



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:51 AM UTC

PDB ID : 8BOT / pdb_00008bot
EMDB ID : EMD-16145
Title : Cryo-EM structure of NHEJ supercomplex(trimer)
Authors : Hardwick, S.W.; Chaplin, A.K.
Deposited on : 2022-11-15
Resolution : 7.76 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

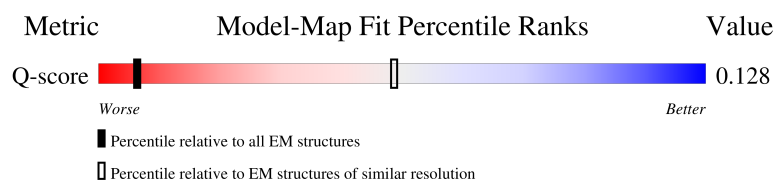
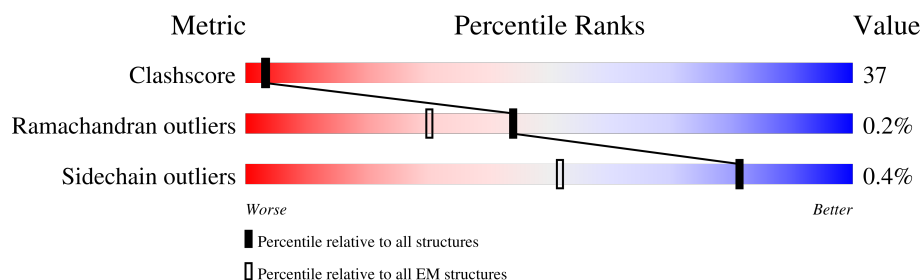
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.76 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.



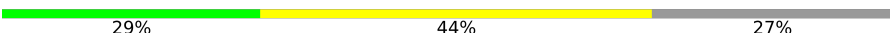
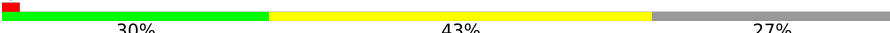
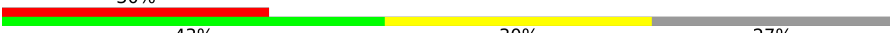
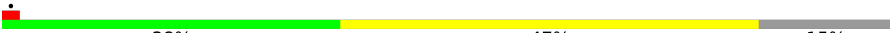
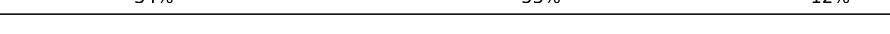
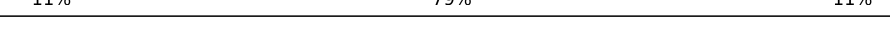
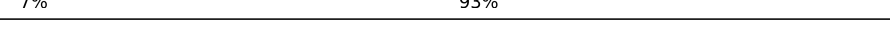
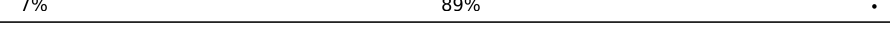
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	355 (7.28 - 8.25)

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	K	336	 27% 31% 40%
1	L	336	 21% 35% 42%
1	N	336	 25% 35% 40%
1	O	336	 28% 30% 42%

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Mol	Chain	Length	Quality of chain
2	M	911	
2	P	911	
3	Q	299	
3	R	299	
3	X	299	
3	Y	299	
4	A	4128	
4	F	4128	
4	S	4128	
5	B	609	
5	G	609	
5	T	609	
6	C	732	
6	H	732	
6	U	732	
7	I	28	
7	V	28	
8	J	27	
8	W	27	
9	D	24	
10	E	24	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 129197 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 repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	201	Total	C	N	O	S	0	0
			1618	1025	277	310	6		
1	L	195	Total	C	N	O	S	0	0
			1579	1001	271	301	6		
1	N	201	Total	C	N	O	S	0	0
			1625	1028	278	312	7		
1	O	195	Total	C	N	O	S	0	0
			1577	999	269	302	7		

- Molecule 2 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	258	Total	C	N	O	S	0	0
			2087	1327	353	394	13		
2	P	258	Total	C	N	O	S	0	0
			2091	1331	353	394	13		

- Molecule 3 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	218	Total	C	N	O	S	0	0
			1723	1099	290	319	15		
3	R	218	Total	C	N	O	S	0	0
			1739	1113	290	321	15		
3	X	218	Total	C	N	O	S	0	0
			1733	1108	290	320	15		
3	Y	218	Total	C	N	O	S	0	0
			1739	1113	290	321	15		

- Molecule 4 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	3535	Total	C	N	O	S	0	0
			27665	17763	4658	5065	179		
4	A	3528	Total	C	N	O	S	0	0
			27365	17573	4573	5050	169		
4	S	3536	Total	C	N	O	S	0	0
			27830	17880	4691	5078	181		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	489	Total	C	N	O	S	0	0
			3924	2515	667	724	18		
5	B	473	Total	C	N	O	S	0	0
			3646	2346	606	676	18		
5	T	470	Total	C	N	O	S	0	0
			3764	2404	644	698	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	642	Total	C	N	O	S	0	0
			5128	3285	860	958	25		
6	C	511	Total	C	N	O	S	0	0
			3968	2535	662	750	21		
6	U	642	Total	C	N	O	S	0	0
			5143	3292	864	962	25		

- Molecule 7 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	28	Total	C	N	O	P	0	0
			576	277	107	164	28		
7	V	28	Total	C	N	O	P	0	0
			576	277	107	164	28		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	27	Total	C	N	O	P	0	0
			557	269	94	167	27		
8	W	27	Total	C	N	O	P	0	0
			557	269	94	167	27		

- Molecule 9 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	24	Total 493	C 238	N 92	O 139	P 24	0	0

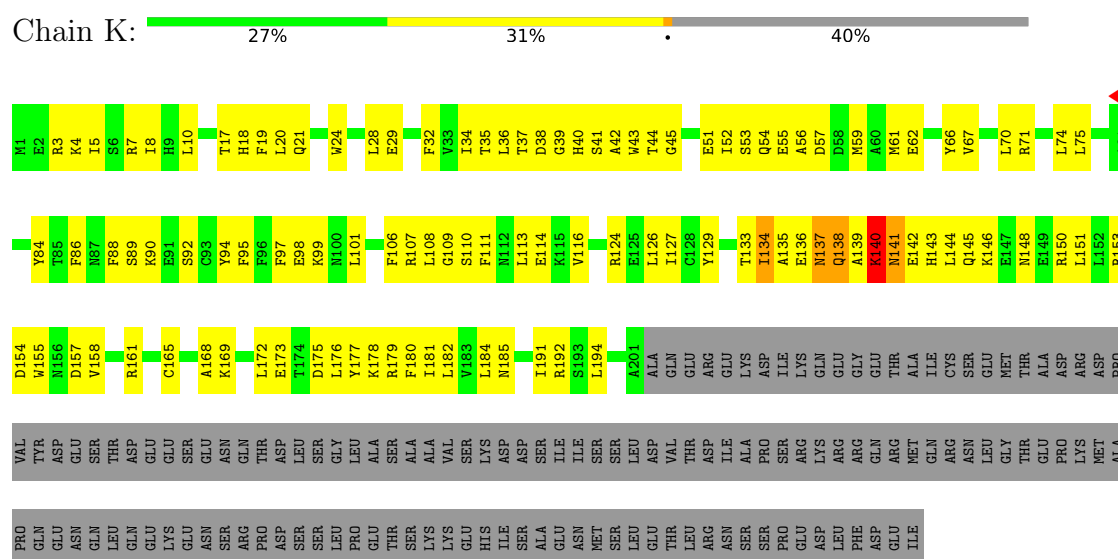
- Molecule 10 is a DNA chain called DNA (24-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	24	Total 494	C 240	N 81	O 149	P 24	0	0

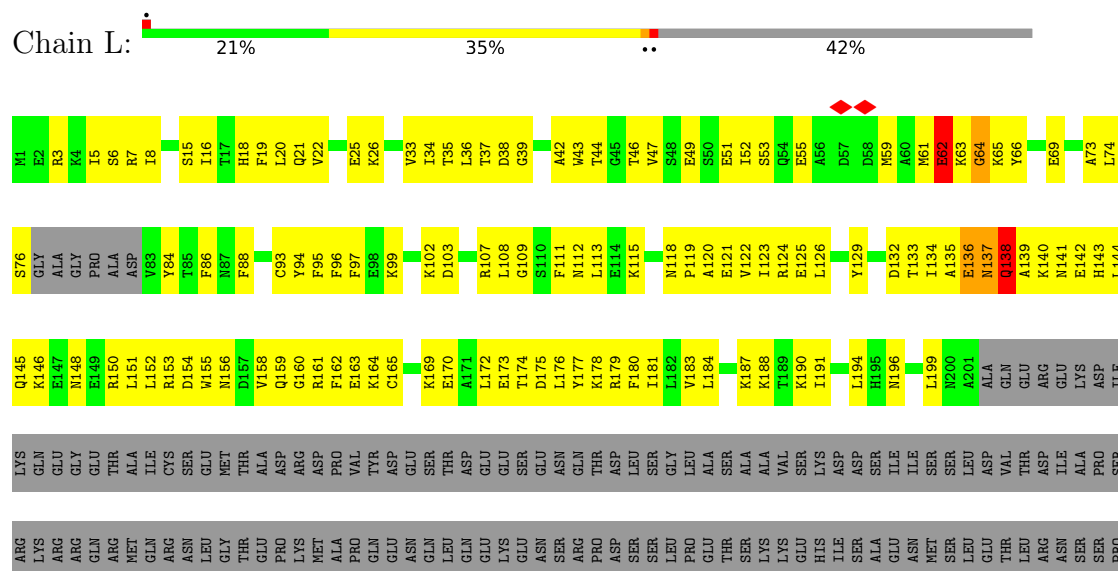
3 Residue-property plots

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.

