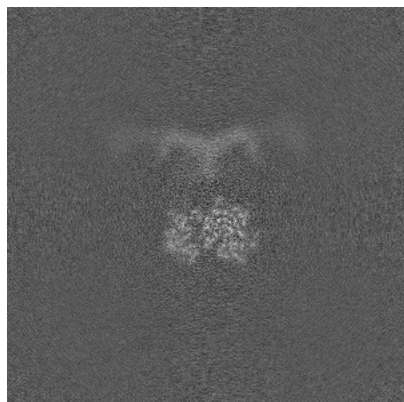


Y Index: 275

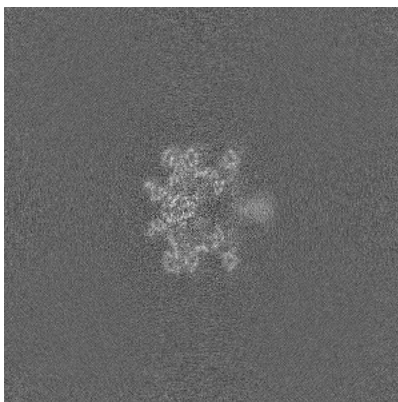


Z Index: 229

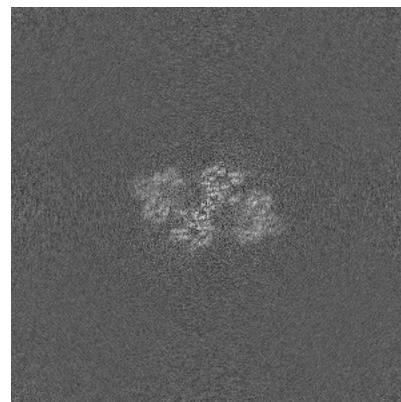
6.3.2 Raw map



X Index: 260



Y Index: 262

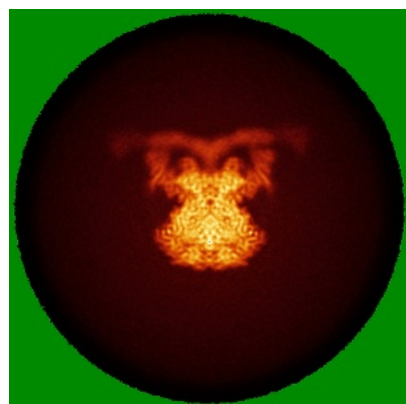


Z Index: 242

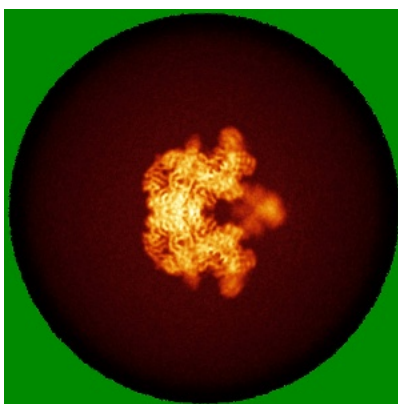
The images above show the largest variance slices of the map in three orthogonal directions.

