



wwPDB EM Validation Summary Report ⓘ

Mar 22, 2026 – 06:06 PM UTC

PDB ID : 8BHY / pdb_00008bhy
EMDB ID : EMD-16074
Title : DNA-PK Ku80 mediated dimer bound to PAXX and XLF
Authors : Hardwick, S.W.; Chaplin, A.K.
Deposited on : 2022-11-01
Resolution : 5.33 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

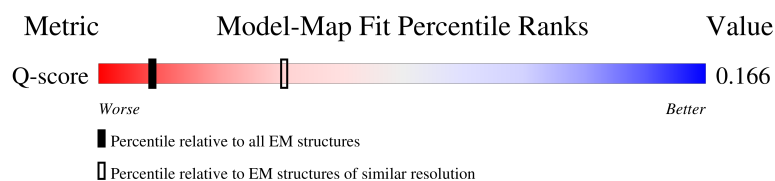
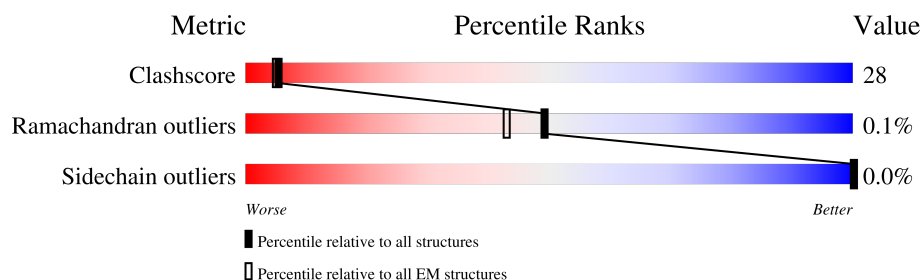
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

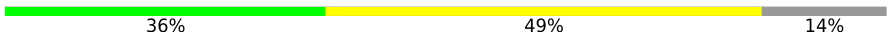
The reported resolution of this entry is 5.33 Å.

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.



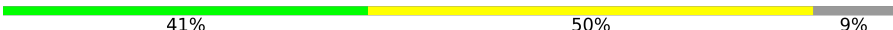
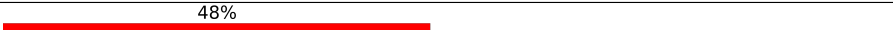
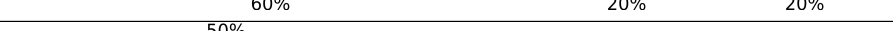
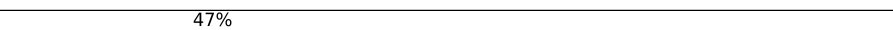
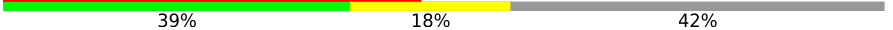
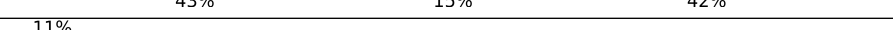
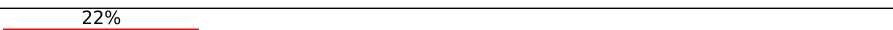
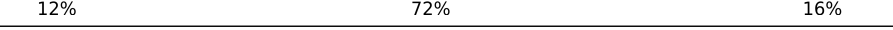
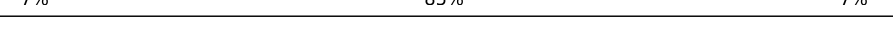
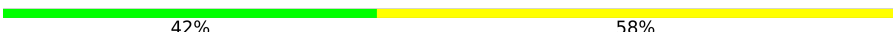
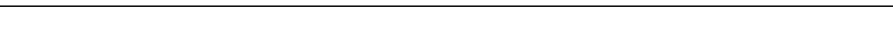
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	504 (4.83 - 5.82)

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	S	4128	
2	B	609	
2	T	609	

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Mol	Chain	Length	Quality of chain
3	C	732	
3	L	732	
4	D	204	 
4	M	204	 
5	G	336	 
5	H	336	 
5	P	336	 
5	Q	336	 
6	I	911	 
6	R	911	 
7	d	25	
8	e	27	
9	i	26	
10	j	24	
11	f	299	
11	m	299	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 90193 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	3547	Total	C	N	O	S	0	0
			28300	18182	4780	5151	187		
1	S	3538	Total	C	N	O	S	0	0
			28342	18207	4793	5154	188		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	507	Total	C	N	O	S	0	0
			4085	2614	693	760	18		
2	T	502	Total	C	N	O	S	0	0
			4037	2587	680	752	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	668	Total	C	N	O	S	0	0
			5318	3397	892	1003	26		
3	L	652	Total	C	N	O	S	0	0
			5204	3324	876	979	25		

- Molecule 4 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	147	Total	C	N	O	S	0	0
			1102	702	190	204	6		
4	M	164	Total	C	N	O	S	0	0
			1219	767	210	236	6		

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
5	H	194	Total	C	N	O	S	0	0
			1589	1009	271	302	7		
5	P	201	Total	C	N	O	S	0	0
			1622	1028	275	312	7		
5	Q	194	Total	C	N	O	S	0	0
			1580	1003	268	302	7		

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	246	Total	C	N	O	S	0	0
			1984	1262	336	373	13		
6	R	246	Total	C	N	O	S	0	0
			1970	1252	335	371	12		

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	d	25	Total	C	N	O	P	0	0
			516	249	87	155	25		

- Molecule 8 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	27	Total	C	N	O	P	0	0
			554	267	102	158	27		

- Molecule 9 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	26	Total	C	N	O	P	0	0
			532	257	97	152	26		

- Molecule 10 is a DNA chain called DNA (5'-D(P*AP*AP*TP*AP*AP*TP*AP*GP*TP*T
P*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	24	Total	C	N	O	P	0	0
			497	240	84	149	24		

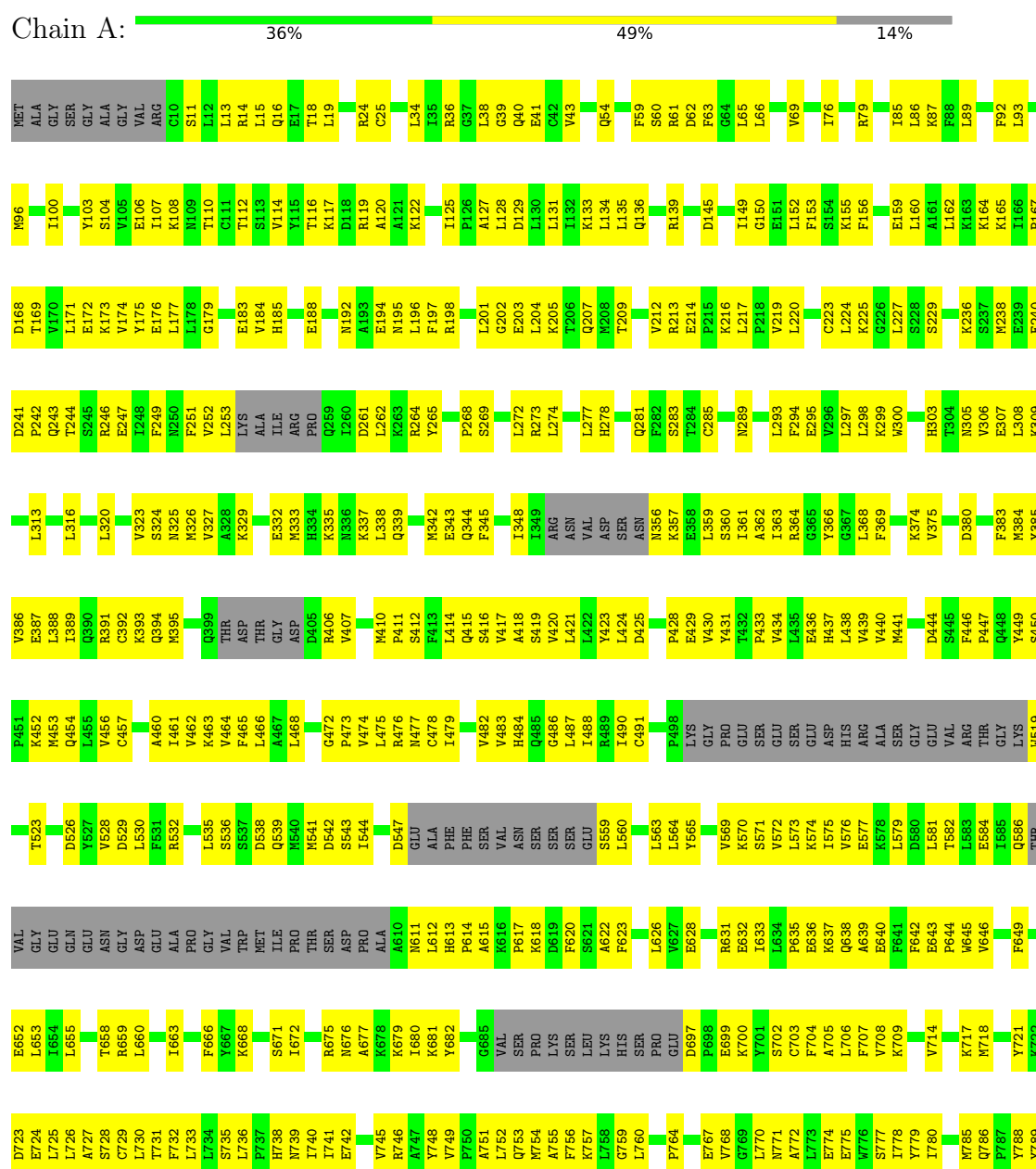
- Molecule 11 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	f	7	Total	C	N	O	0	0
			57	37	11	9		
11	m	7	Total	C	N	O	0	0
			57	37	11	9		