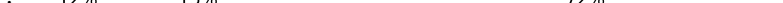
• Molecule 1: DNA repair protein XRCC4



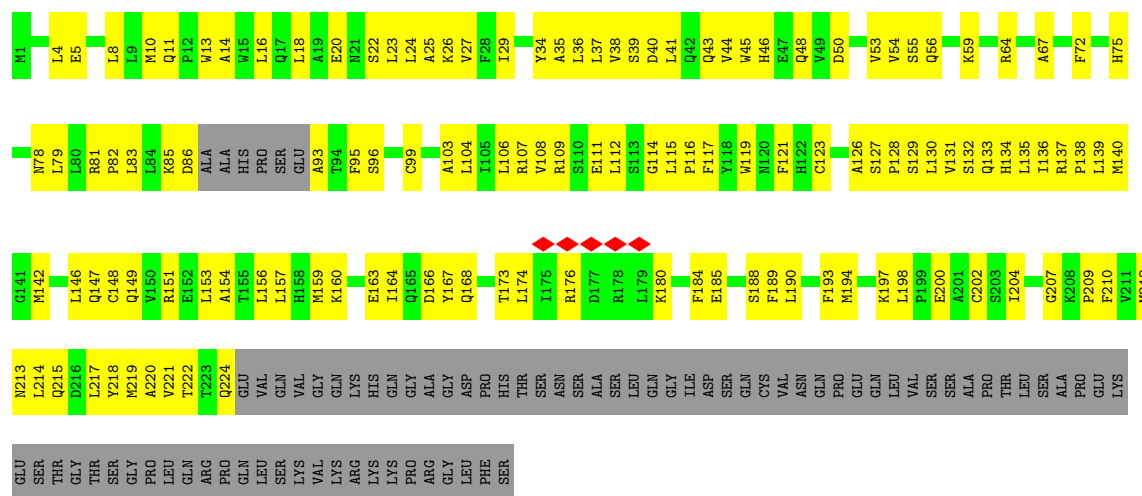
• Molecule 1: DNA repair protein XRCC4



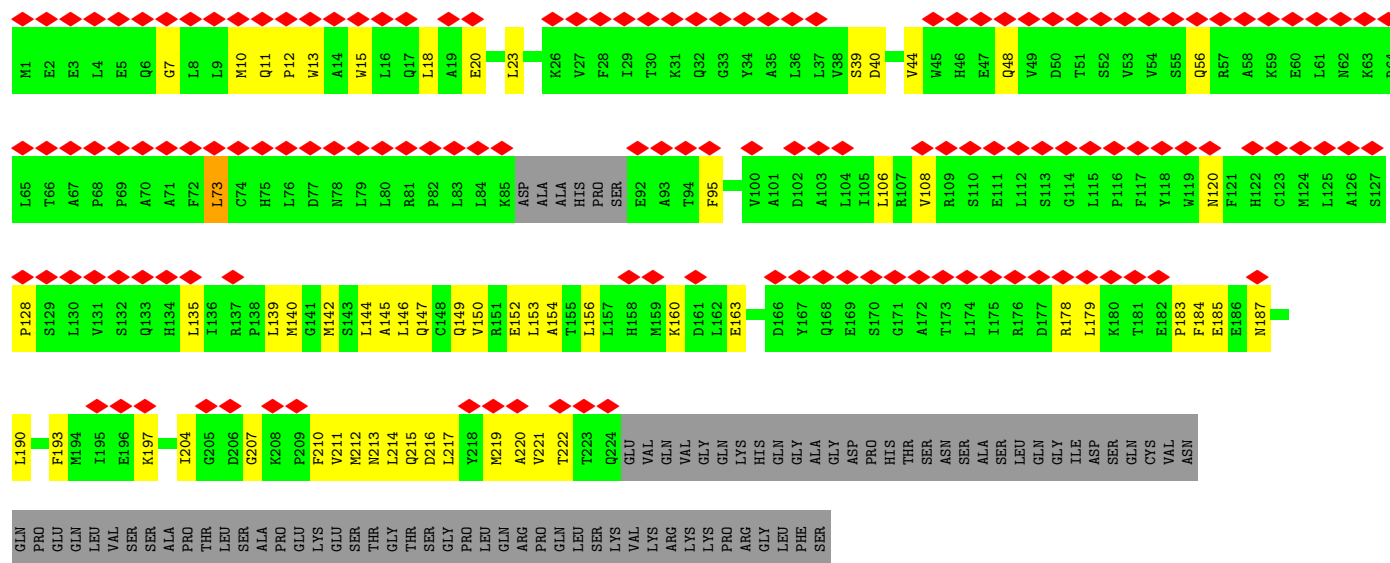
- Molecule 2: DNA ligase 4

Chain P:  12% 15% 72%

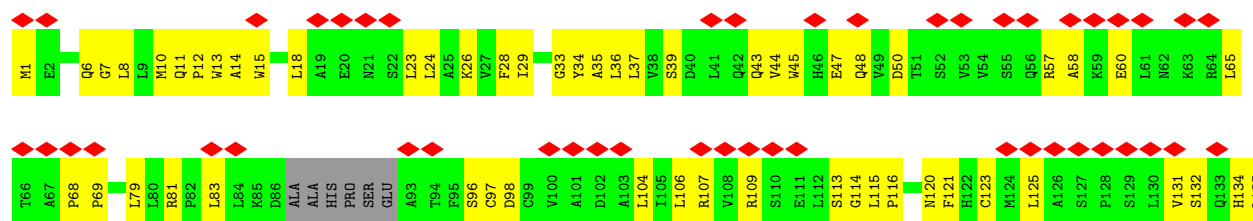
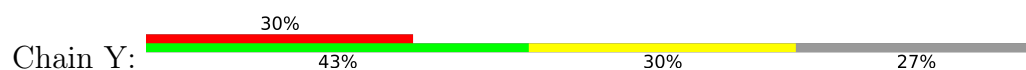
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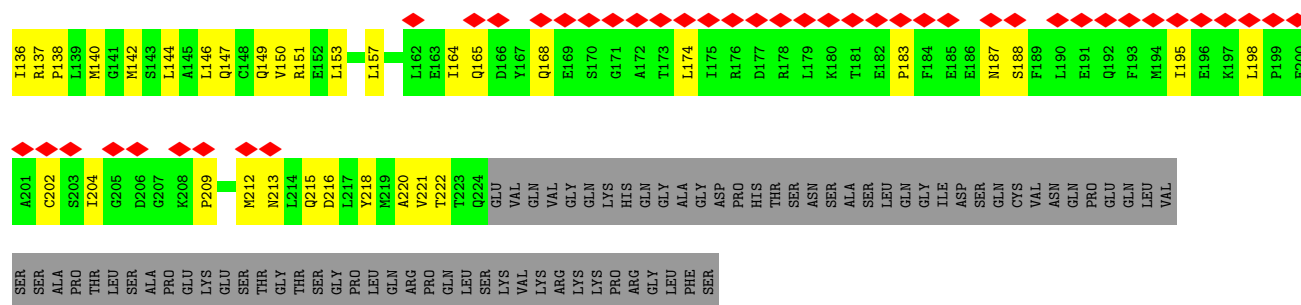