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

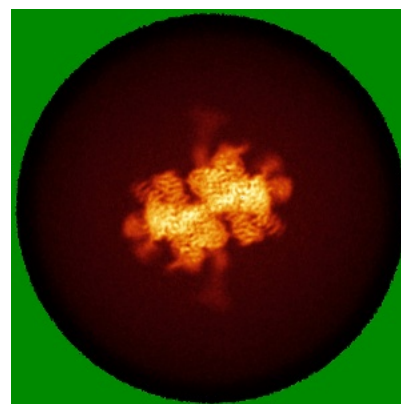
6.4.1 Primary map



X

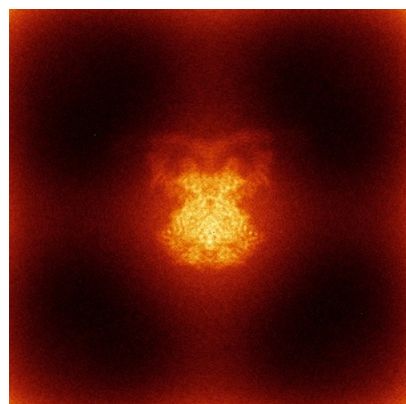


Y

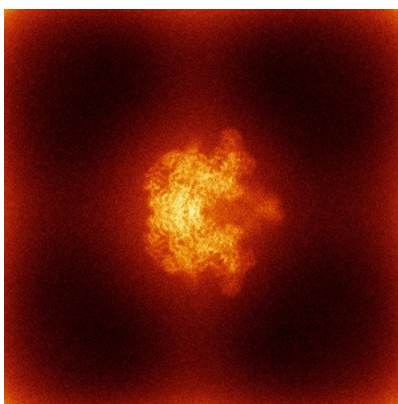


Z

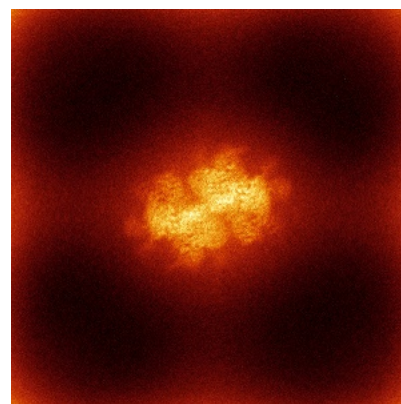
6.4.2 Raw map



X



Y

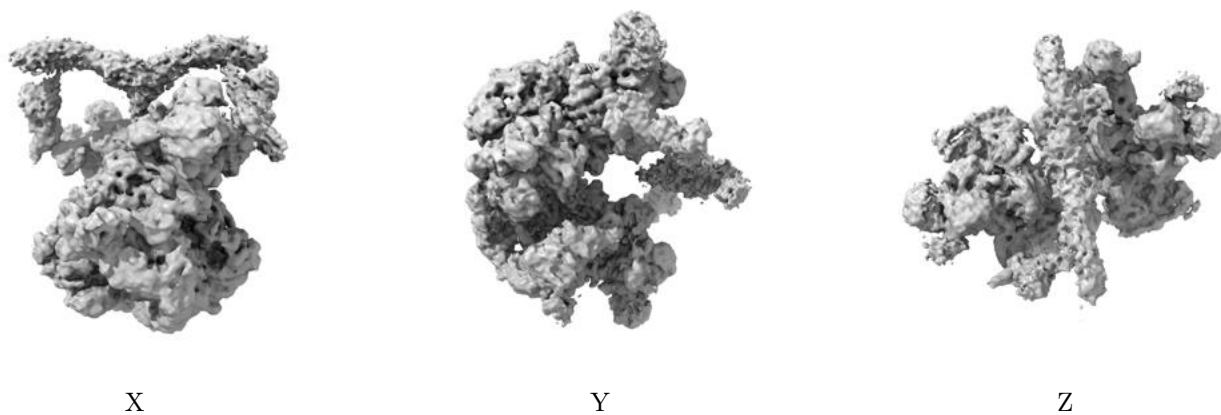


Z

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.

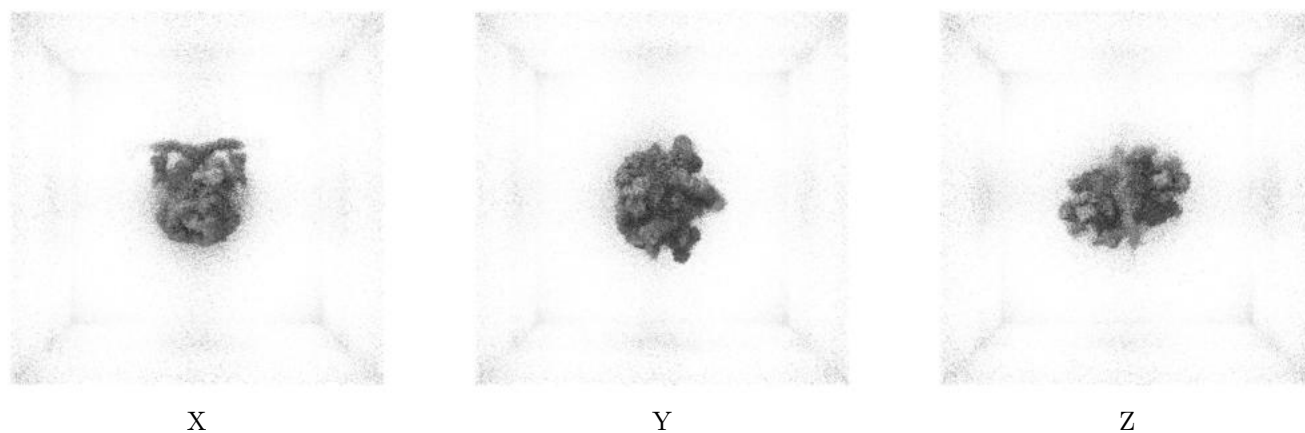
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.168. 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.