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







A3909	P3832	E3765	F3628	P3491	E3428	K3267	GLU	I3138	F3064	E2988	GLY
L3910	R3633	Q3766	R3629	C3492	E3429	T3268	ASP	Q3139	I3065	A2989	LYS
C3912	A3834	L3767	R3629	Q3493	ASN	R3269	ASN	F3140	I3066	A2990	ALA
S3913	P3835	F3768	Q3494	Q3494	ALA	D3270	SER	F3141	K3067	K2991	ARG
S3914	Q3769	K3631	K3631	F3495	SER	D3271	MET	I3142	M3068	W2994	L2916
H3915	E3838	Q3704	P3632	I3496	VAL	W3272	ASN	S3143	M3069	W2994	P2917
	Y3839	K3771	I3633	S3497	ILE	L3273	VAL	F3144	K3074	P2918	P2918
		N3772	Q3634	W3498	ASP	V3274	ASP		Q3075	W2919	W2919
I3920	W3842	R3708	F3636	W3498	SER	S3275	GLN	K3147	K3076	V2920	V2920
G3921	L3843	G3709	T3635	I3499	GLU	W3276	ASP	Q3148	A3076	D3000	R2921
D3922	THR	P3713	G3637	M3502	LEU	V3277	GLY	Q3149	L3077	C3001	R2922
R3923	LYS	H3716	K3638	V3503	GLN	Q3278	ASP	K3150	L3078	Y3002	W2923
H3924	MET	Y3715	E3639	A3504	GLN	R3282	PRD	L3151		M3003	W2924
L3925	SER	S3779		L3505	A3441	L3283	SER	S3152	H3081	E2925	E2925
	GLY	D3777	G3645	D3506	A3444	L3283	ASP	Q3153	Y3082	W3008	L2926
F3928	R3780	H3716	K3646	D3507	A3444	C3286	ASP	Q3154	Y3082	K3009	A2927
M3929	LYS	V3717	K3647	K3508	V3446	R3287	MET	F3155	E3085	S3010	K2928
W3930	HIS	R3718	G3647	S3509	V3447	S3288	GLU	P3156	L3086	L3011	L2929
A3931	D3851	Q3783	SER	Q3510	E3448	R3289	VAL	L3157	S3087	E3012	Y2930
	V3852	A3720	LYS	A3511	E3448	R3289	GLN	K3158	L3088	Y3013	R2931
		G3721	LEU	V3512	E3448	R3289	GLN	R3159	L3089	C3014	C3014
G3935	Y3855	F3722	LEU	A3513	N3450	E3295	GLU	L3160	Y3090	S3015	E2935
G3936	M3856	E3723	ARG	V3514	L3451	E3295	GLU	L3161	Y3090	S3015	E2936
V3937		E3724	LYS	Q3515	K3452	L3298	GLU	W3164	D3094	S3018	D2937
I3938	Y3859	R3789	MET	K3516	A3453	T3299	GLU	K3165	D3095		W2938
G3939	K3860	T3790	LEU	S3517	L3454	V3300		T3166		E3022	L2939
L3940		S3722	S3657	V3518	K3455	L3301		R3167	R3098	ASN	F2943
D3941		V3793		E3519	L3456	K3302		Q3167	R3099	PRO	T2944
G3943	T3867	V3794	N3660	E3520	L3456	T3303		Y3168	K3100	ASP	
H3944	Y3868	M3795	K3661	S3521	S3457	F3304		P3169	P3169	ASP	
A3945	T3869	R3733		T3522	K3458	E3395		S3236	L3103	LEU	T2947
	S3870	R3734	M3685	Q3527	N3459	ALA		D3170	L3103	ASN	Q2948
	L3800	K3736	L3666	A3528	E3460	GLN		A3171		K3029	
L3963	R3801	R3737	L3667	A3529	A3461	PRD		K3172	L3107		
P3964	L3802	I3738	L3668	I3529	R3462	PRD		M3173		I3030	Q2954
V3965	I3803	R3739	K3669	V3530	L3463	SER		D3174	F3110	W3031	S2955
	E3804	I3740	M3670	Y3531	K3464	TRP		P3175		A2956	
	E3805	R3741	N3671	P3532	F3465	SER		M3176	N3113	E3033	
M3969	K3877	G3742		F3533	P3466	CYS		N3177	Y3114	P3034	A2969
P3960	V3878	H3743	S3674	F3533	R3467	GLY		I3178			
F3961		D3744		I3534	L3468	PRD		W3179	L3117	Q3037	R2962
R3962	A3880	E3745	P3677	I3535	L3469	ALA		D3180	D3118		S2963
L3963	D3881	R3746	G3678	S3537	Q3470	K3248		D3181	L3119	Y3040	D2964
T3964		E3747	N3679	E3538	I3471	Q3249		I3182	L3120	L3041	P2965
R3965	K3884	H3748	L3680	F3538	I3472	D3244		I3183	L3121	P3042	S2966
Q3966	R3885	P3749	K3681	S3539	E3473	D3244		T3184	H3122	Y3043	E2967
F3967		F3750	E3682	THR	R3474	S3245		R3185	Q3123	M3044	
I3968	V3888	L3751	C3683	PHE		S3253		S3124	S3124	R3046	Q2971
N3969	R3889	T3818	C3684	LYS	E3477	L3254		C3187	R3125	S3047	D2972
L3970	M3820	K3612	P3685	ASP	T3479	A3255		F3188	L3126	S3047	W2973
M3971	S3891	R3613	W3686	T3545	L3480	M3257		F3189	T3127	K3048	
		Q3822	M3687	T3545	S3481	K3257		L3190	K3128	L3049	L2976
	P3894	E3823	S3688	T3546	L3482	L3258		S3191	L3129	K3050	R2977
		E3824	D3689	T3547	M3483	L3259		K3192	Q3130	L3051	K2978
T3977	L3998	K3825	F3690	H3549	K3484	K3260		I3193	V3132	L3052	Q2979
G3978		Q3760	K3691	P3620	K3485	E3261			Q3133	L3053	D2980
L3979	R3901	D3761	V3692	N3551	E3486	L3262			A3134	Q3054	W2981
M3980		Q3762		K3552		H3263			L3136		E2985
Y3981	F3904	V3764	R3696	K3552	S3489	E3265			T3136	LEU	P2986
			N3697	V3555	V3490	E3265			E3137	PRO	T2987



A1943	L1877	K1744	L1878	R1606	A1536	Q1457	Q1374	S1289	V1211	Q1048	F966	S893
C1947	D1878	K1745	L1879	E1607	V1537	L1458	T1375	K1292	L1212	Q1049	Y976	F894
A1948	V1879	F1746	M1880	R1608	LEU	H1459	E1378	K1296	K1213	K1050	D977	A895
S1950	Y1881	D1747	L1682	E1609	SER	H1460	E1378	A1296	E1215	K1051	Q978	V896
V1951	P1885	L1683	T1683	Q1611	THR	L1464	L1382	F1297	F1219	M1055	V979	F897
I1952	LYS	L1750	D1685	K1612	ALA	H1465	L1382	F1297	F1219	T1066	T980	F898
C1953	ASP	E1751	L1686	H1613	SER	N1466	G1387	L1298	L1220	K1062	R981	R899
C1954	ASP	L1752	H1687	H1614	LEU	N1467	D1388	E1299	L1221	R1063	E982	E900
L1959	VAL	Q1753	L1688	L1688	GLY	L1468	V1389	I1301	T1223	K1064	E985	M901
K1960	HIS	Q1754	K1689	K1617	SER	P1469	Q1390	H1304	T1223	Y1064	P986	P903
Q1963	ALA	S1755	Q1690	I1622	SER	S1470	V1391	H1307	E1225	S1065	P987	V904
GLY	LYS	M1756	Q1691	L1623	GLN	Q1471	A1393	I1307	G1226	L1066	Y989	I905
PHE	GLU	L1757	A1692	Q1624	VAL	D1474	H1394	K1312	Q1231	A1067	Y992	F910
LEU	LYS	L1758	V1693	H1625	ILE	L1475	L1395	C1312	I1235	L1068	H993	P912
LEU	LYS	E1760	L1696	W1626	THR	H1476	P1396	F1313	Q1238	L1069	Y994	R913
GLY	ILE	L1761	P1697	K1627	HIS	V1479	D1397	GLY	P1239	P1070	F995	V914
PHE	ASN	M1762	F1698	K1628	PHE	G1480	V1398	ALA	LEU	M1071	T996	L919
SER	GLN	T1763	F1699	C1629	S1554	G1481	C1399	ASN	TYR	K1074	F1001	T920
GLU	VAL	E1764	THR	D1630	H1555	L1481	V1400	ARG	LEU	R1075	E1002	A921
LYS	PHE	V1765	SER	S1631	Y1558	L1484	M1403	ALA	ARG	L1076	S1003	D923
PRO	HIS	L1766	LEU	W1632	F1559	L1484	K1404	ALA	GLY	G1077	Q1004	R924
GLY	GLY	C1767	THR	W1633	Y1560	V1487	A1405	GLY	PRO	A1078	D1005	T926
LYS	LYS	E1768	GLY	K1634	S1561	V1487	A1406	ASN	PHE	F1082	T1006	K927
ASN	CYS	E1769	GLY	K1635	L1562	G1490	S1409	ARG	THR	L1085	L1009	L934
LEU	ILE	Q1770	SER	D1636	E1565	L1491	K1412	ALA	LEU	Y1086	L1010	H935
LEU	ILE	Q1771	LEU	S1631	T1566	L1492	D1413	ASP	LEU	R1087	E1011	S936
LEU	GLY	Q1772	THR	W1639	H1567	GLY	L1414	GLY	PRO	L1088	A1012	M937
PHE	GLY	W1773	E1708	L1639	I1568	ASP	L1416	ARG	PRO	L1089	L1013	V938
GLY	GLY	E1774	E1709	E1640	T1569	GLU	L1417	GLN	GLY	E1091	L1014	M939
ASN	ASN	E1775	L1710	T1641	K1573	LEU	H1418	CYS	THR	E1092	F940	F940
LEU	ILE	E1776	R1711	K1642	M1574	PRO	L1419	S1333	D1258	E1093	M941	M941
ILE	ILE	E1777	R1712	M1643	A1578	S1502	E1421	K1334	L1259	S1094	V1018	L942
ASP	ASP	F1778	V1713	W1644	V1579	S1506	K1422	T1335	L1260	L1095	D1019	G943
LEU	LEU	Q1779	L1714	A1644	E1570	ARG	L1423	T1336	A1261	V1096	P1020	K944
LYS	V1850	Q1780	E1715	V1645	K1573	GLN	T1424	V1337	A1262	F1099	R1026	A945
ARG	L1851	Q1781	Q1716	L1646	M1574	LEU	L1419	S1333	E1265	V1100	D1027	T946
ARG	K1852	S1781	L1717	L1646	N1574	PRO	E1420	S1333	E1266	F1101	R1031	Q947
ARG	SER	F1782	I1718	L1649	L1577	S1502	I1428	T1341	C1266	E1102	R1031	G952
TYR	ARG	R1783	LEU	A1650	A1578	S1506	E1429	T1345	I1271	L1106	R1034	Q953
ASN	PHE	R1784	H1721	K1651	V1579	S1506	E1430	P1196	R1274	L1114	E1035	G954
PHE	THR	I1785	F1722	L1652	L1580	Q1509	L1431	L1197	T1275	L1115	F1036	A955
PRO	LYS	A1786	Q1725	L1653	L1581	Q1509	L1431	L1198	V1276	L1116	F1036	P956
VAL	ASN	R1787	S1726	Q1654	S1586	E1516	Y1437	P1199	E1285	L1117	E1036	M958
GLU	GLU	R1788	R1727	T1663	S1586	L1517	Y1443	L1359	E1286	D1117	W1039	Y959
VAL	GLU	T1793	E1728	H1665	Q1584	L1518	V1443	K1361	E1287	L1118	S1040	Q960
PRO	GLU	Q1794	F1729	G1666	L1584	L1517	R1447	L1361	L1279	L1119	Q1043	L961
MET	ASN	G1796	G1732	F1667	M1589	L1518	L1448	L1361	L1282	L1120	I1044	Y962
GLU	GLN	L1797	R1735	F1668	M1592	F1521	L1448	M1369	L1282	L1121	T1045	K963
ARG	LEU	L1798	F1736	E1670	V1593	F1521	L1448	M1369	L1282	L1122	P1046	R964
LYS	LYS	Y1802	M1737	V1671	V1596	L1524	L1448	M1369	L1282	L1123	Q1047	T965
LYS	LYS	E1803	M1738	F1672	L1597	L1524	L1448	M1369	L1282	L1123	Q1047	T965
TYR	TYR	M1804	M1739	T1673	L1597	L1524	L1448	M1369	L1282	L1123	Q1047	T965
ILE	ILE	F1805	V1740	T1674	M1600	R1527	V1452	R1370	E1285	L1123	Q1047	T965
GLU	GLU	R1806	D1741	I1675	L1601	L1528	S1453	V1371	E1286	L1123	Q1047	T965
ILE	ILE	LYS	C1742	I1676	L1601	L1528	S1453	V1371	E1286	L1123	Q1047	T965
ARG	ARG	ASP	M1743	S1677	D1602	L1531	K1456	V1373	S1288	L1123	Q1047	T965