• Molecule 3: Non-homologous end-joining factor 1

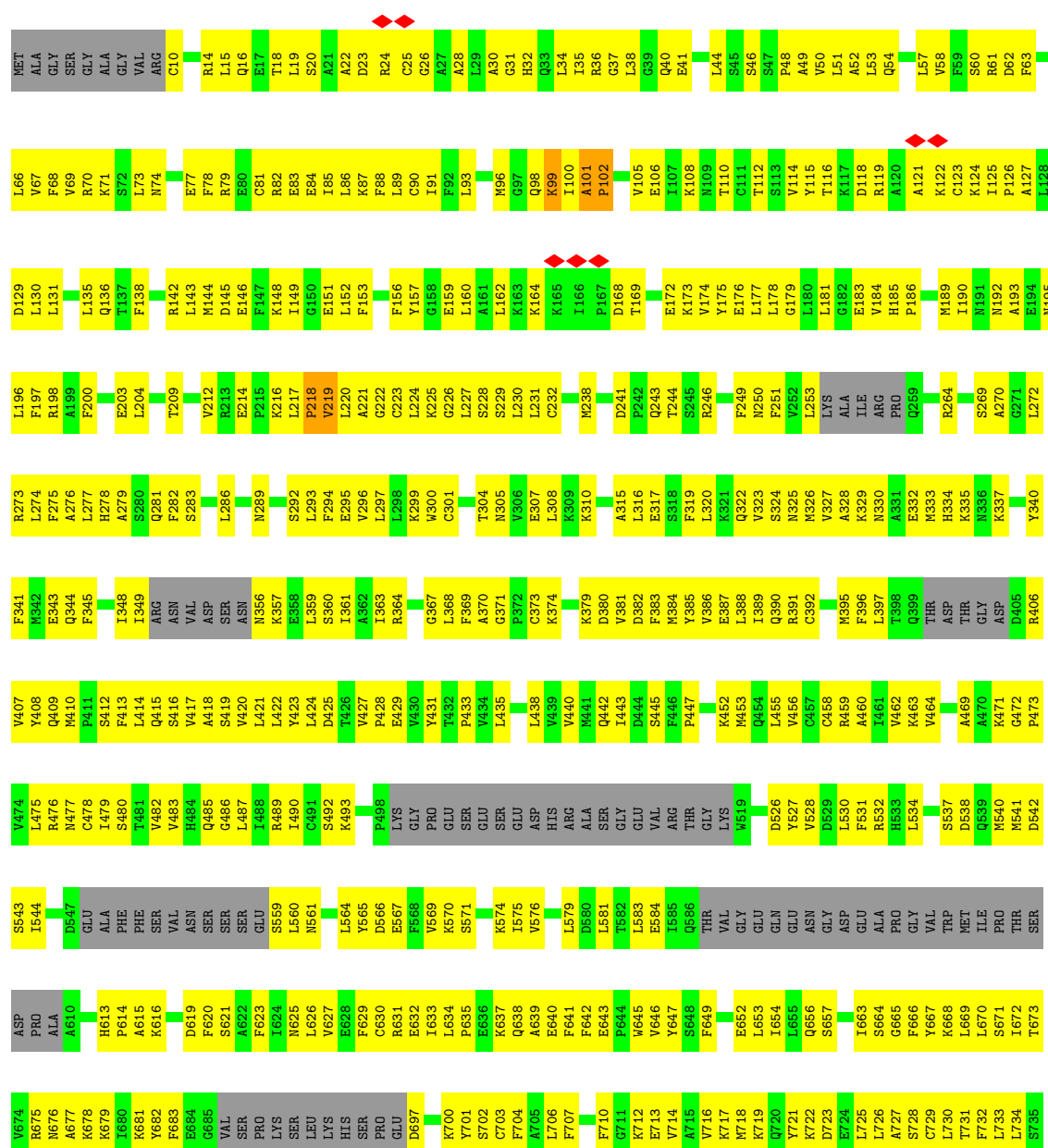


• Molecule 3: Non-homologous end-joining factor 1





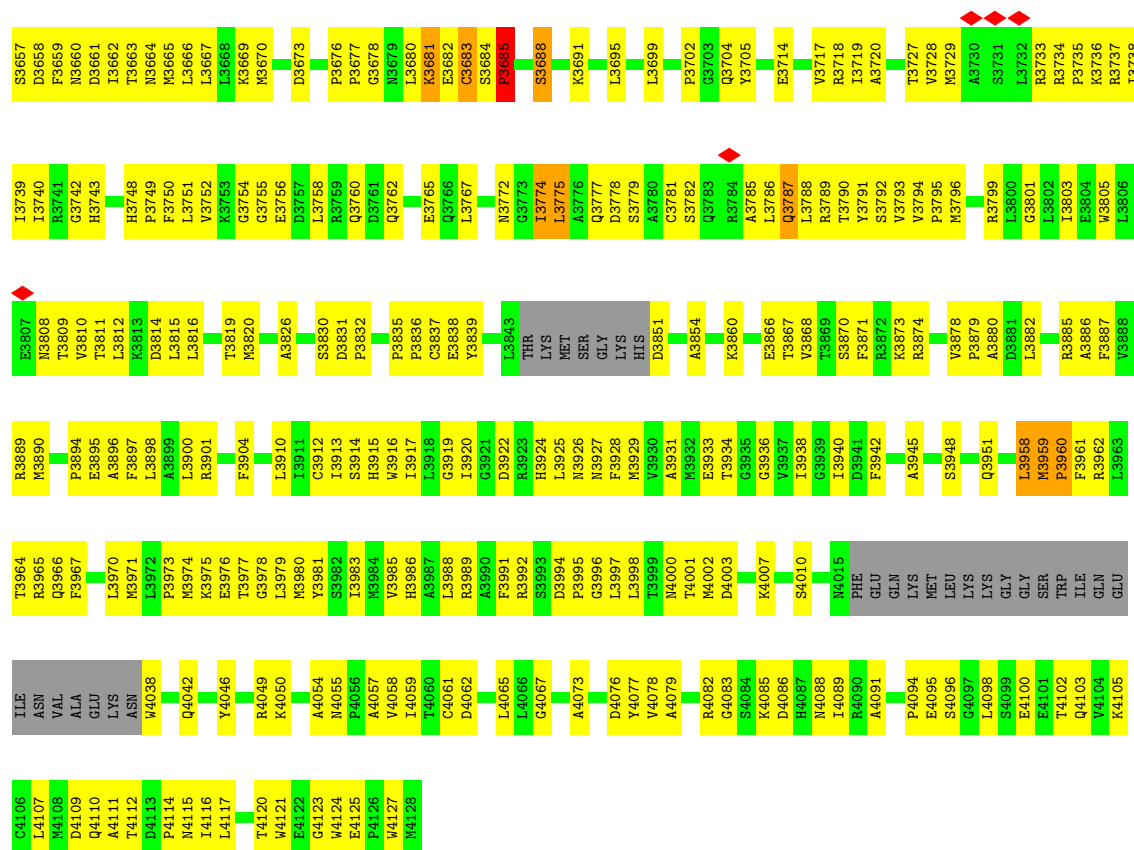
● Molecule 4: DNA-dependent protein kinase catalytic subunit



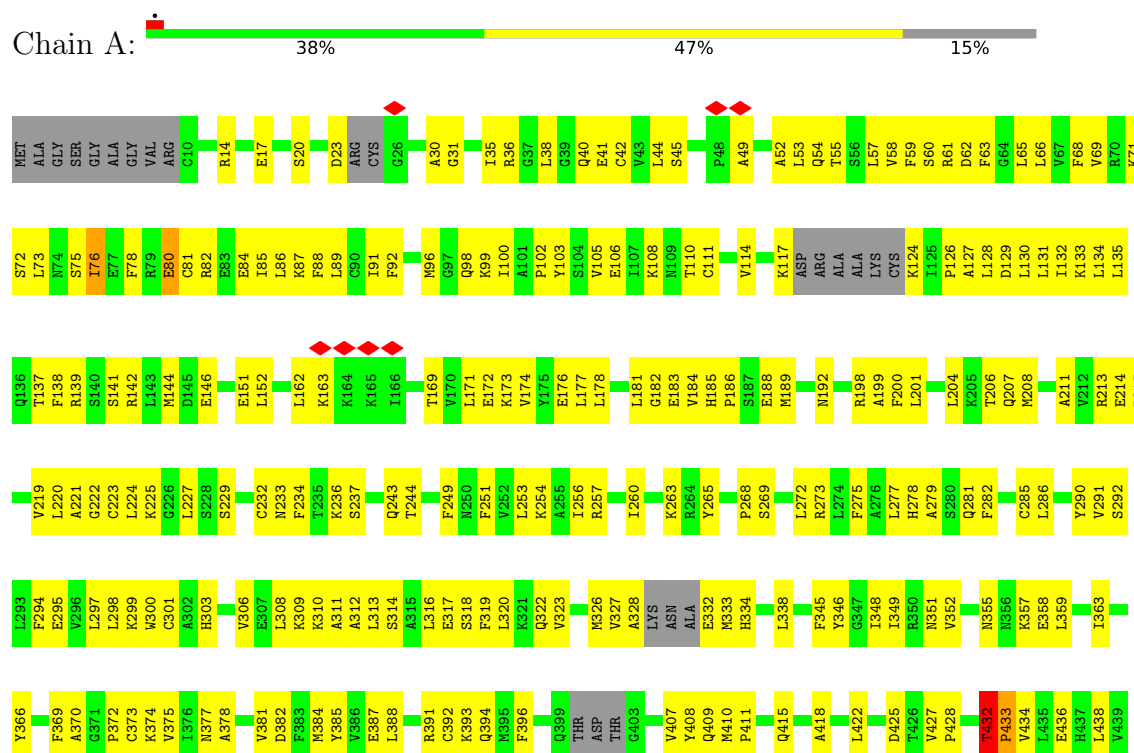








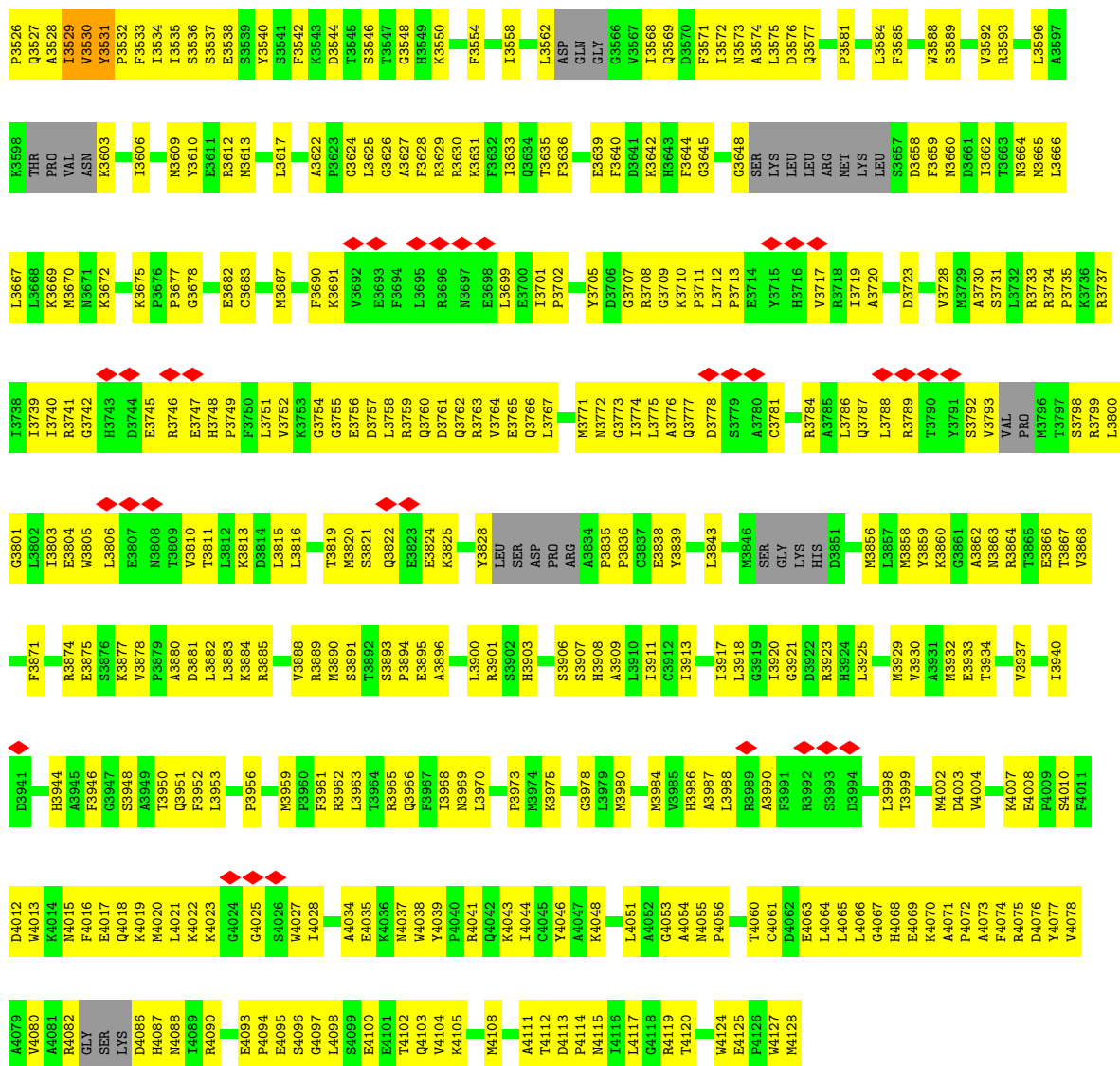
● Molecule 4: DNA-dependent protein kinase catalytic subunit