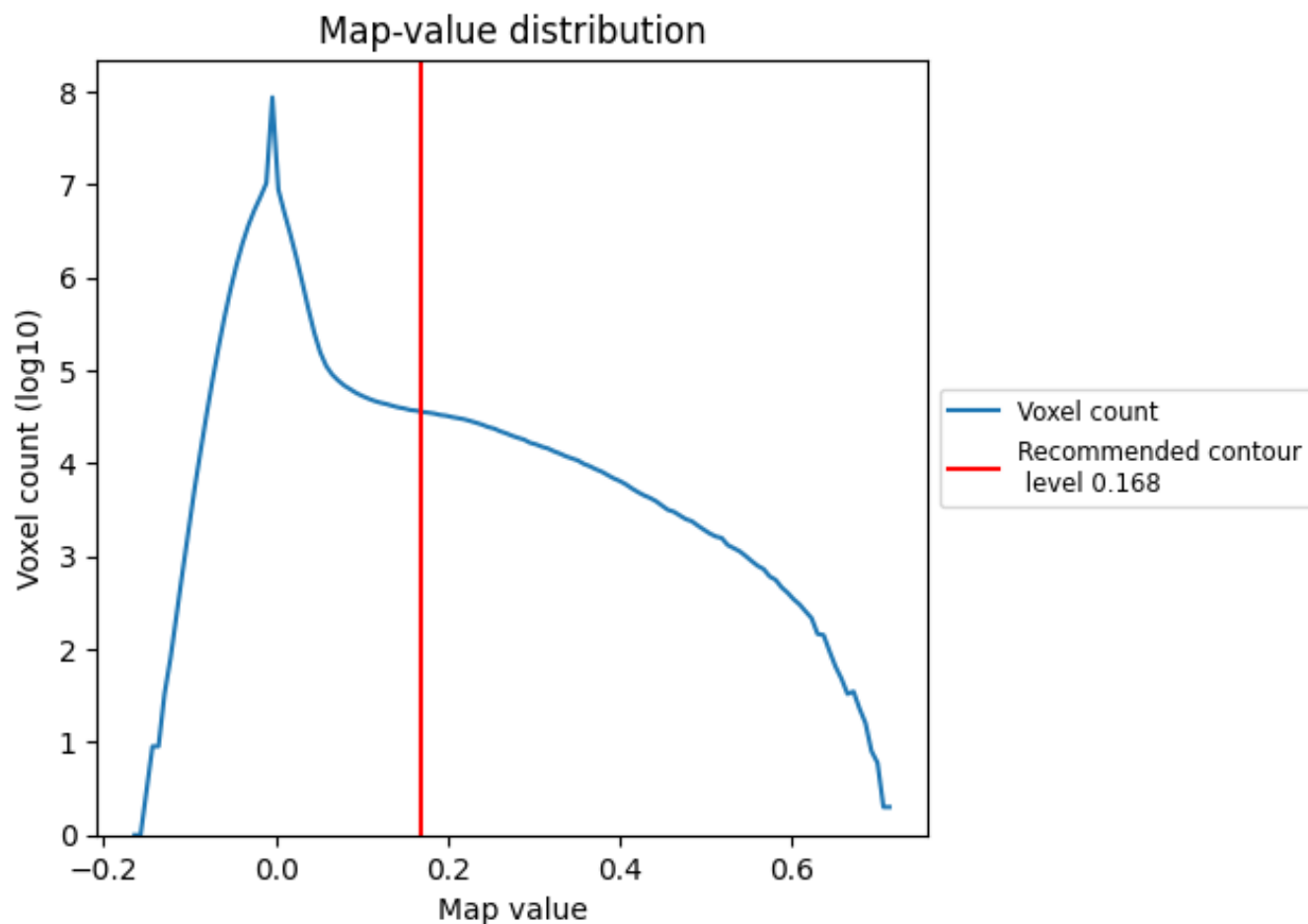
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