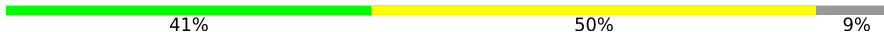
- Molecule 2: X-ray repair cross-complementing protein 6

Response	Percentage
Yes	32%
No	52%
Don't know	17%

MET	SER	GLY	TRP	GLU	SER	TYR	LYS	THR	GLU	GLY	ASP	GLU	ALA	GLU	V85	GLU	V86	GLU	V87	GLN	GLU	GLU	ASN	GLU	LEU	LEU	ALA	SER	GLY	ASP	TYR	LYS	Y32	Y33	G34	R35	D36	S37	L38	I39	F40	L41	A44	S45	K46	A47	M48	F49	D55	E56	P59	M62	S63	I64	Q65	C66	I67																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
Q68	S69	V70	Y71	I72	S73	K74	I75	I76	D79	R80	D81	L82	L83	A84	V85	V86	V87	V88	V89	V90	V91	V92	V93	V94	V95	V96	V97	V98	V99	V100	V101	V102	V103	V104	V105	V106	V107	V108	V109	V110	V111	V112	V113	V114	V115	V116	V117	V118	V119	V120	V121	V122	V123	V124	V125	V126	V127	V128	V129	V130	V131	V132	V133	V134	V135	V136	V137																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
G138	S139	S140	S141	S142	S143	S144	S145	S146	V149	L153	F154	S155	D156	V157	Q158	V159	V160	V161	V162	V163	V164	V165	V166	V167	V168	V169	V170	V171	V172	V173	V174	V175	V176	V177	V178	V179	V180	V181	V182	V183	V184	V185	V186	V187	V188	V189	V190	V191	V192	V193	V194	V195	V196	V197	V198	V199	V200	V201	V202	V203	V204	V205																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
K206	K207	P208	G209	G210	F211	D212	I213	S214	F216	V217	L218	D219	I220	I221	D228	L229	R230	V231	H232	F233	K234	E235	E236	S237	V238	V239	V240	V241	V242	V243	V244	V245	V246	V247	V248	V249	V250	V251	V252	V253	V254	V255	V256	V257	V258	V259	V260	V261	V262	V263	V264	V265	V266	V267	V268	V269	V270	V271	V272	V273																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
V274	N275	L276	V277	K282	P283	P284	P285	I286	K287	L288	V289	R290	E291	N292	N293	E294	P295	V296	K297	T298	F299	T300	R301	T302	F303	N304	T305	S306	E307	T308	G309	L310	L311	L312	D315	T316	K317	S318	S319	Q320	V321	R325	Q326	I327	I328	L329	E330	K331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018	E1019	E1020	E1021	E1022	E1023	E1024	E1025	E1026	E1027	E1028	E1029	E1030	E1031	E1032	E1033	E1034	E1035	E1036	E1037	E1038	E1039	E1040	E1041	E1042	E1043	E1044	E1045	E1046	E1047	E1048	E1049	E1050	E1051	E1052	E1053	E1054	E1055	E1056	E1057	E1058	E1059	E1060	E1061	E1062	E1063	E1064	E1065	E1066	E1067	E1068	E1069	E1070	E1071	E1072	E1073	E1074	E1075	E1076	E1077	E1078	E1079	E1080	E1081	E1082	E1083	E1084	E1085	E1086	E1087	E1088	E1089	E1090	E1091	E1092	E1093	E1094	E1095	E1096	E1097	E1098	E1099	E1100	E1101	E1102	E1103	E1104	E1105	E1106	E1107	E1108	E1109	E1110	E1111	E1112	E1113	E1114	E1115	E1116	E1117	E1118	E1119	E1120	E1121	E1122	E1123	E1124	E1125	E1126	E1127	E1128	E1129	E1130	E1131	E1132	E1133	E1134	E1135	E1136	E1137	E1138	E1139	E1140	E1141	E1142	E1143	E1144	E1145	E1146	E1147	E1148	E1149	E1150	E1151	E1152	E1153	E1154	E1155	E1156	E1157	E1158	E1159	E1160	E1161	E1162	E1163	E1164	E1165	E1166	E1167	E1168	E1169	E1170	E1171	E1172	E1173	E1174	E1175	E1176	E1177	E1178	E1179	E1180	E1181	E1182	E1183	E1184	E1185	E1186	E1187	E1188	E1189	E1190	E1191	E1192	E1193	E1194	E1195	E1196	E1197	E1198	E1199	E1200	E1201	E1202	E1203	E1204	E1205	E1206	E1207	E1208	E1209	E1210	E1211	E1212	E1213	E1214	E1215	E1216	E1217	E1218	E1219	E1220	E1221	E1222	E1223	E1224	E1225	E1226	E1227	E1228	E1229	E1230	E1231	E1232	E1233	E1234	E1235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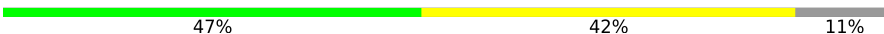
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K463	LYS	THR
K464	HIS	LYS
I465	ASP	HIS
V466	ASN	PHE
E467	GLU	GLN
K468	SER	ASP
Y473	GLY	
E474	LYS	
S475	ARG	
D476	PRO	
S477	LYS	
F478	VAL	
E479	GLU	
M480	TVR	
Q484	SER	
Q485	GLU	
H486	LEU	
F487	LYS	
R488	THR	
M489	HIS	
E491	ILE	
L495	LYS	
P500	GLY	
E501	THR	
A513	LEU	
M514	PHE	
R517	THR	
L518	VAL	
L521	PRO	
V522	MET	
D523	LEU	
E524	LYS	
F525	GLU	
K526	ALA	
E527	ARG	
L528	ALA	
W529	TVR	
Y530	GLY	
P531	LEU	
Y534	LYS	
N535	GLY	
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E537	LYS	
G538	GLN	
Y539	GLU	
VAL	LEU	

• Molecule 3: X-ray repair cross-complementing protein 5

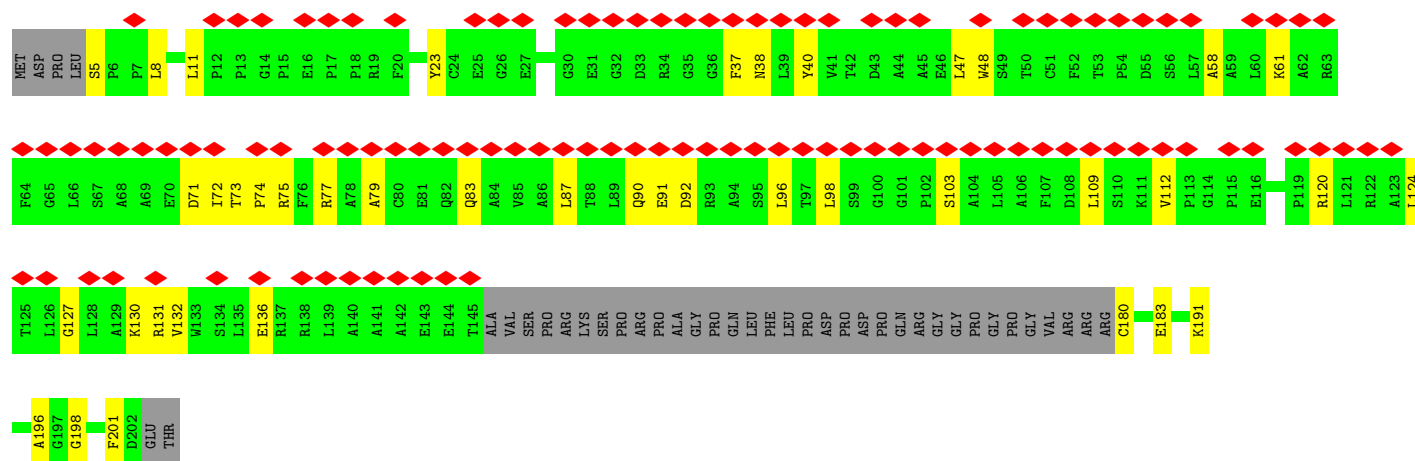
Chain C:  41% 50% 9%

MET	VAL	ARG	SER	GLY	N6	K7	A8	A9	V10	V11	L12	C13	M14	D15	V16	G17	F18	T19	M20	I27	F31	E32	Q33	A34	V37	V38	T39	M40	F41	V42	Q43	R44	Q45	V46	A48	E49	N50	A55	L56	W57	L58	F59	D62	D65	L68	G71	D72	Q73	Y74	Q75																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
	VAL	SER	GLY	VAL	F594	A595	F598	R599	L601	V602	Q603	Q604	K605	F609	E610	E611	A612																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										</