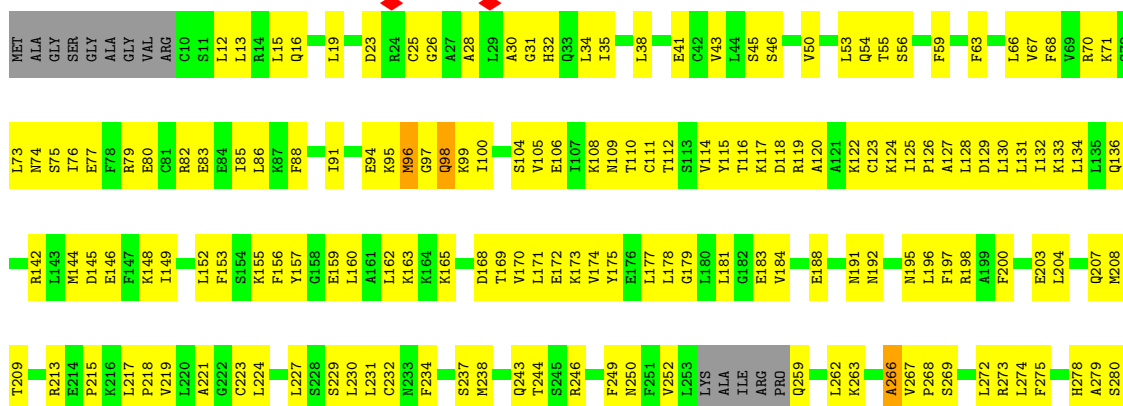
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K1361	Q1390	C1135	Y1064	L991	I866	S803	T731	Q656	THR	GLY	VAL	GLY	M441
D1362	V1391	R1136	S1065	L992	R867	A804	L733	R659	GLY	W519	F732	GLY	Q442
L1363	V1392	I1137	L1068	H993	R868	A804	L733	P661	GLU	K520	F732	GLY	I443
G1364	V1393	E1138	L1068	W994	R869	LEU	L734	L660	GLN	K520	F732	GLY	D444
G1365	V1394	E1139	L1068	W995	L870	SER	L735	P661	GLN	T523	F732	GLY	S445
T1366	V1395	K1140	P1070	N998	L871	GLU	L736	I663	ASN	T523	F732	GLY	F446
H1367	V1396	K1141	M1071	N999	T872	THR	P737	I663	ASN	Y524	F732	GLY	P451
L1368	V1397	H1142	A1072	K999	T873	LYS	I741	S664	GLY	K525	F732	GLY	K452
M1369	V1398	V1143	F1073	K1000	T874	ASN	Y745	G665	ASP	K526	F732	GLY	K452
R1370	V1399	S1144	F1074	F1001	S875	ASP	R746	F666	GLU	Y527	F732	GLY	L455
L1371	V1400	L1145	R1075	E1002	S876	TRP	R745	Y667	ALA	V528	F732	GLY	V456
A1302	V1401	N1146	L1076	F940	S877	GLU	A747	K668	P80	D529	F732	GLY	C457
M1303	V1402	K1147	G1077	L942	D877	VAL	V749	L670	VAL	L530	F732	GLY	C458
H1304	V1403	A1148	L1077	G943	E878	GLY	V749	S671	TRP	HE33	F732	GLY	C459
A1309	V1404	K1149	A1081	Q943	E879	SER	V749	I672	MET	L534	F732	GLY	R459
E1310	V1405	R1150	F1082	Q944	R879	ALA	L752	R675	ILE	L534	F732	GLY	K463
K1311	V1406	L1151	N1083	T946	R880	LEU	Q753	R676	P80	S537	F732	GLY	V464
CYS	V1407	R1152	N1084	GLN	R881	SER	M754	A677	THR	D538	F732	GLY	F465
PHE	V1408	L1153	I1085	PRO	Y882	ARG	A755	K678	S606	M541	F732	GLY	L466
GLY	V1409	R1155	I1087	GLY	Y883	ALA	A755	K679	D607	D542	F732	GLY	A469
THR	V1410	G1156	E1088	GLY	Y884	ALA	K757	F883	P808	S543	F732	GLY	A470
GLY	V1411	F1157	E1089	GLY	Y885	GLN	T763	P888	A610	I544	F732	GLY	P473
ALA	V1412	L1163	R1090	GLN	D887	LYS	P764	P888	B611	L545	F732	GLY	V474
ALA	V1413	L1164	E1091	GLY	R888	PHE	L765	P888	L612	L545	F732	GLY	L475
GLY	V1414	C1164	E1092	PRO	E889	ASN	A766	P888	LYS	A549	F732	GLY	A549
ASN	V1415	L1165	E1093	PRO	K890	LYS	E767	P888	LYS	PHE	F732	GLY	S480
THR	V1416	L1166	S1094	PRO	R891	VAL	V768	LEU	S621	SER	F732	GLY	T481
THR	V1417	L1168	S1095	PRO	L892	VAL	G769	LYS	A622	VAL	F732	GLY	V482
SER	V1418	L1169	V1096	PRO	S893	LYS	L770	HIS	F623	ASN	F732	GLY	V483
P1324	V1419	K1170	E1097	PRO	P894	LYS	L770	SER	I624	S555	F732	GLY	R489
Q1325	V1420	W1171	E1098	PRO	R895	HIS	L770	GLU	V627	S557	F732	GLY	I490
E1326	V1421	L1175	F1100	PRO	R896	LYS	A772	P698	E628	L560	F732	GLY	P494
G1327	V1422	C1176	V1099	PRO	R897	LYS	E774	P698	F629	N561	F732	GLY	V495
E1328	V1423	G1177	F1101	PRO	R898	LYS	E774	P698	C630	N561	F732	GLY	V496
R1329	V1424	L1178	E1102	PRO	R899	LYS	E774	P698	R631	N561	F732	GLY	L497
S1333	V1425	L1179	A1103	PRO	R900	LYS	E774	P698	E632	N561	F732	GLY	P498
K1334	V1426	L1180	L1104	PRO	R901	LYS	E774	P698	I633	N561	F732	GLY	LYS
C1335	V1427	Q1180	V1105	PRO	R902	LYS	E774	P698	L634	N561	F732	GLY	GLY
T1336	V1428	L1181	I1106	PRO	R903	LYS	E774	P698	K637	N561	F732	GLY	PRO
V1337	V1429	E1182	Y1107	PRO	R904	LYS	E774	P698	Q638	N561	F732	GLY	GLU
V1338	V1430	C1183	M1108	PRO	R905	LYS	E774	P698	A639	N561	F732	GLY	SER
V1339	V1431	R1184	E1109	PRO	R906	LYS	E774	P698	F642	N561	F732	GLY	SER
R1340	V1432	S1187	S1110	PRO	R907	LYS	E774	P698	E643	N561	F732	GLY	GLU
I1341	V1433	L1188	L1111	PRO	R908	LYS	E774	P698	P644	N561	F732	GLY	GLU
M1342	V1434	F1194	A1112	PRO	R909	LYS	E774	P698	W645	N561	F732	GLY	GLU
E1343	V1435	L1195	L1113	PRO	R910	LYS	E774	P698	V646	N561	F732	GLY	GLU
F1344	V1436	P1196	S1120	PRO	R911	LYS	E774	P698	F649	N561	F732	GLY	GLU
T1345	V1437	L1197	L1121	PRO	R912	LYS	E774	P698	K719	N561	F732	GLY	GLU
T1346	V1438	P1198	G1122	PRO	R913	LYS	E774	P698	Q720	N561	F732	GLY	GLU
L1347	V1439	L1199	T1123	PRO	R914	LYS	E774	P698	W645	N561	F732	GLY	GLU
T1348	V1440	G1200	L1124	PRO	R915	LYS	E774	P698	V646	N561	F732	GLY	GLU
L1421	V1441	Q1280	Q1125	PRO	R916	LYS	E774	P698	F649	N561	F732	GLY	GLU
K1422	V1442	V1281	Q1126	PRO	R917	LYS	E774	P698	K719	N561	F732	GLY	GLU
I1423	V1443	L1282	Q1126	PRO	R918	LYS	E774	P698	Q720	N561	F732	GLY	GLU
I1428	V1444	L1283	Q1126	PRO	R919	LYS	E774	P698	W645	N561	F732	GLY	GLU
L1431	V1445	T1284	Q1126	PRO	R920	LYS	E774	P698	V646	N561	F732	GLY	GLU
V1434	V1446	E1285	Q1126	PRO	R921	LYS	E774	P698	F649	N561	F732	GLY	GLU
Y1437	V1447	S1288	Q1126	PRO	R922	LYS	E774	P698	K719	N561	F732	GLY	GLU
G1438	V1448	L1208	Q1126	PRO	R923	LYS	E774	P698	Q720	N561	F732	GLY	GLU
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	V1452	L1208	Q1126	PRO	R927	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1453	L1208	Q1126	PRO	R928	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1454	L1208	Q1126	PRO	R929	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1455	L1208	Q1126	PRO	R930	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1456	L1208	Q1126	PRO	R931	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1457	L1208	Q1126	PRO	R932	LYS	E774	P698	K719	N561	F732	GLY	GLU
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	V1461	L1208	Q1126	PRO	R936	LYS	E774	P698	F649	N561	F732	GLY	GLU
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	V1464	L1208	Q1126	PRO	R939	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1465	L1208	Q1126	PRO	R940	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1466	L1208	Q1126	PRO	R941	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1467	L1208	Q1126	PRO	R942	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1468	L1208	Q1126	PRO	R943	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1469	L1208	Q1126	PRO	R944	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1470	L1208	Q1126	PRO	R945	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1471	L1208	Q1126	PRO	R946	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1472	L1208	Q1126	PRO	R947	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1473	L1208	Q1126	PRO	R948	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1474	L1208	Q1126	PRO	R949	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1475	L1208	Q1126	PRO	R950	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1476	L1208	Q1126	PRO	R951	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1477	L1208	Q1126	PRO	R952	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1478	L1208	Q1126	PRO	R953	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1479	L1208	Q1126	PRO	R954	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1480	L1208	Q1126	PRO	R955	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1481	L1208	Q1126	PRO	R956	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1482	L1208	Q1126	PRO	R957	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1483	L1208	Q1126	PRO	R958	LYS	E774	P698	Q720	N561	F732	GLY	GLU
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	V1485	L1208	Q1126	PRO	R960	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1486	L1208	Q1126	PRO	R961	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1487	L1208	Q1126	PRO	R962	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1488	L1208	Q1126	PRO	R963	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1489	L1208	Q1126	PRO	R964	LYS	E774	P698	W645	N561	F732	GLY	GLU
	V1490	L1208	Q1126	PRO	R965	LYS	E774	P698	V646	N561	F732	GLY	GLU
	V1491	L1208	Q1126	PRO	R966	LYS	E774	P698	F649	N561	F732	GLY	GLU
	V1492	L1208	Q1126	PRO	R967	LYS	E774	P698	K719	N561	F732	GLY	GLU
	V1493	L1208	Q1126	PRO	R968	LYS	E774	P698	Q720	N561	F732	GLY	GLU
	V1494	L1208	Q1126	PRO	R969	LYS	E774	P698	W645	N561	F732		