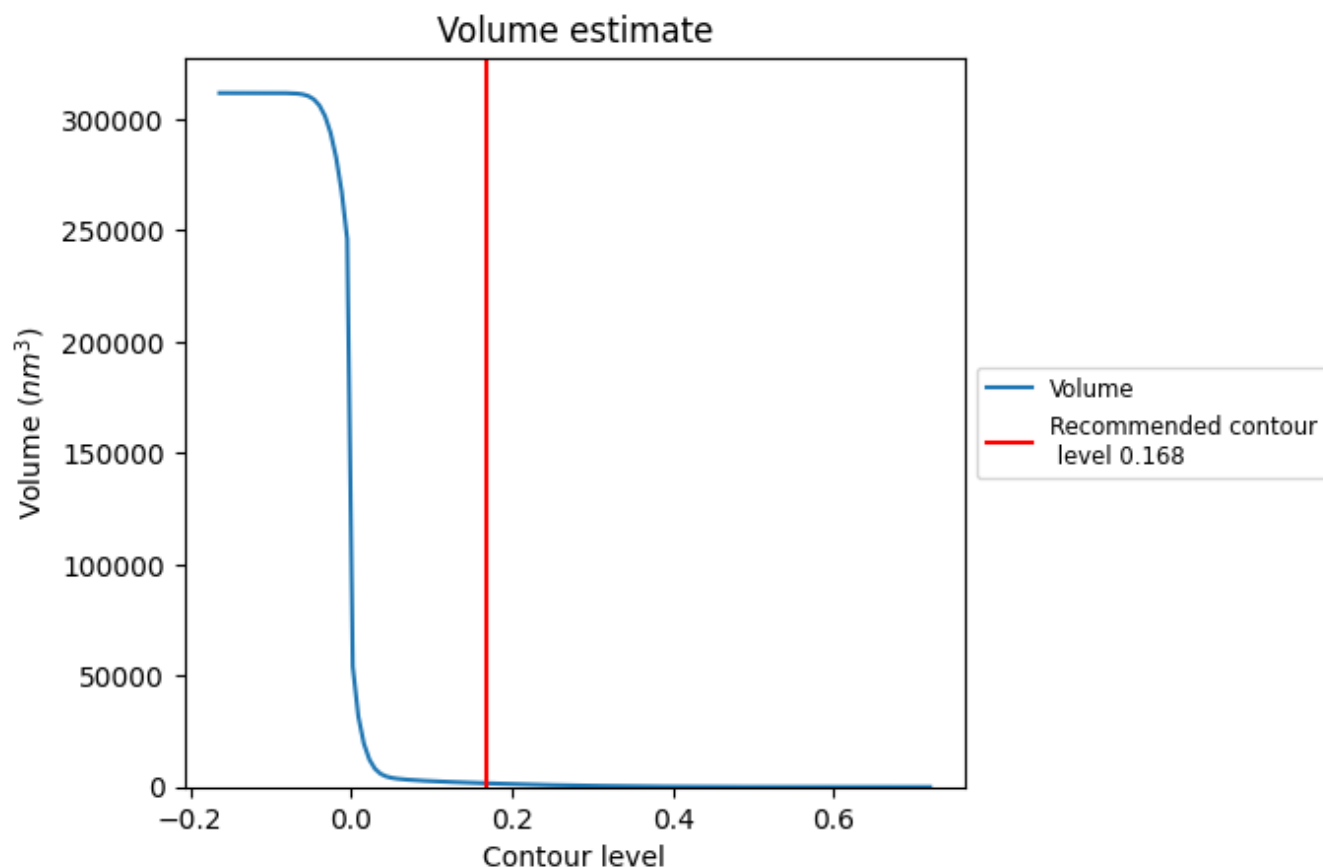
This section contains the results of statistical analysis of the map.

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.