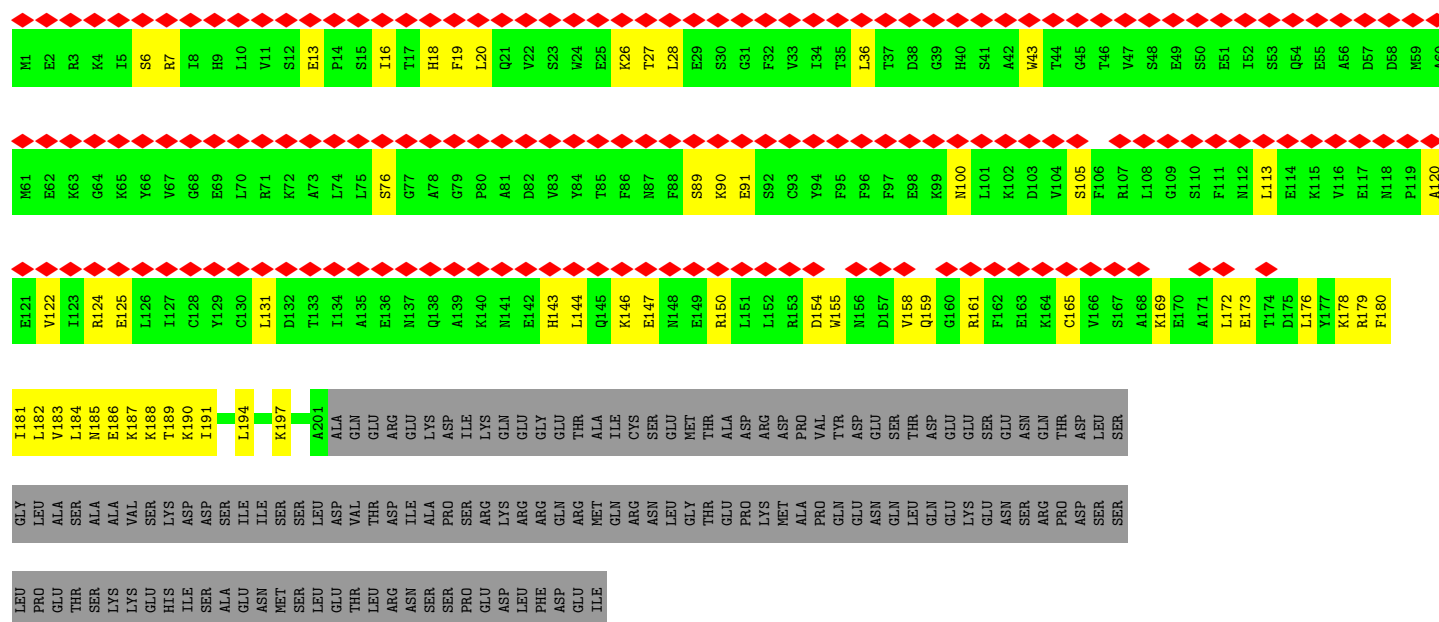
• Molecule 3: X-ray repair cross-complementing protein 5

Chain L:  47% 42% 11%

MET	VAL	ARG	SER	GLY	N6	K7	A8	A9	V10	L12	C13	M14	D15	G17	F18	T19	M20	S21	I27	P30	Q33	A34	V37	I38	K39	T39	M40	F41	A55	L56	V57	F59	N66	G71	D72	Q73	Y74	Q75	W76	I77	R81	H82	L83	M84	L85	D93	S96
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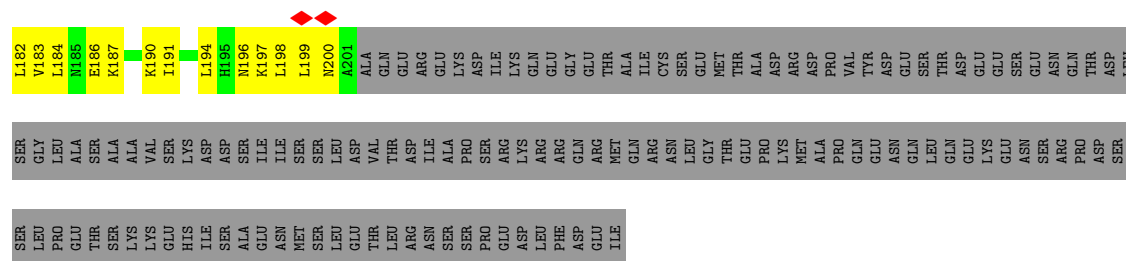


• Molecule 5: DNA repair protein XRCC4

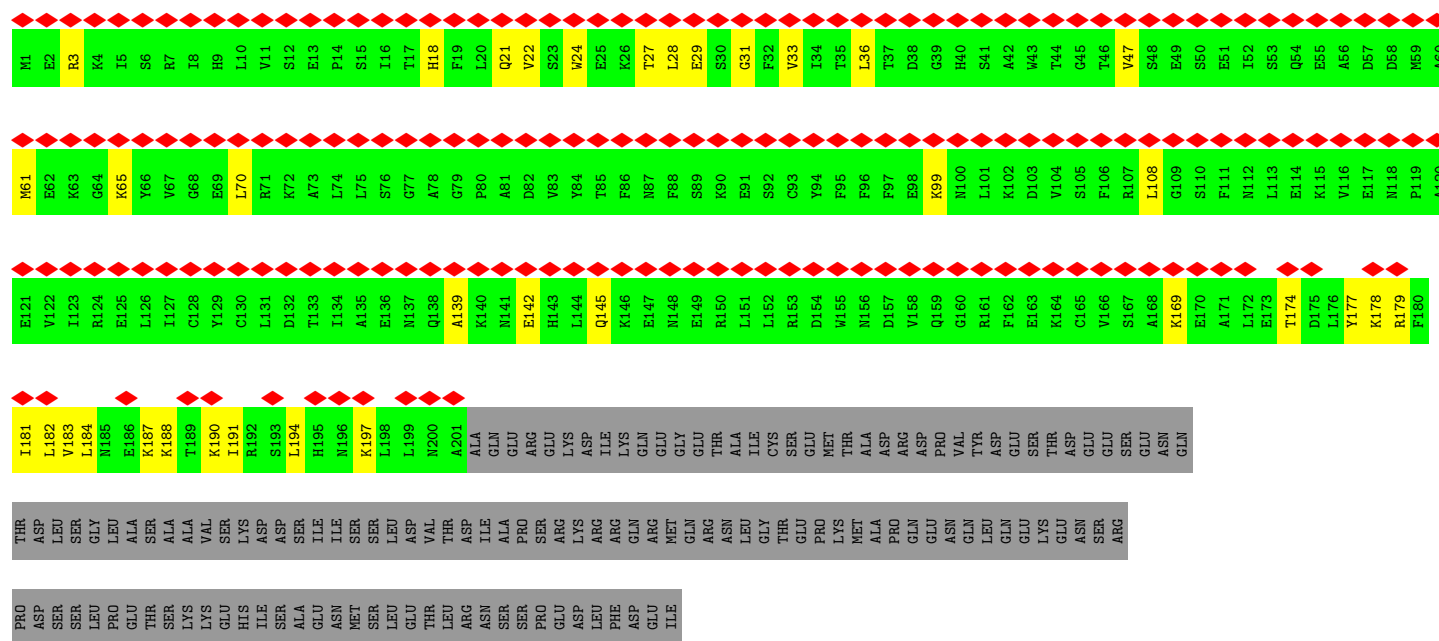


• Molecule 5: DNA repair protein XRCC4

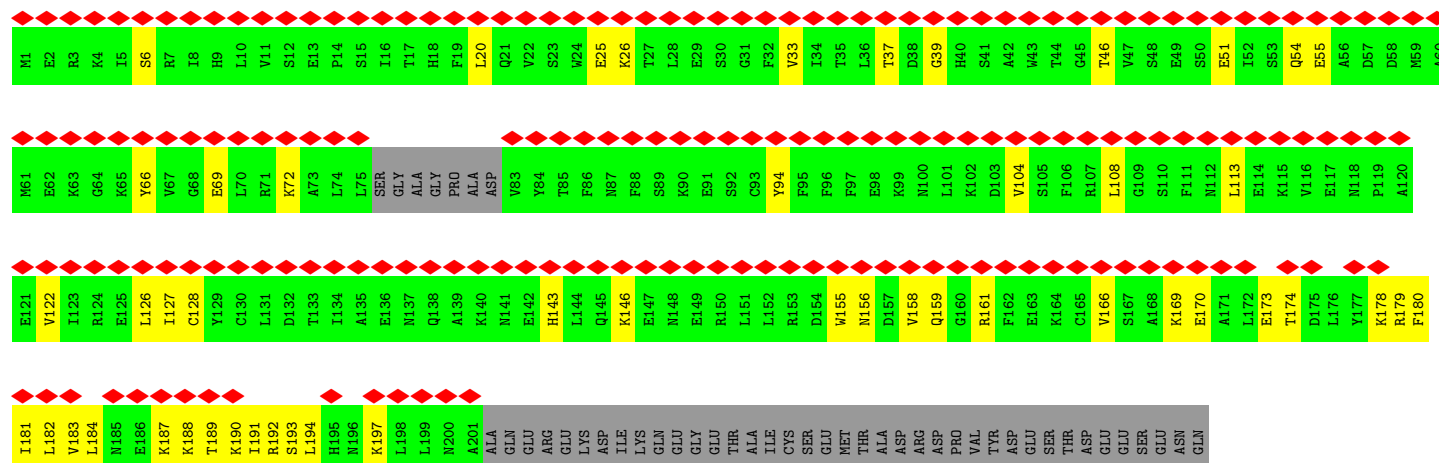




• Molecule 5: DNA repair protein XRCC4



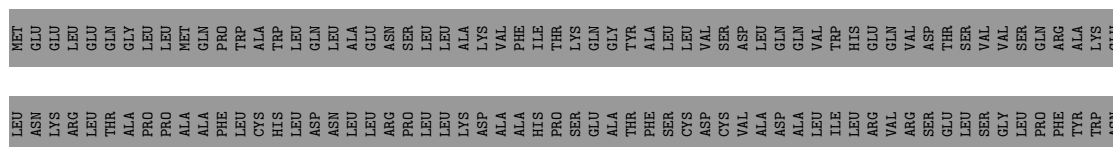
• Molecule 5: DNA repair protein XRCC4



[illegible]

- Molecule 6: DNA ligase 4

[illegible]



THR	PHE
GLU	HIS
PRO	CYS
PHE	MET
GLU	LEU
GLU	ALA
ASN	SER
PRO	PRO
SER	SER
PHE	LEU
LEU	VAL
GLU	SER
GLN	GLN
PHE	HIS
MET	LEU
ILE	ILE
ASN	GLN
GLN	ARG
PRO	LEU
GLU	PRO
GLN	LEU
LEU	MET
VAL	GLY
SER	GLY
SER	MET
SER	SER
ALA	ILE
ALA	LEU
PRO	GLY
THR	ASP
LEU	GLN
SER	LYS
GLY	CYS
LEU	GLN
ALA	PRO
ALA	PHE
PRO	VAL
GLU	ARG
LYS	GLU
GLU	LEU
SER	ASN
GLU	LEU
SER	ALA
THR	GLN
GLY	THR
THR	ASP
SER	LEU
GLY	LEU
PRO	HIS
LEU	MET
GLN	LYS
ARG	ASP
PRO	LEU
GLN	THR
GLN	ILE
LEU	GLN
SER	VAL
LYS	TYR
VAL	GLN
VAL	GLY
LYS	GLU
ARG	SER
LYS	GLY
LYS	ALA
LYS	THR
P294	LEU
R295	ILE
G296	ARG
L297	ASP
F298	PRO
S299	HIS
	LEU
	THR
	LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30390	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)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.204	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.045	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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/28856	0.44	0/38971
1	S	0.16	0/28899	0.40	0/39012
2	B	0.17	0/4166	0.38	0/5615
2	T	0.15	0/4116	0.35	0/5547
3	C	0.15	0/5419	0.36	0/7303
3	L	0.15	0/5303	0.36	1/7147 (0.0%)
4	D	0.11	0/1128	0.30	0/1533
4	M	0.10	0/1247	0.27	0/1695
5	G	0.10	0/1657	0.28	0/2228
5	H	0.11	0/1616	0.27	0/2170
5	P	0.11	0/1651	0.30	0/2221
5	Q	0.13	0/1607	0.34	0/2159
6	I	0.12	0/2028	0.37	0/2735
6	R	0.19	0/2014	0.43	0/2719
7	d	0.42	0/577	0.78	4/890 (0.4%)
8	e	0.33	0/622	0.53	2/957 (0.2%)
9	i	0.23	0/597	0.41	0/918
10	j	0.30	0/556	0.62	2/858 (0.2%)
11	f	0.30	0/58	0.80	0/74
11	m	0.17	0/58	0.60	0/74
All	All	0.18	0/92175	0.40	9/124826 (0.0%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	j	27	DT	P-O3'-C3'	-8.38	107.62	120.20
7	d	26	DT	P-O3'-C3'	-7.36	109.16	120.20
7	d	21	DA	P-O3'-C3'	-6.97	109.74	120.20
8	e	31	DA	P-O3'-C3'	-6.21	110.88	120.20
8	e	30	DA	P-O3'-C3'	-5.75	111.58	120.20