S3458	S3459	S3460	S3461	S3462	S3463	S3464	S3465	S3466	S3467	S3468	S3469	S3470	S3471	S3472	S3473	S3474	S3475	S3478	S3479	S3480	S3481	S3482	S3483	S3484	S3485	S3486	S3487	S3490	S3491	S3492	S3493	S3494	S3495	S3496	S3497	S3498	S3499	S3500	S3501	S3502	S3503	S3504	S3505	S3508	S3511	S3512	S3515	S3518	S3519	S3520	S3524	S3525											
A3381	F3382	Q3383	H3384	L3385	V3389	E3394	GLU	ALA	GLN	PRO	PRO	SER	TRP	SER	CYS	GLY	PRO	ALA	ALA	G3408	V3409	Y3413	K3414	T3415	L3416	A3417	D3418	F3419	C3420	L3421	Q3422	R3425	E3429	ASN	ALA	SER	VAL	ILE	ASP	SER	ALA	GLU	L3439	L3445	V3446	V3447	E3448	K3449	K3450	L3454	K3455												
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H3081	Y3082	S3083	L3086	S3087	L3088	L3089	Y3090	L3091	L3092	Q3093	R3098	A3099	K3100	Y3101	Y3102	I3103	Q3104	N3105	G3106	I3107	Q3108	M3111	G3112	N3113	S3124	K3128	V3132	Q3133	A3134	L3135	E3137	I3138	F3141	I3142	S3143	S3146	K3147	N3150	L3151	S3152	S3153	Q3154	V3155	P3156	L3157	K3158	L3159	L3160	L3161														
A2997	D3000	N3003	H3004	S3010	Y3013	C3014	S3015	S3018	I3019	P3024	L3027	W3031	P3034	Y3035	F3036	Q3037	E3038	T3039	Y3040	L3041	M3044	I3045	R3046	K3050	Q3054	GLY	GLU	ALA	ASP	Q3059	S3060	L3061	I3065	D3066	M3069	H3070	G3071	E3072	L3073	A3076	I3077	L3078	E3079	L3080																			
D2919	V2920	L2921	R2922	Y2923	Y2924	E2925	L2926	A2927	K2928	L2929	Y2930	R2931	S2932	L2933	G2934	E2935	Y2936	D2937	Y2938	L2939	R2940	G2941	I2942	F2943	T2944	Q2945	E2946	I2947	Q2948	E2967	A2968	K2969	Q2970	Q2971	L2976	Y2977	K2978	Q2979	D2980	V2981	E2985	P2986	K2991	D2992	F2993	L2994	E2995	L2996															
F2848	L2763	Q2784	L2785	K2786	H2787	S2788	S2789	D2860	I2861	S2862	H2865	A2866	L2868	S2870	L2871	D2872	A2873	A2875	C2880	L2884	Q2885	Q2886	P2887	V2888	G2889	L2890	R2891	L2892	L2893	E2894	E2895	A2896	L2897	L2898	R2899	LEU	PRO	ALA	LEU	PRO	ALA	LYS	ARG	VAL	F2840	G2841	R2842	F2843	L2844	N2845	T2846	T2847											
D2762	L2763	Q2784	L2785	K2786	H2787	S2788	S2789	D2860	I2861	S2862	H2865	A2866	L2868	S2870	L2871	D2872	A2873	A2875	C2880	L2884	Q2885	Q2886	P2887	V2888	G2889	L2890	R2891	L2892	L2893	E2894	E2895	A2896	L2897	L2898	R2899	LEU	PRO	ALA	LEU	PRO	ALA	LYS	ARG	VAL	R2773	S2774	Y2775	R2776	R2777	G2778	L2779	L2780	P2781										
ARG	THR	ASP	LEU	ARG	LEU	LEU	ARG	ARG	ARG	ARG	MET	ASP	GLN	ASP	LYS	LEU	LEU	ALA	TYR	ALA	ARG	ARG	GLY	VAL	ALA	GLN	TRP	PRO	ALA	LYS	ARG	LEU	GLU	LEU	LEU	MET	LYS	ASP	PHE	GLN	GLN	ASP	VAL	R2773	S2774	Y2775	R2776	R2777	G2778	L2779	L2780	P2781											
LEU	THR	PRO	MET	PHE	VAL	GLU	THR	THR	GLN	ALA	SER	SER	THR	LEU	THR	ARG	THR	ALA	GLN	GLY	LEU	SER	ALA	ARG	GLY	LEU	GLN	TRP	PRO	ALA	LYS	ARG	LEU	GLY	LEU	LEU	LYS	ASP	PHE	GLN	GLN	ASP	VAL	R2773	S2774	Y2775	R2776	R2777	G2778	L2779	L2780	P2781											



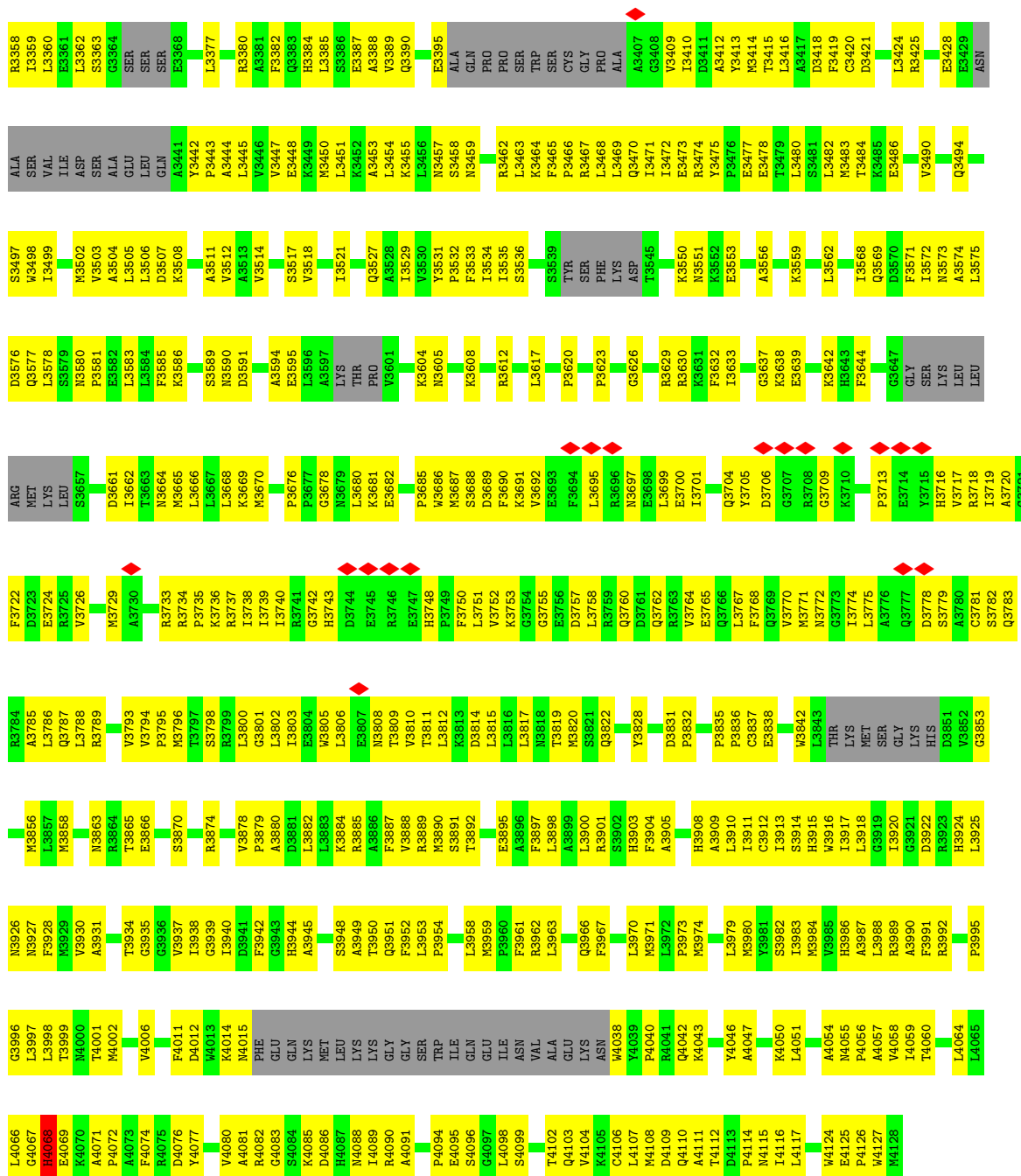
• Molecule 4: DNA-dependent protein kinase catalytic subunit