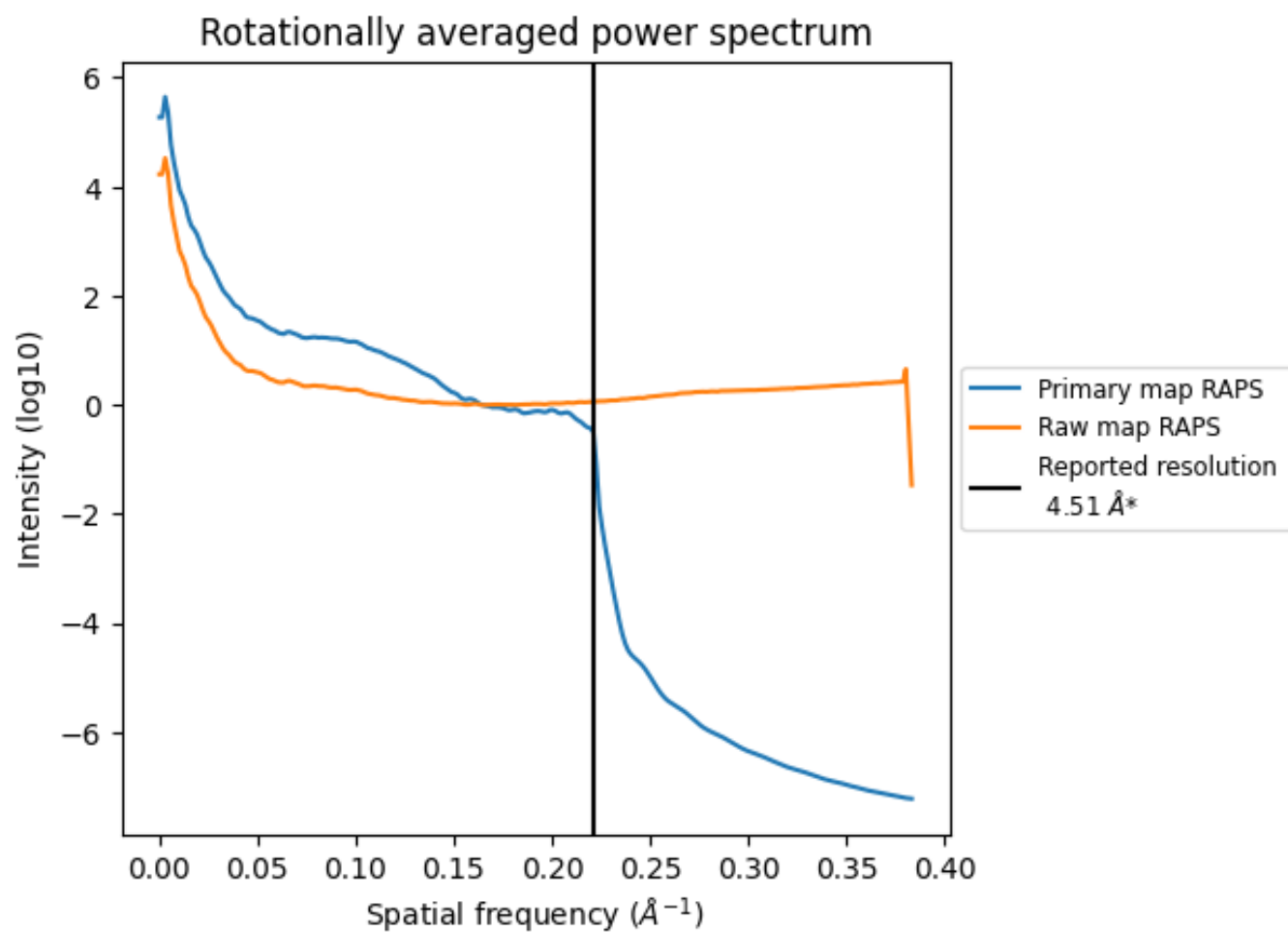
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1663 nm^3 ; this corresponds to an approximate mass of 1502 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 ⓘ