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	28300	0	28587	1832	0
1	S	28342	0	28717	1599	0
2	B	4085	0	4143	352	0
2	T	4037	0	4105	258	0
3	C	5318	0	5327	369	0
3	L	5204	0	5210	279	0
4	D	1102	0	1098	43	0
4	M	1219	0	1197	32	0
5	G	1628	0	1620	39	0
5	H	1589	0	1587	55	0
5	P	1622	0	1609	27	0
5	Q	1580	0	1567	43	0
6	I	1984	0	1940	84	0
6	R	1970	0	1916	66	0
7	d	516	0	288	43	0
8	e	554	0	307	54	0
9	i	532	0	296	23	0
10	j	497	0	277	23	0
11	f	57	0	60	16	0
11	m	57	0	60	15	0
All	All	90193	0	89911	4936	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 28.

The worst 5 of 4936 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)
3:C:461:MET:HE3	3:C:526:SER:HB3	1.33	1.07
3:L:236:VAL:HA	11:m:298:PHE:HA	1.46	0.98
6:I:814:ARG:H	6:I:850:ALA:H	1.19	0.91
1:A:1871:MET:HE1	1:A:1940:TYR:HA	1.49	0.91
1:S:2225:HIS:HB2	1:S:2231:PHE:HB2	1.51	0.90

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	3473/4128 (84%)	3140 (90%)	330 (10%)	3 (0%)	48	82
1	S	3462/4128 (84%)	3180 (92%)	280 (8%)	2 (0%)	48	82
2	B	505/609 (83%)	468 (93%)	37 (7%)	0	100	100
2	T	498/609 (82%)	468 (94%)	30 (6%)	0	100	100
3	C	660/732 (90%)	619 (94%)	41 (6%)	0	100	100
3	L	644/732 (88%)	608 (94%)	35 (5%)	1 (0%)	43	77
4	D	139/204 (68%)	132 (95%)	7 (5%)	0	100	100
4	M	160/204 (78%)	156 (98%)	4 (2%)	0	100	100
5	G	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
5	H	190/336 (56%)	188 (99%)	2 (1%)	0	100	100
5	P	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
5	Q	190/336 (56%)	184 (97%)	6 (3%)	0	100	100
6	I	242/911 (27%)	213 (88%)	29 (12%)	0	100	100
6	R	242/911 (27%)	215 (89%)	27 (11%)	0	100	100
11	f	5/299 (2%)	3 (60%)	2 (40%)	0	100	100
11	m	5/299 (2%)	4 (80%)	1 (20%)	0	100	100
All	All	10813/15110 (72%)	9969 (92%)	838 (8%)	6 (0%)	49	82

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3304	VAL
1	S	3304	VAL
1	A	1960	LYS
3	L	236	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	956	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	3123/3671 (85%)	3121 (100%)	2 (0%)	88	88
1	S	3142/3671 (86%)	3142 (100%)	0	100	100
2	B	455/548 (83%)	455 (100%)	0	100	100
2	T	452/548 (82%)	452 (100%)	0	100	100
3	C	589/649 (91%)	589 (100%)	0	100	100
3	L	576/649 (89%)	575 (100%)	1 (0%)	87	85
4	D	116/160 (72%)	116 (100%)	0	100	100
4	M	127/160 (79%)	127 (100%)	0	100	100
5	G	180/303 (59%)	180 (100%)	0	100	100
5	H	177/303 (58%)	177 (100%)	0	100	100
5	P	179/303 (59%)	179 (100%)	0	100	100
5	Q	175/303 (58%)	175 (100%)	0	100	100
6	I	220/808 (27%)	220 (100%)	0	100	100
6	R	217/808 (27%)	217 (100%)	0	100	100
11	f	6/262 (2%)	6 (100%)	0	100	100
11	m	6/262 (2%)	6 (100%)	0	100	100
All	All	9740/13408 (73%)	9737 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1958	GLU
1	A	3161	LEU
3	L	233	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 159 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	2335	ASN
2	T	95	ASN
1	S	2560	ASN
1	S	3150	ASN
2	T	326	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

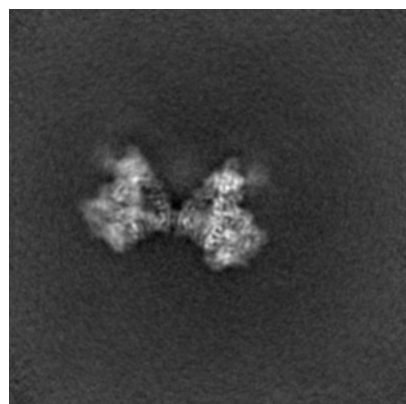
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16074. These allow visual inspection of the internal detail of the map and identification of artifacts.

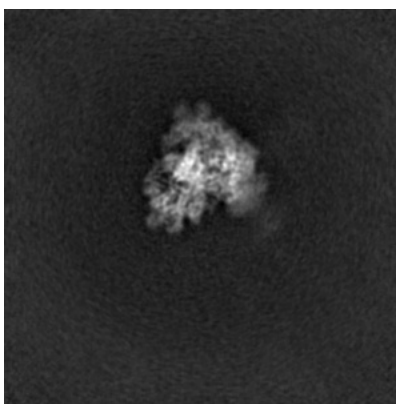
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

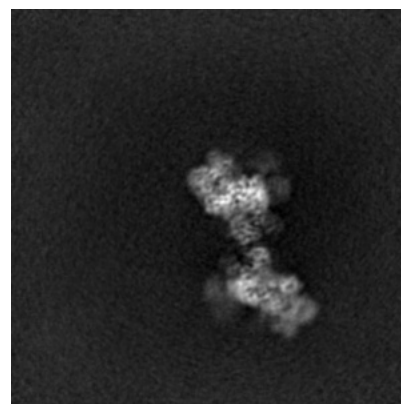
6.1.1 Primary map



X

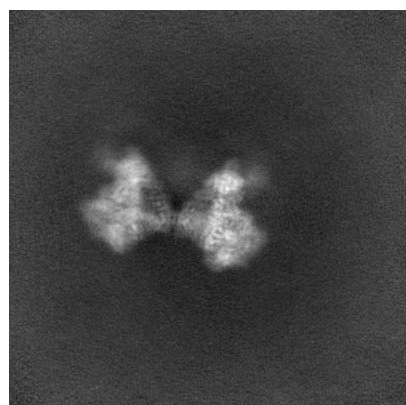


Y

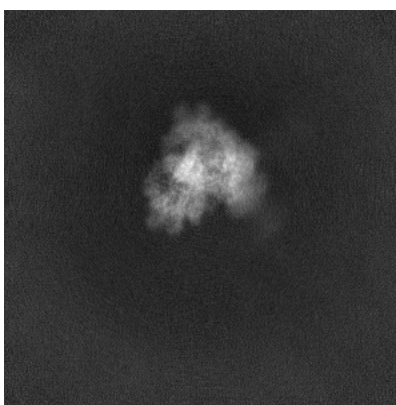


Z

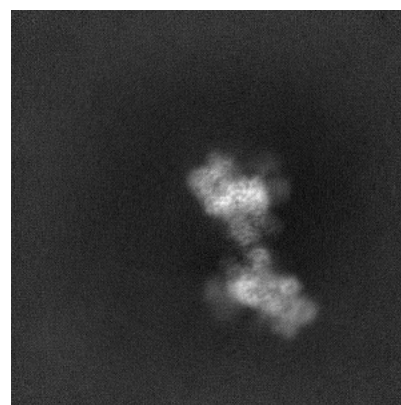
6.1.2 Raw map



X



Y

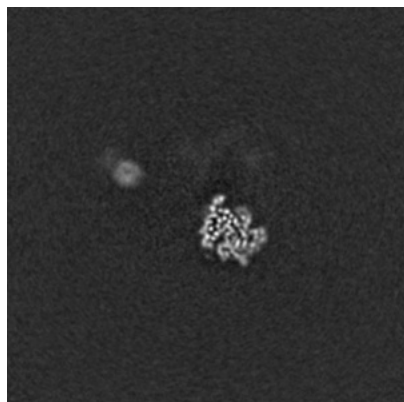


Z

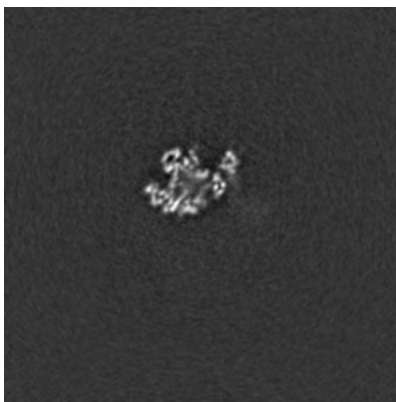
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

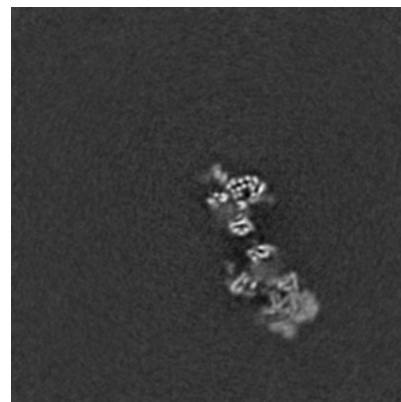
6.2.1 Primary map



X Index: 260

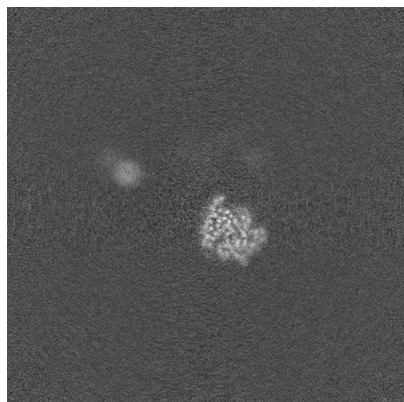


Y Index: 260



Z Index: 260

6.2.2 Raw map



X Index: 260



Y Index: 260

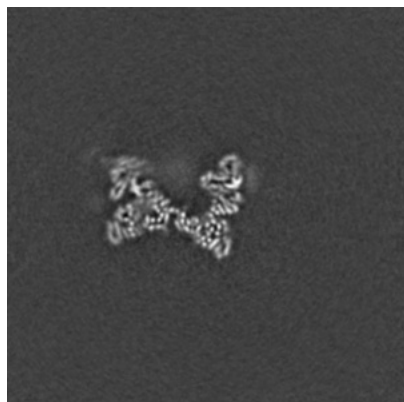


Z Index: 260

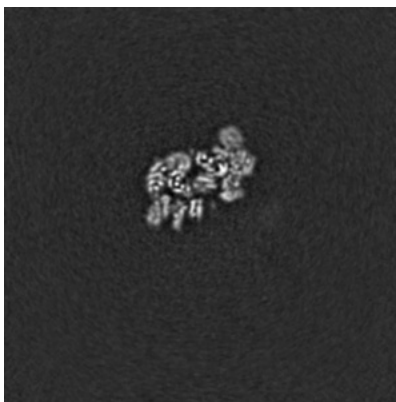
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