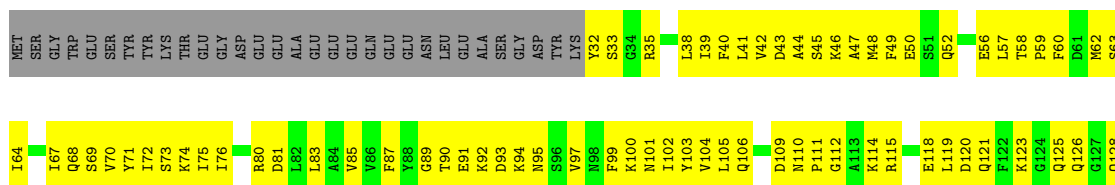
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Q2300	L2235	A2172	R2106	ASP	L1850	R1787	A1719	V1645	E1565	S1486	A1405	V1339
Q2301	E2236	A2173	L1851	LEU	L1852	G1789	A1720	L1646	I1566	Y1487	L1406	R1340
L2302	E2175	S2174	GLY	LEU	SER	P1723	P1723	A1647	I1567	Y1488	K1407	I1341
L2303	E2176	S2175	PRO	ARG	ARG	M1724	M1724	L1648	I1568	N1489	M1408	M1342
V2304	N2176	N2176	PRO	ARG	PHE	Q1726	Q1726	L1649	T1569	G1490	P1409	E1343
N2305	ASN	ASN	GLN	ARG	THR	Q1795	Q1795	A1650	E1570	I1491	P1410	F1344
N2306	GLY	GLY	GLN	THR	LEU	G1796	G1796	K1651	A1492	PRO	Y1411	F1345
G2179	G2179	GLY	GLY	LEU	LEU	L1797	L1797	L1652	GLY	ASP	K1412	T1346
H2183	GLY	PHE	GLY	ASN	ASN	L1798	L1798	Q1654	ASP	GLY	D1413	T1347
H2184	VAL	VAL	VAL	VAL	GLU	E1799	E1799	L1655	GLU	ARG	I1414	L1348
M2185	SER	SER	SER	SER	SER	S1800	P1731	D1656	E1577	LEU	L1415	L1349
V2186	VAL	VAL	VAL	VAL	THR	L1862	G1732	L1657	N1574	ARG	H1418	N1350
V2187	PRO	PRO	PRO	PRO	THR	Y1801	G1732	L1658	N1575	GLN	L1419	T1351
E2188	SER	SER	SER	SER	ASP	Y1802	T1733	L1659	D1576	ARG	L1419	T1351
E2189	GLN	GLN	GLN	GLN	ASP	L1803	T1733	L1660	E1578	CYS	R1420	W1356
R2190	VAL	VAL	VAL	VAL	ASP	M1804	P1734	N1662	V1579	LEU	R1420	K1357
A2191	MET	MET	MET	MET	LEU	R1805	R1735	H1665	E1581	PRO	T1423	L1358
P2123	GLU	GLU	GLU	GLU	L1866	R1806	F1736	F1668	Q1583	S1562	L1424	L1359
S2124	ARG	ARG	ARG	ARG	L1868	L1867	N1737	F1671	Q1584	D1504	A1425	K1360
W2125	ALA	ALA	ALA	ALA	K1869	ASP	M1743	F1672	S1585	C1507	L1431	D1362
M2126	LYS	LYS	LYS	LYS	ASP	ASP	F1746	T1673	V1587	L1436	L1363	L1363
K2127	TYR	TYR	TYR	TYR	M1871	PRO	D1747	L1676	L1588	A1511	L1437	N1365
K2132	ILE	ILE	ILE	ILE	G1872	LEU	D1748	I1677	S1594	S1512	L1437	N1366
L2133	GLU	GLU	GLU	GLU	Y1873	LEU	A1749	L1679	L1597	G1513	D1440	H1367
G2134	ARG	ARG	ARG	ARG	Y1874	PHE	E1751	L1679	L1597	L1514	L1441	L1368
N2135	ARG	ARG	ARG	ARG	L1876	L1815	E1751	L1679	L1597	L1515	Q1442	M1369
V2138	GLY	GLY	GLY	GLY	L1877	Q1817	S1753	K1683	L1601	E1516	V1443	R1370
P2139	ALA	ALA	ALA	ALA	D1878	S1818	Q1754	L1684	D1602	F1519	D1444	V1371
L2140	ARG	ARG	ARG	ARG	Y1879	F1819	S1755	D1685	Q1603	R1527	R1445	L1372
N2141	GLU	GLU	GLU	GLU	M1880	S1819	S1756	L1686	S1604	L1528	V1452	L1376
P2207	ALA	ALA	ALA	ALA	S1881	D1820	M1757	H1687	F1605	V1529	S1483	C1377
D2208	ALA	ALA	ALA	ALA	R1882	R1821	L1758	L1688	R1606	L1530	A1484	E1378
E2209	ASN	ASN	ASN	ASN	L1884	S1823	L1758	F1689	E1607	L1531	C1455	P1379
GLY	GLY	GLY	GLY	GLY	P1885	L1824	L1761	V1693	Q1611	L1538	G1383	G1383
ASP	ASP	ASP	ASP	ASP	LYS	L1825	M1762	L1696	K1612	L1539	L1384	N1385
ASP	ASP	ASP	ASP	ASP	ASP	T1826	T1763	L1697	H1613	T1540	H1459	N1386
GLY	GLY	GLY	GLY	GLY	VAL	L1827	E1764	P1697	Q1614	ALA	R1460	I1386
PRO	PRO	PRO	PRO	PRO	HIS	Y1829	V1765	F1698	G1615	SER	L1463	V1389
SER	SER	SER	SER	SER	ALA	H1830	L1766	F1699	L1616	LEU	L1467	Q1390
TYR	TYR	TYR	TYR	TYR	LYS	C1831	Q1767	THR	A1619	GLY	I1468	V1391
PHE	PHE	PHE	PHE	PHE	GLU	S1832	R1768	SER	Q1622	GLY	Q1471	M1392
LEU	LEU	LEU	LEU	LEU	LYS	L1833	E1769	THR	H1625	SER	H1394	A1393
ASN	ASN	ASN	ASN	ASN	ILE	L1836	Q1770	THR	W1626	V1550	D1474	L1395
VAL	VAL	VAL	VAL	VAL	ASN	R1837	H1771	GLY	K1627	I1551	P1396	P1396
LEU	LEU	LEU	LEU	LEU	GLN	E1838	V1772	GLY	Q1624	GLY	L1475	V1397
TYR	TYR	TYR	TYR	TYR	GLN	R1837	M1773	SER	H1632	H1552	H1476	C1399
ALA	ALA	ALA	ALA	ALA	VAL	F1839	E1775	L1707	W1632	GLY	H1477	V1399
ASP	ASP	ASP	ASP	ASP	PHE	F1840	F1778	E1708	K1628	I1550	D1474	C1399
SER	SER	SER	SER	SER	HIS	S1841	V1773	L1710	W1632	H1552	L1475	C1399
THR	THR	THR	THR	THR	GLY	T1842	Q1769	R1711	W1632	H1552	H1477	V1399
LEU	LEU	LEU	LEU	LEU	GLY	T1843	S1780	R1711	W1632	H1552	H1477	V1399
ILE	ILE	ILE	ILE	ILE	CYS	V1844	S1781	R1711	W1632	H1552	H1477	V1399
THR	THR	THR	THR	THR	GLY	V1845	F1782	L1714	K1635	Y1558	G1480	N1401
GLU	GLU	GLU	GLU	GLU	THR	V1846	F1783	E1715	D1636	F1559	T1481	L1402
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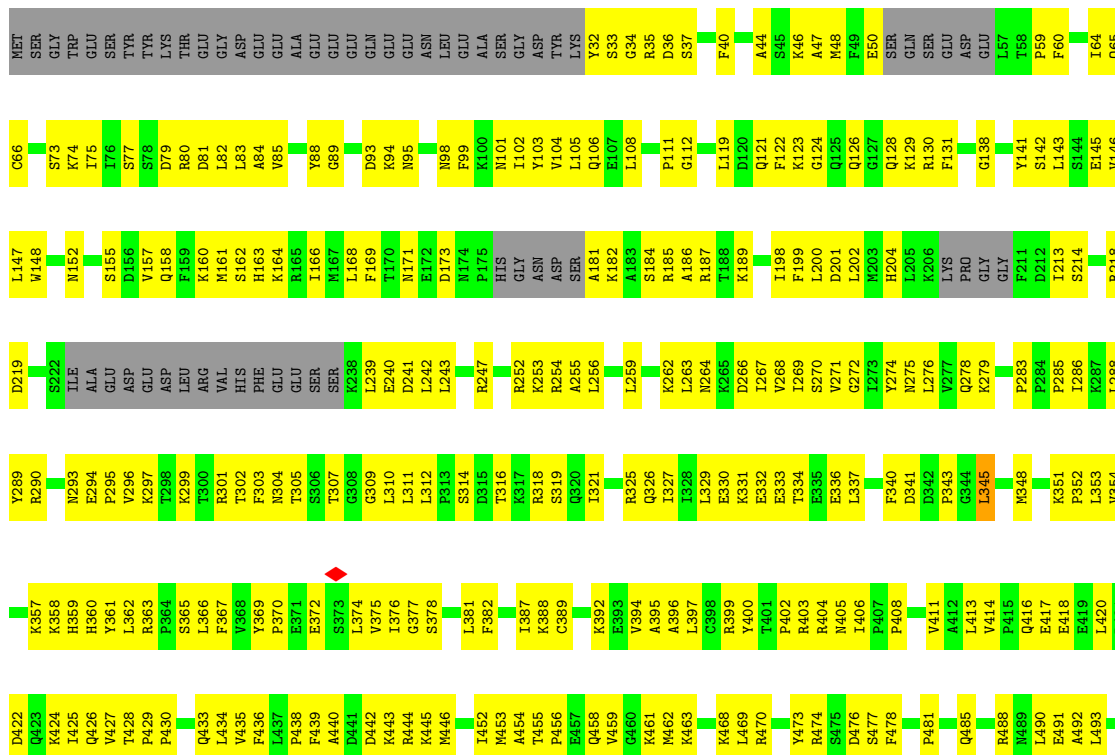