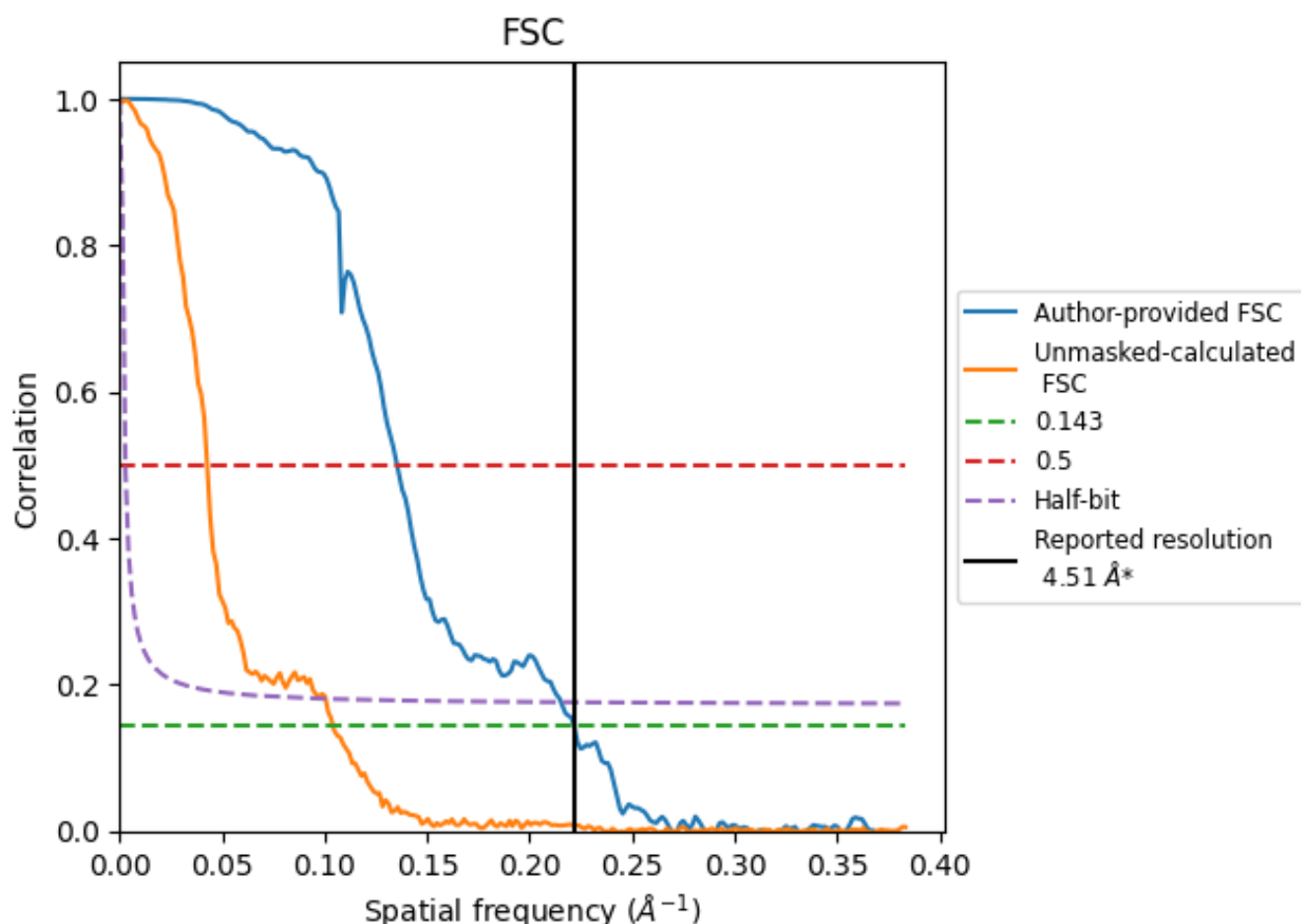


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

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 Å⁻¹

8.2 Resolution estimates [i](#)

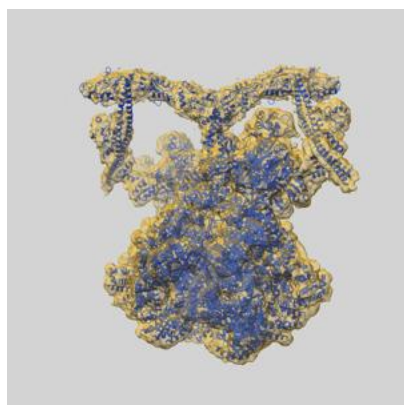
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.51	-	-
Author-provided FSC curve	4.51	7.39	4.64
Unmasked-calculated*	9.60	23.42	9.95

*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 9.60 differs from the reported value 4.51 by more than 10 %

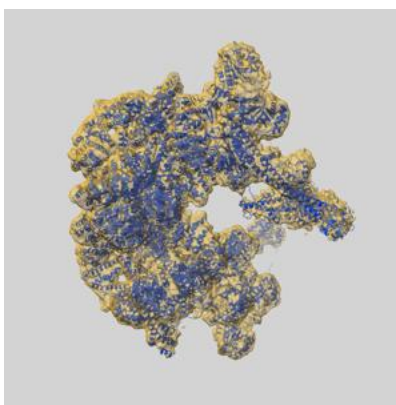
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16070 and PDB model 8BHV. Per-residue inclusion information can be found in section [3](#) on page [7](#).