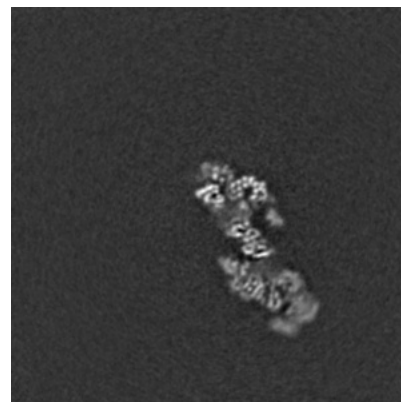
6.3.1 Primary map



X Index: 316

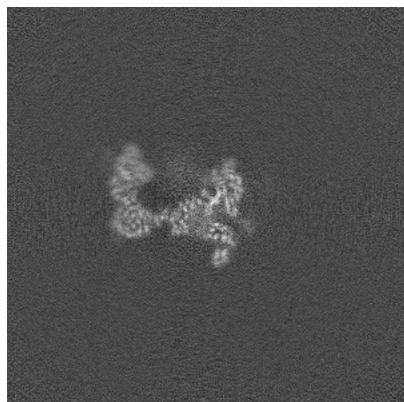


Y Index: 283

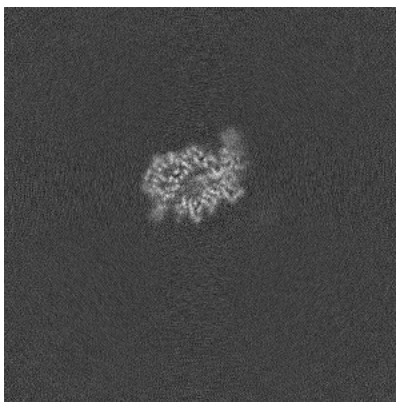


Z Index: 253

6.3.2 Raw map



X Index: 302



Y Index: 275

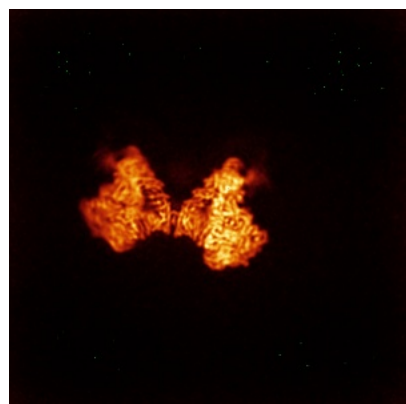


Z Index: 242

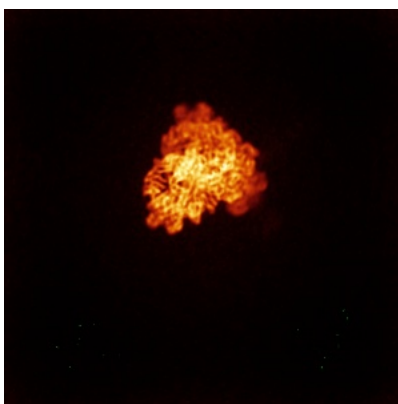
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

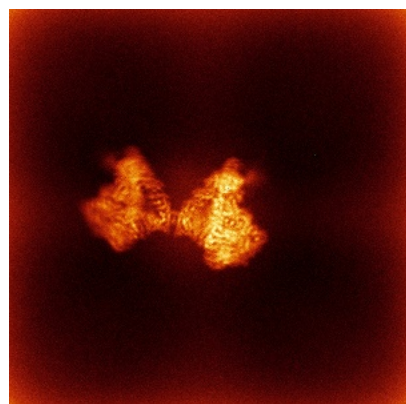


Y

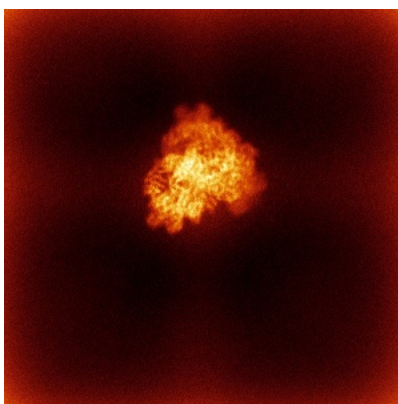


Z

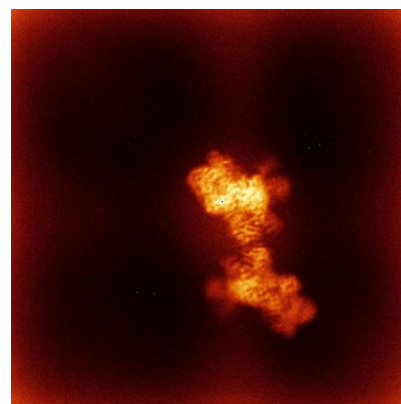
6.4.2 Raw map



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



X



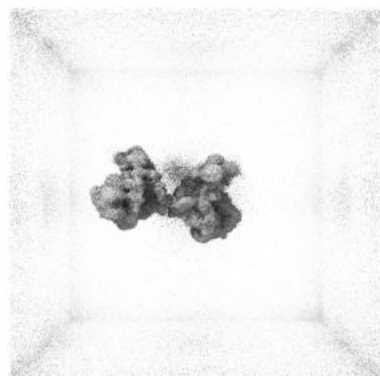
Y



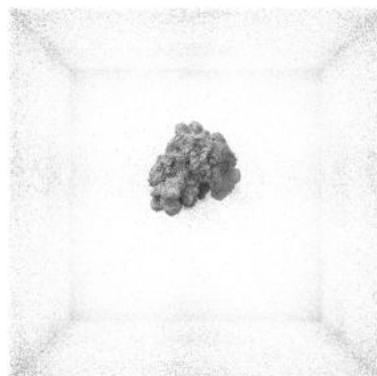
Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

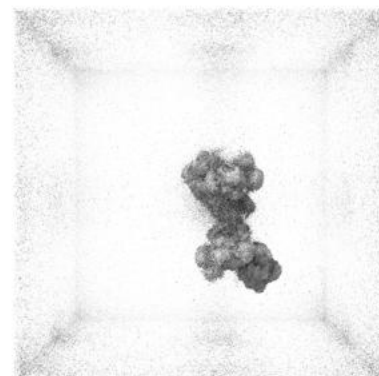
6.5.2 Raw map



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.

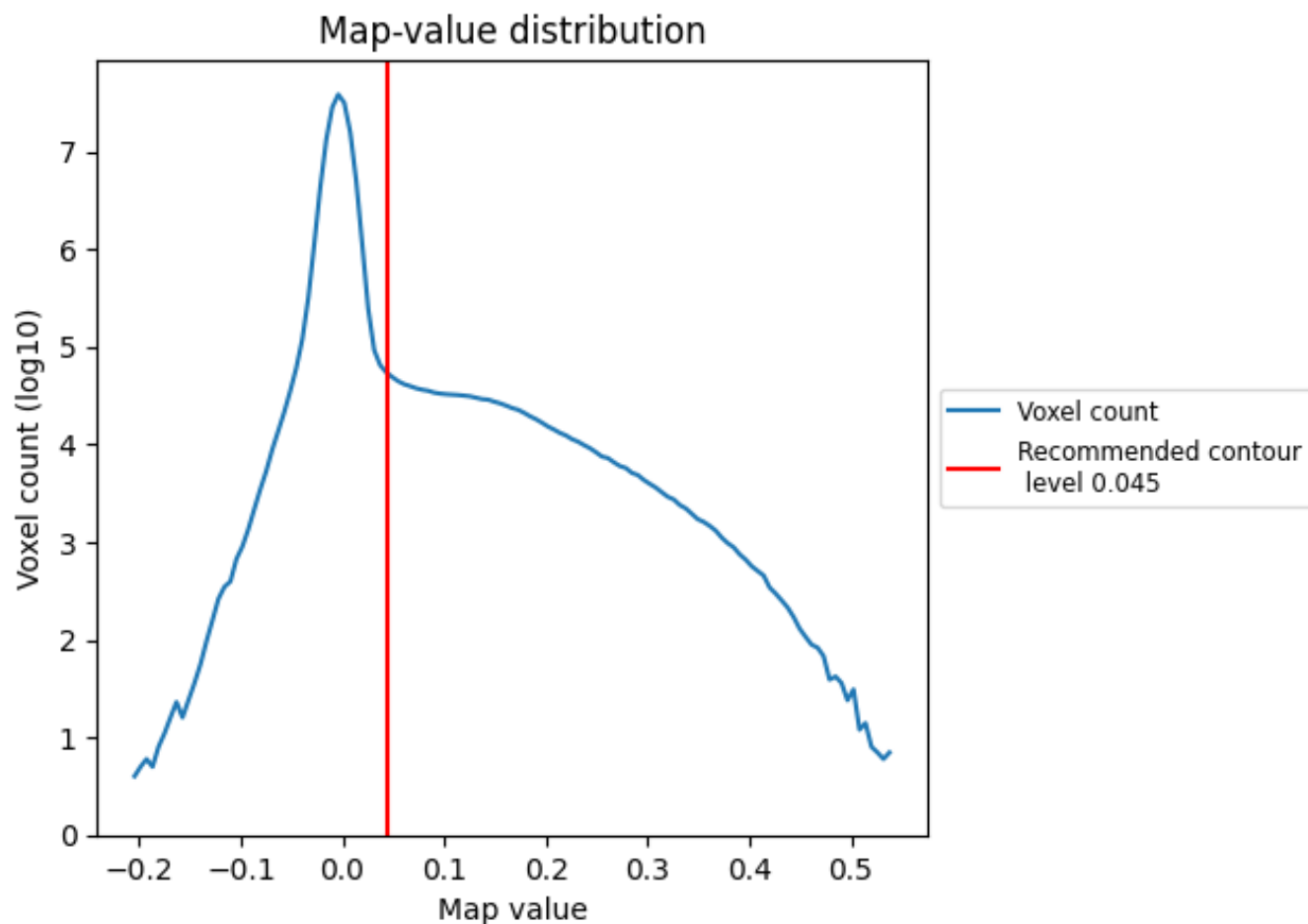
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