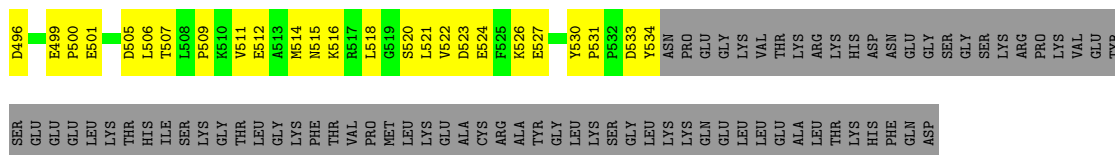


● Molecule 5: X-ray repair cross-complementing protein 6

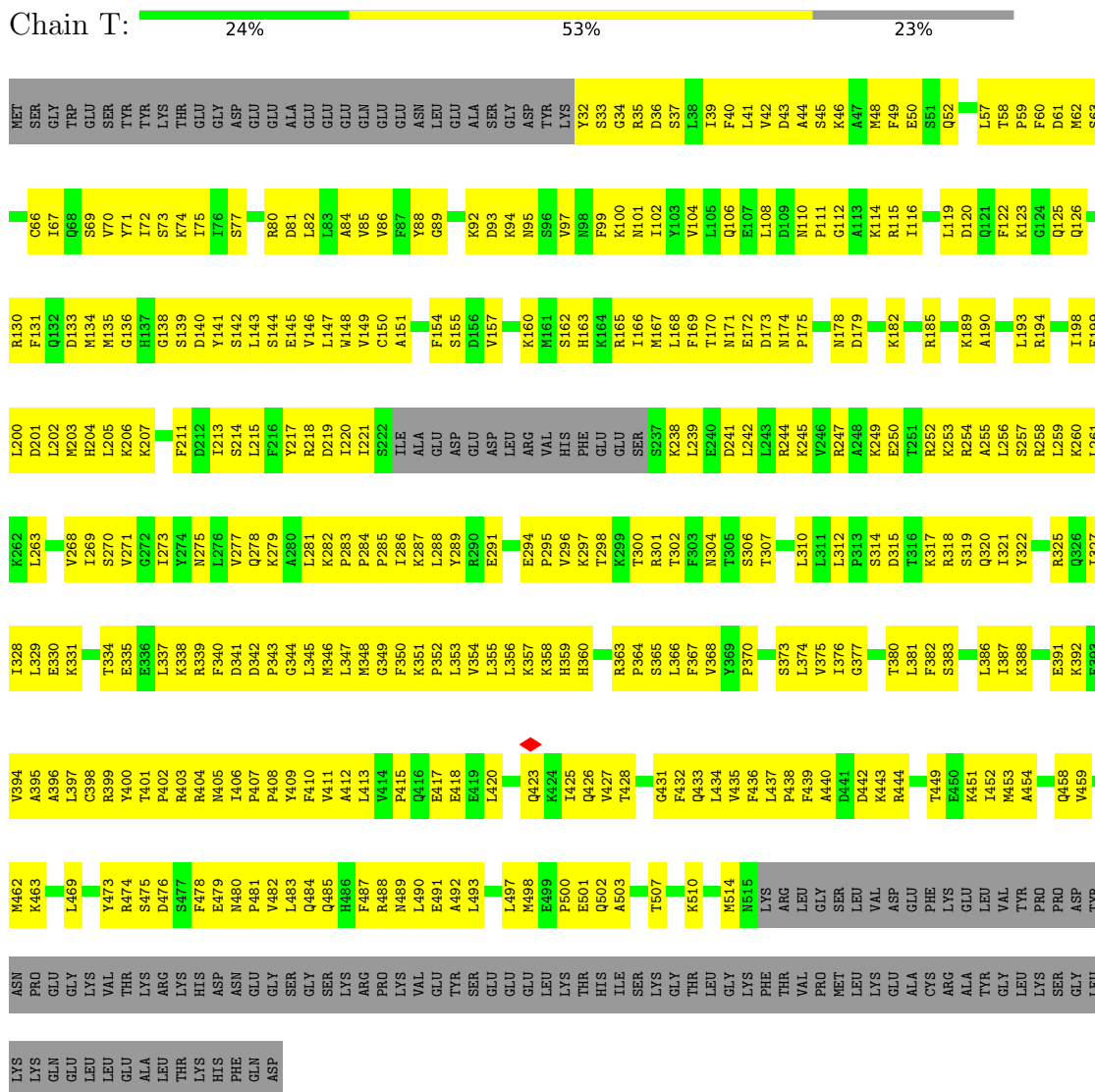
Chain G: 26% 54% 20%



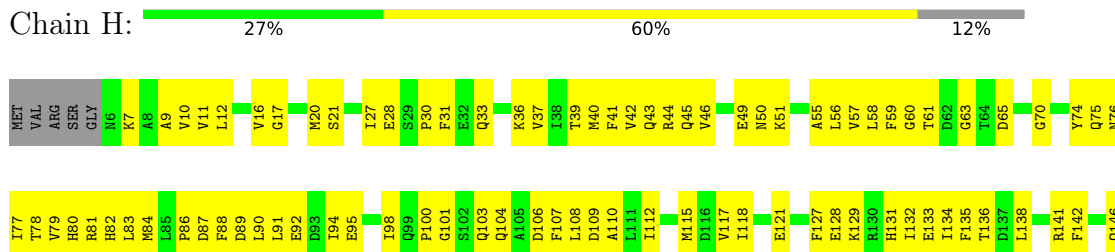


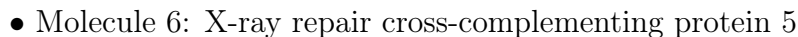


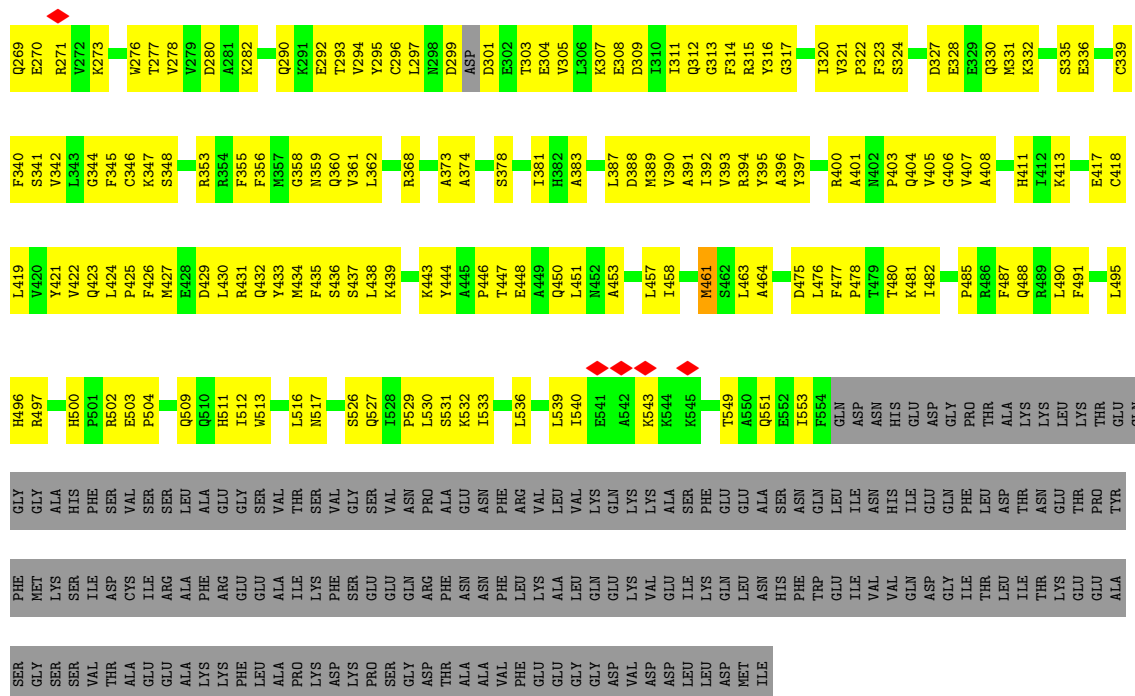
• Molecule 5: X-ray repair cross-complementing protein 6



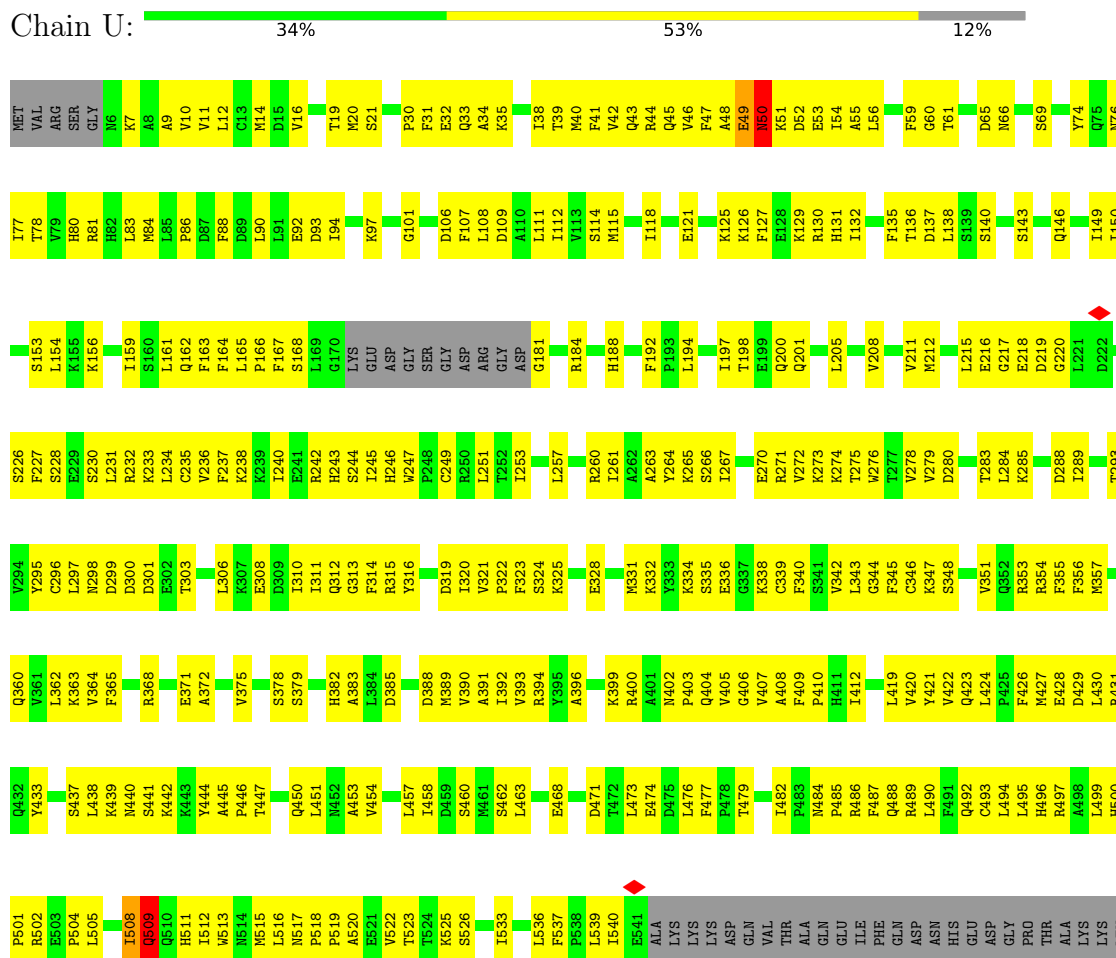
• Molecule 6: X-ray repair cross-complementing protein 5

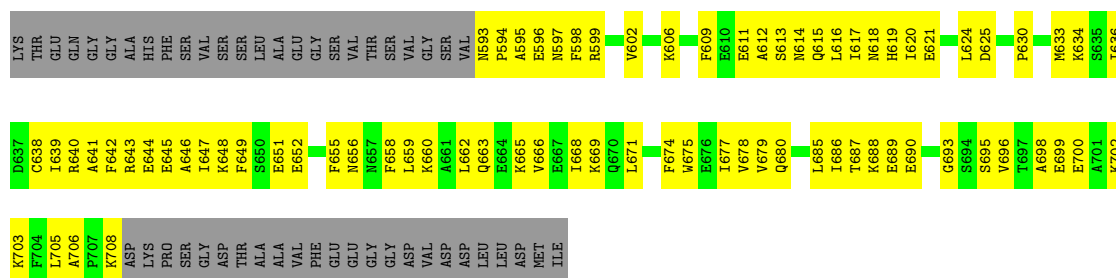




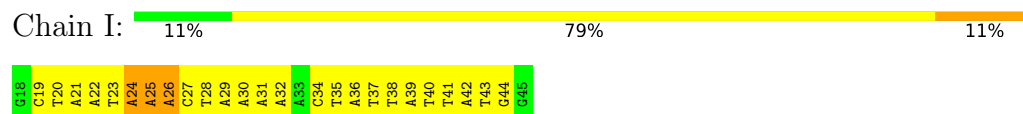


• Molecule 6: X-ray repair cross-complementing protein 5

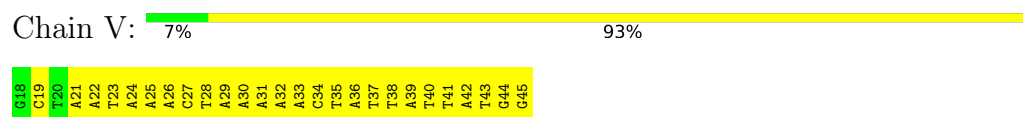




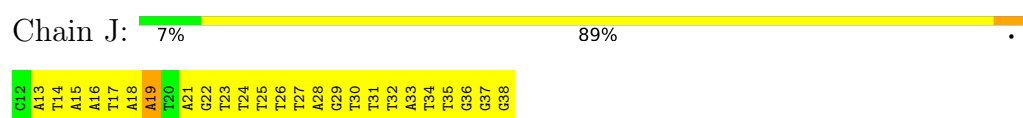
- Molecule 7: DNA (28-MER)