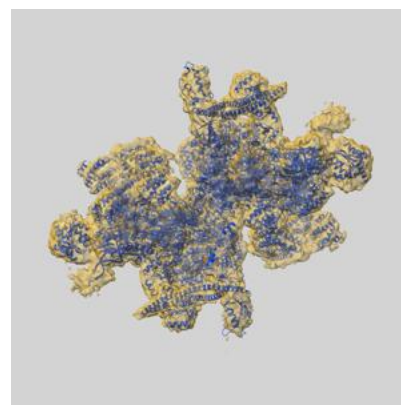
9.1 Map-model overlay [i](#)



X



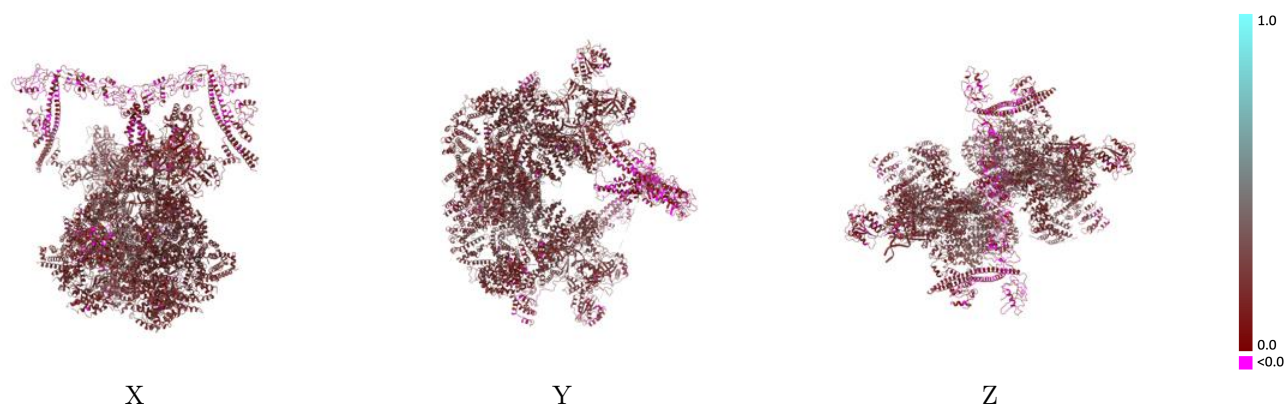
Y



Z

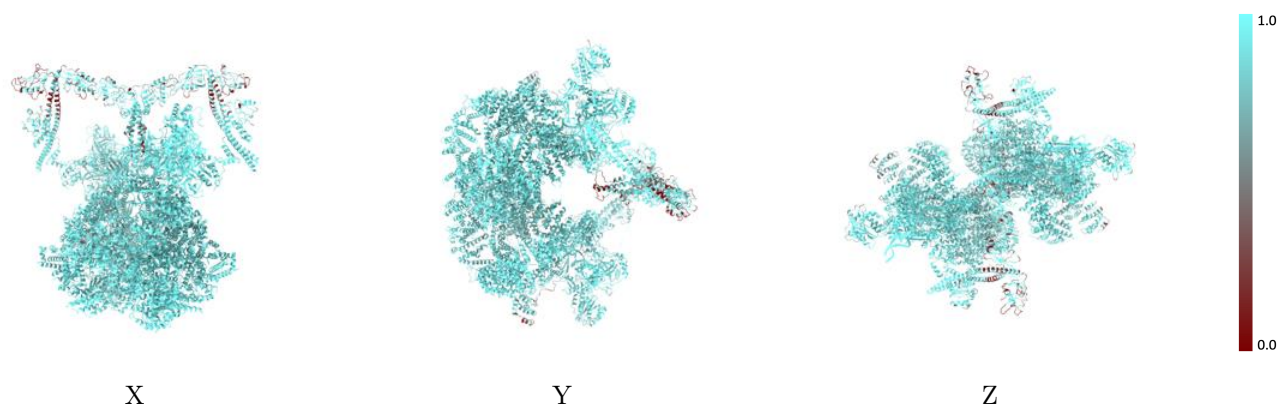
The images above show the 3D surface view of the map at the recommended contour level 0.168 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