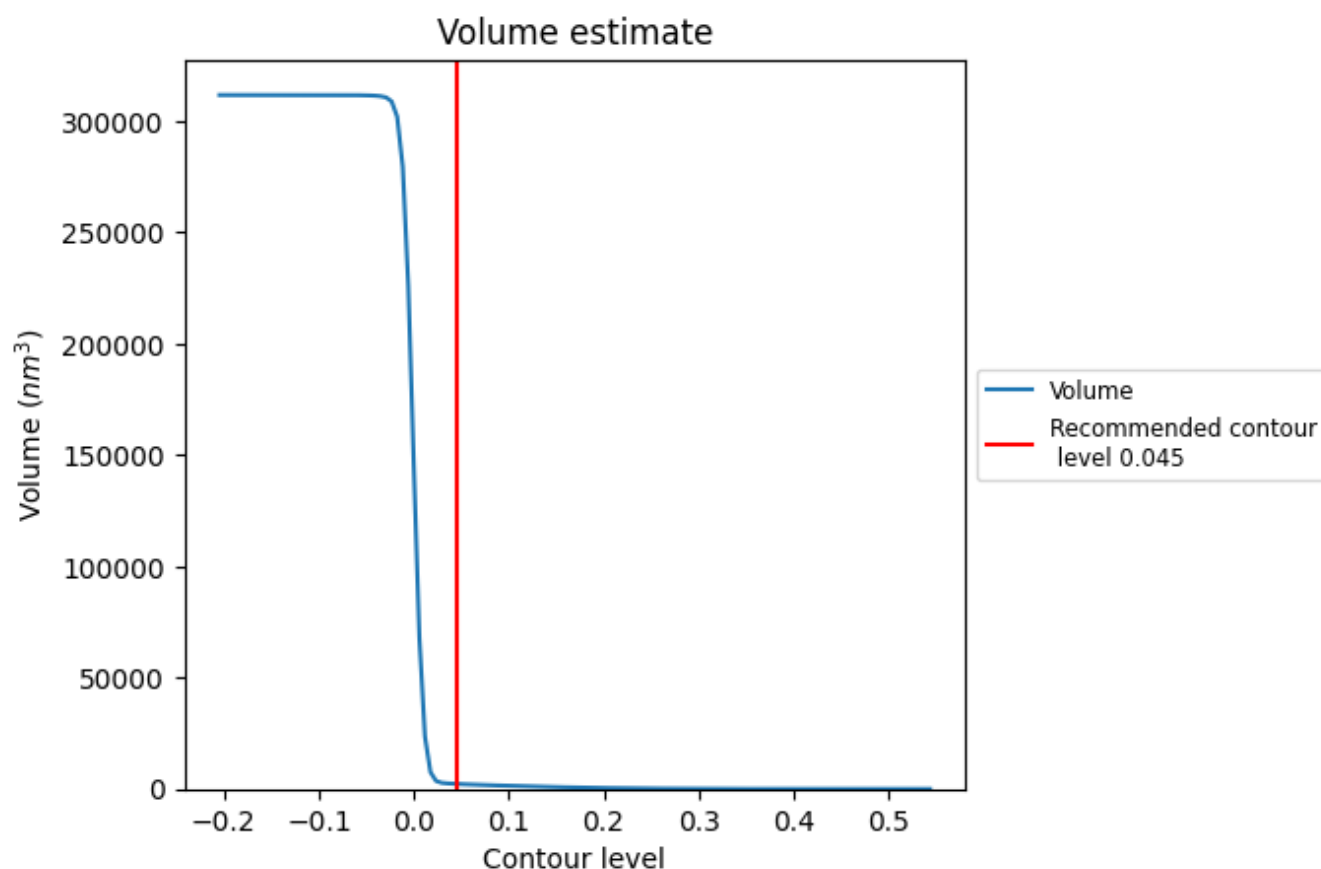
This section contains the results of statistical analysis of the map.

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.

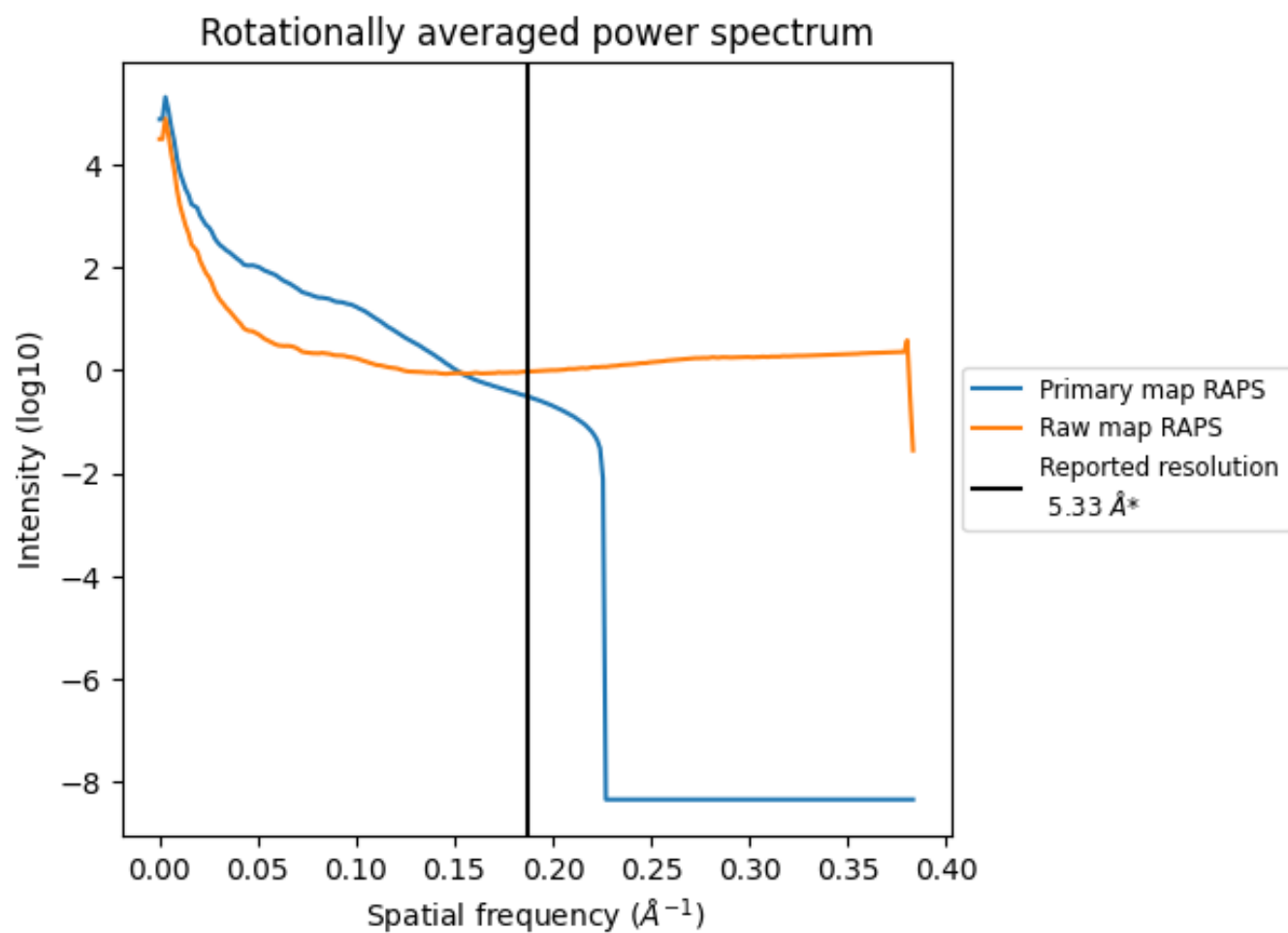
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2267 nm^3 ; this corresponds to an approximate mass of 2048 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 ⓘ

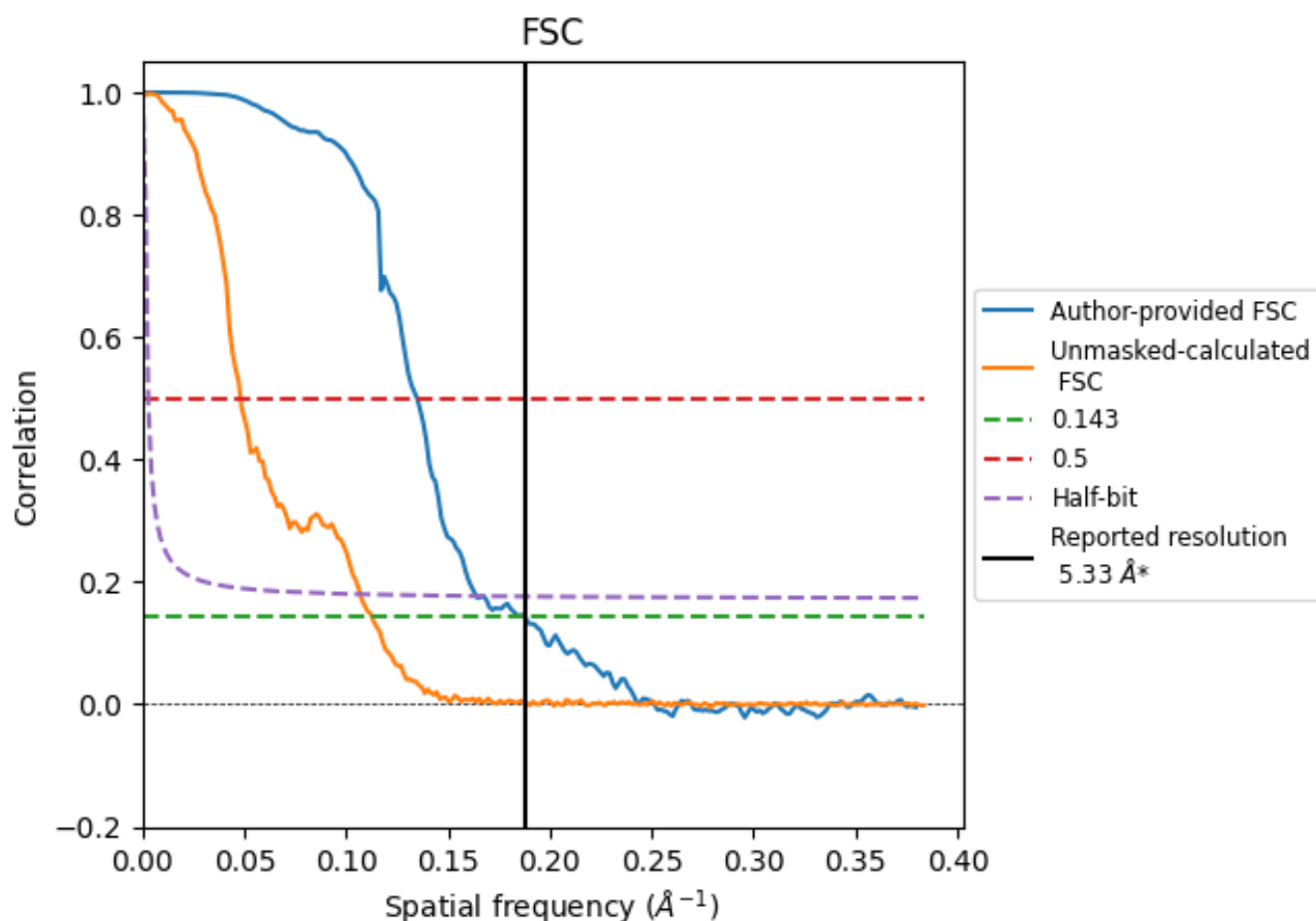


*Reported resolution corresponds to spatial frequency of 0.188 $\text{\AA}^{-1}$

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 0.188 Å⁻¹

8.2 Resolution estimates [i](#)

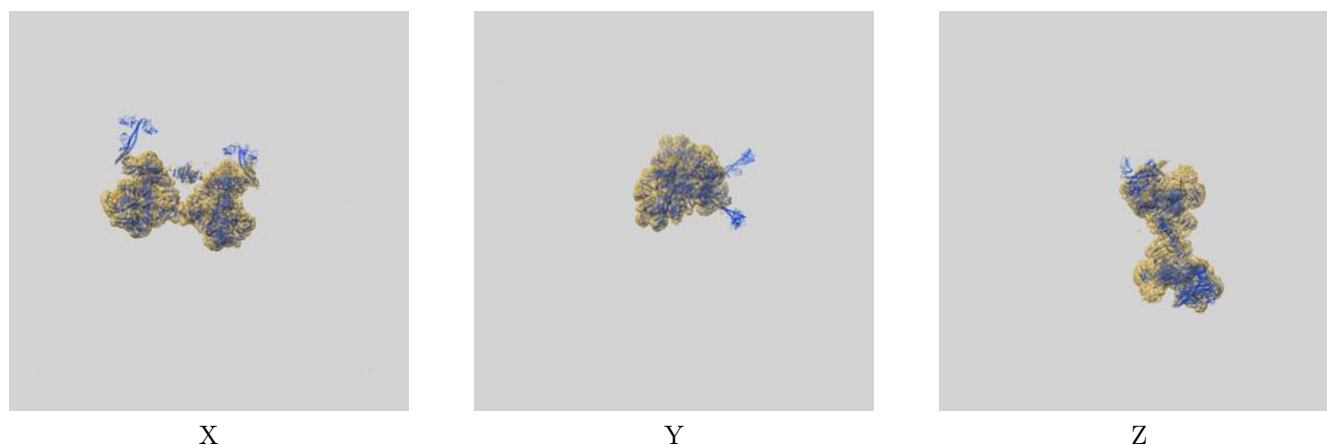
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.33	-	-
Author-provided FSC curve	5.33	7.42	6.10
Unmasked-calculated*	8.88	20.79	9.35

*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 8.88 differs from the reported value 5.33 by more than 10 %

9 Map-model fit [i](#)

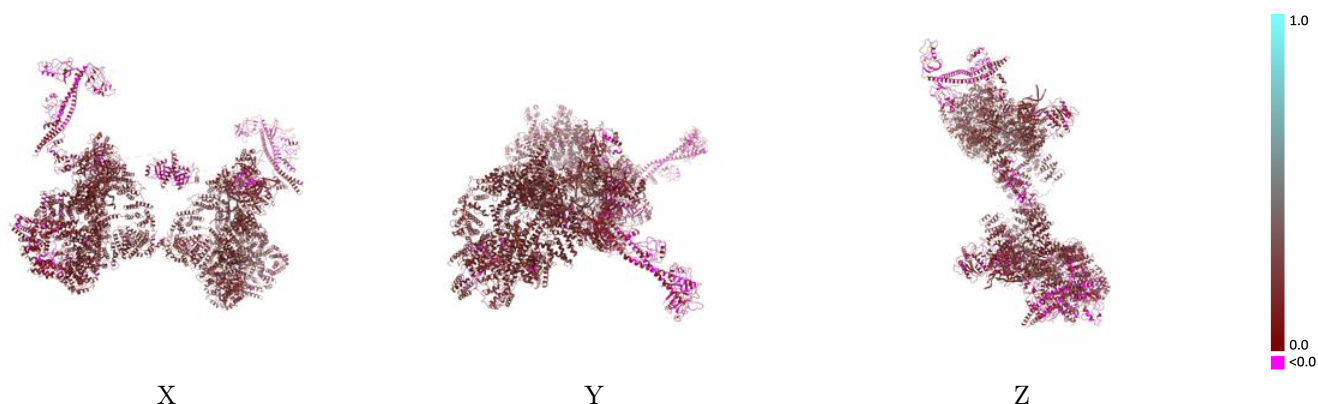
This section contains information regarding the fit between EMDB map EMD-16074 and PDB model 8BHY. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



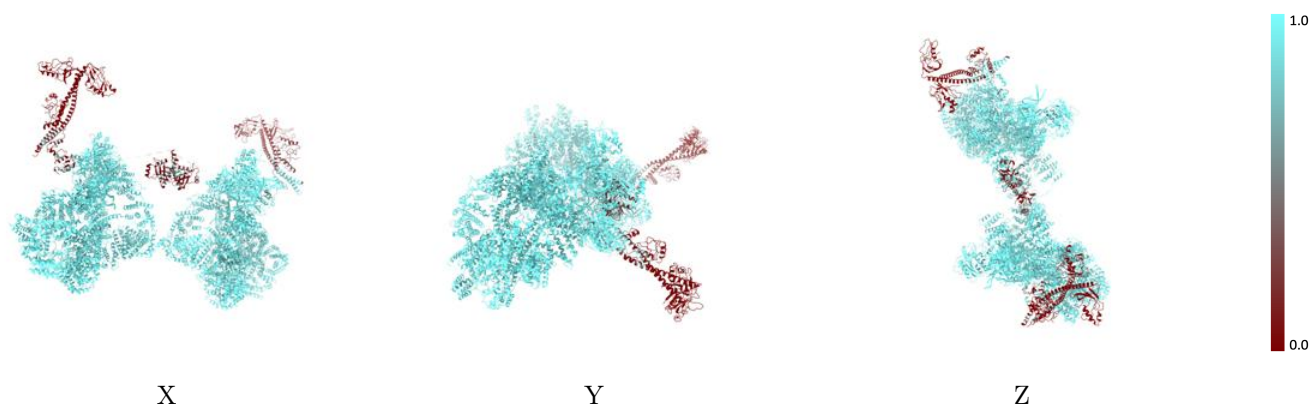
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



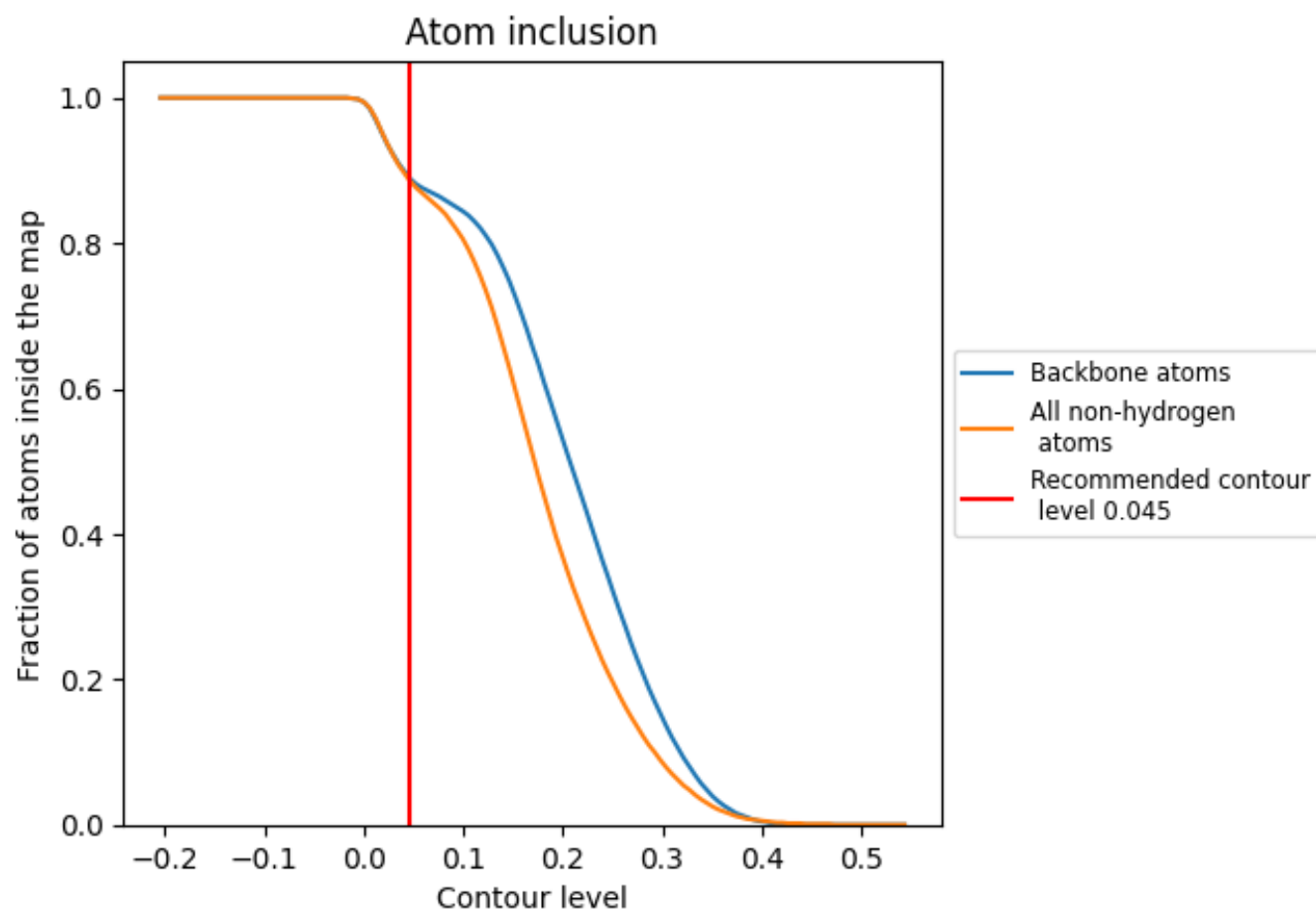
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 89% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.1660
A	 0.9940	 0.1980
B	 0.9970	 0.2050
C	 0.9930	 0.1680
D	 0.3220	 0.0840
G	 0.1640	 0.0630
H	 0.1830	 0.0900
I	 0.5710	 0.1120
L	 0.9970	 0.1310
M	 0.3140	 0.0980
P	 0.0650	 0.0810
Q	 0.0430	 0.0600
R	 0.1750	 0.0790
S	 0.9950	 0.1680
T	 0.9970	 0.1550
d	 1.0000	 0.2620
e	 1.0000	 0.2710
f	 0.9820	 0.0580
i	 1.0000	 0.2200
j	 1.0000	 0.2340
m	 1.0000	 0.0260