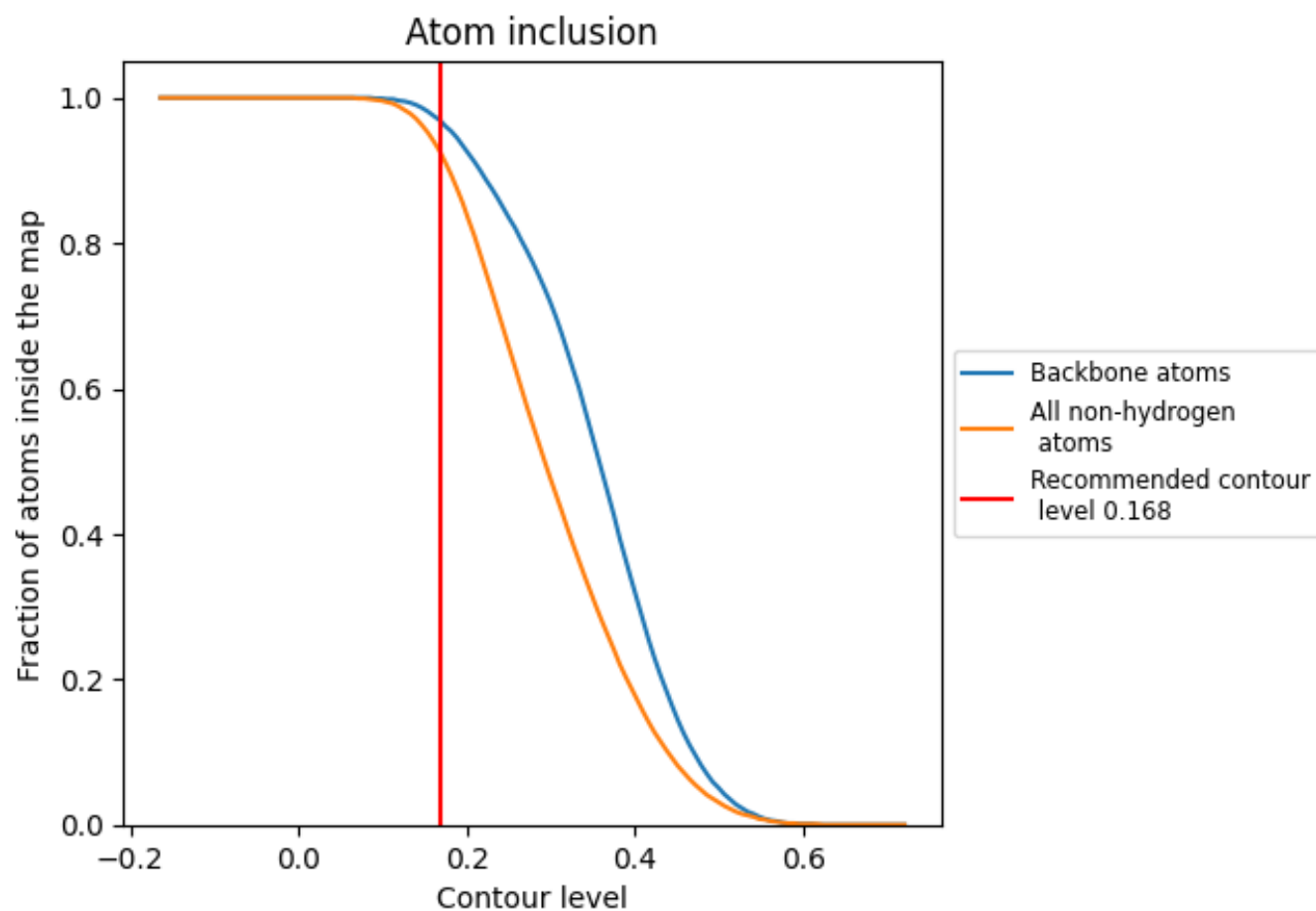
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.168).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 93% 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 (0.168) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.2030
A	 0.9500	 0.2210
D	 0.9570	 0.2520
E	 0.9790	 0.2310
F	 0.9560	 0.2290
I	 0.9720	 0.2110
J	 0.9800	 0.2680
K	 0.7510	 0.0990
L	 0.6330	 0.1040
M	 0.9080	 0.1520
N	 0.8230	 0.0990
O	 0.6800	 0.1210
P	 0.9420	 0.1500
Q	 0.8030	 0.0910
R	 0.7830	 0.0720
a	 0.9610	 0.2170
b	 0.8810	 0.1760
c	 0.9700	 0.2440
h	 0.9610	 0.2310
i	 0.9940	 0.2550
j	 0.9380	 0.1920