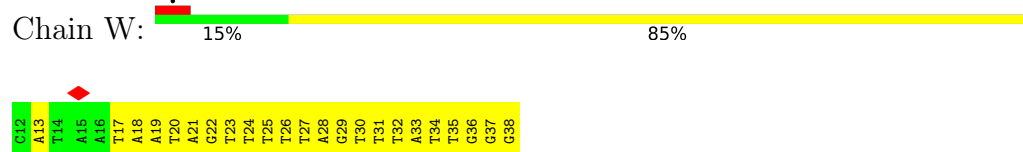
- Molecule 7: DNA (28-MER)



- Molecule 8: DNA (27-MER)



- Molecule 8: DNA (27-MER)



- Molecule 9: DNA (24-MER)



- Molecule 10: DNA (24-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9114	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 ($e^-/\text{\AA}^2$)	46.8	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	0.338	Depositor
Minimum map value	-0.177	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.066	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	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	K	0.27	0/1647	0.52	3/2215 (0.1%)
1	L	0.29	0/1605	0.52	1/2155 (0.0%)
1	N	0.20	0/1654	0.41	0/2224
1	O	0.19	0/1603	0.42	0/2154
2	M	0.13	0/2135	0.34	0/2883
2	P	0.24	0/2140	0.41	0/2890
3	Q	0.16	0/1755	0.42	0/2377
3	R	0.15	0/1773	0.36	0/2402
3	X	0.24	0/1766	0.40	0/2392
3	Y	0.11	0/1773	0.34	0/2402
4	A	0.18	0/27902	0.41	4/37795 (0.0%)
4	F	0.26	0/28192	0.52	15/38135 (0.0%)
4	S	0.19	0/28373	0.44	7/38372 (0.0%)
5	B	0.20	0/3712	0.43	1/5018 (0.0%)
5	G	0.21	0/4000	0.44	0/5388
5	T	0.17	0/3833	0.43	0/5160
6	C	0.18	0/4039	0.39	1/5457 (0.0%)
6	H	0.19	0/5232	0.43	0/7057
6	U	0.18	0/5246	0.46	1/7075 (0.0%)
7	I	0.43	0/647	0.72	3/996 (0.3%)
7	V	0.21	0/647	0.44	0/996
8	J	0.31	0/623	0.58	1/961 (0.1%)
8	W	0.26	0/623	0.55	0/961
9	D	0.27	0/554	0.48	0/852
10	E	0.23	0/552	0.47	0/851
All	All	0.21	0/132026	0.45	37/179168 (0.0%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3577	GLN	N-CA-C	-11.42	99.17	113.55
4	F	1142	HIS	N-CA-C	-8.92	102.12	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	219	VAL	N-CA-C	-8.34	104.57	112.83
1	K	140	LYS	N-CA-C	-8.33	103.28	113.19
4	S	956	PRO	N-CA-CB	7.75	110.60	103.08

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	K	1618	0	1597	160	0
1	L	1579	0	1564	149	0
1	N	1625	0	1611	130	0
1	O	1577	0	1557	112	0
2	M	2087	0	2036	196	0
2	P	2091	0	2042	170	0
3	Q	1723	0	1733	163	0
3	R	1739	0	1754	168	0
3	X	1733	0	1749	61	0
3	Y	1739	0	1754	83	0
4	A	27365	0	26865	1779	0
4	F	27665	0	27584	2231	0
4	S	27830	0	27817	1981	0
5	B	3646	0	3608	314	0
5	G	3924	0	3997	419	0
5	T	3764	0	3852	422	0
6	C	3968	0	3876	306	0
6	H	5128	0	5128	513	0
6	U	5143	0	5166	496	0
7	I	576	0	318	69	0
7	V	576	0	318	66	0
8	J	557	0	311	59	0
8	W	557	0	311	66	0
9	D	493	0	273	46	0
10	E	494	0	278	33	0
All	All	129197	0	127099	9393	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 37.

The worst 5 of 9393 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)
4:S:1082:PHE:HB3	4:S:1129:ASP:H	1.09	1.09
4:S:1077:GLY:HA2	4:S:1124:ILE:HA	1.36	1.05
4:F:3574:ALA:H	4:F:3685:PRO:HD3	1.21	1.02
4:F:728:SER:O	4:F:732:PHE:HB2	1.61	1.00
4:F:175:TYR:HB2	4:F:221:ALA:HA	1.44	0.99

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	K	199/336 (59%)	178 (89%)	19 (10%)	2 (1%)	12	49
1	L	191/336 (57%)	169 (88%)	19 (10%)	3 (2%)	7	38
1	N	199/336 (59%)	179 (90%)	20 (10%)	0	100	100
1	O	191/336 (57%)	171 (90%)	20 (10%)	0	100	100
2	M	256/911 (28%)	234 (91%)	22 (9%)	0	100	100
2	P	256/911 (28%)	233 (91%)	22 (9%)	1 (0%)	30	67
3	Q	214/299 (72%)	191 (89%)	23 (11%)	0	100	100
3	R	214/299 (72%)	196 (92%)	18 (8%)	0	100	100
3	X	214/299 (72%)	190 (89%)	24 (11%)	0	100	100
3	Y	214/299 (72%)	198 (92%)	16 (8%)	0	100	100
4	A	3448/4128 (84%)	3149 (91%)	294 (8%)	5 (0%)	48	83
4	F	3463/4128 (84%)	3030 (88%)	419 (12%)	14 (0%)	30	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S	3464/4128 (84%)	3094 (89%)	361 (10%)	9 (0%)	36	72
5	B	463/609 (76%)	403 (87%)	59 (13%)	1 (0%)	43	78
5	G	485/609 (80%)	436 (90%)	49 (10%)	0	100	100
5	T	466/609 (76%)	412 (88%)	54 (12%)	0	100	100
6	C	499/732 (68%)	443 (89%)	54 (11%)	2 (0%)	30	67
6	H	636/732 (87%)	549 (86%)	87 (14%)	0	100	100
6	U	636/732 (87%)	552 (87%)	82 (13%)	2 (0%)	36	72
All	All	15708/20769 (76%)	14007 (89%)	1662 (11%)	39 (0%)	44	78

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	138	GLN
4	F	218	PRO
4	F	955	ALA
4	F	956	PRO
4	F	2291	GLN

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	K	176/303 (58%)	175 (99%)	1 (1%)	78	83
1	L	173/303 (57%)	168 (97%)	5 (3%)	37	58
1	N	179/303 (59%)	176 (98%)	3 (2%)	53	69
1	O	173/303 (57%)	173 (100%)	0	100	100
2	M	232/808 (29%)	232 (100%)	0	100	100
2	P	233/808 (29%)	229 (98%)	4 (2%)	53	69
3	Q	191/262 (73%)	191 (100%)	0	100	100
3	R	194/262 (74%)	194 (100%)	0	100	100
3	X	193/262 (74%)	191 (99%)	2 (1%)	68	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Y	194/262 (74%)	194 (100%)	0	100	100
4	A	2916/3671 (79%)	2911 (100%)	5 (0%)	87	87
4	F	2987/3671 (81%)	2964 (99%)	23 (1%)	73	80
4	S	3020/3671 (82%)	3009 (100%)	11 (0%)	84	84
5	B	387/548 (71%)	386 (100%)	1 (0%)	86	86
5	G	436/548 (80%)	435 (100%)	1 (0%)	87	87
5	T	422/548 (77%)	422 (100%)	0	100	100
6	C	426/649 (66%)	426 (100%)	0	100	100
6	H	567/649 (87%)	566 (100%)	1 (0%)	87	87
6	U	573/649 (88%)	570 (100%)	3 (0%)	81	83
All	All	13672/18480 (74%)	13612 (100%)	60 (0%)	81	84

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	3685	PRO
6	U	50	ASN
4	F	3959	MET
4	S	4068	HIS
3	X	73	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 194 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	3177	ASN
4	S	1201	ASN
4	A	3339	ASN
5	B	152	ASN
4	S	1614	GLN

5.3.3 RNA ⓘ

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.

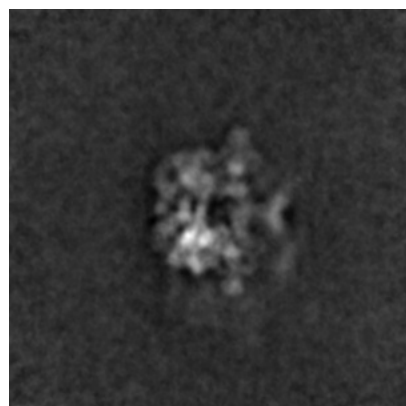
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16145. These allow visual inspection of the internal detail of the map and identification of artifacts.

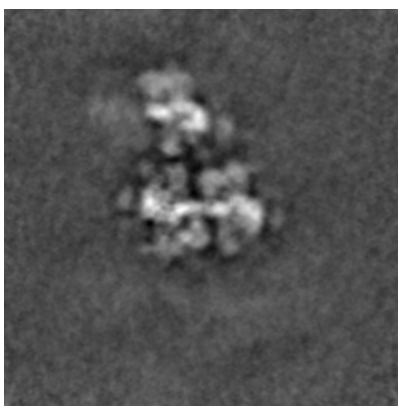
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

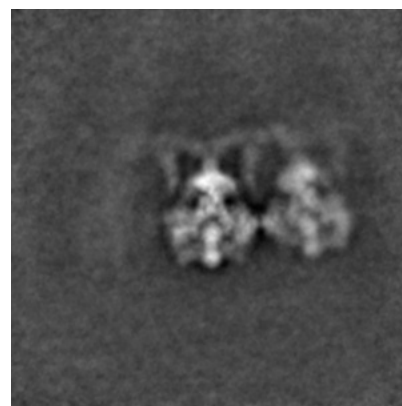
6.1.1 Primary map



X

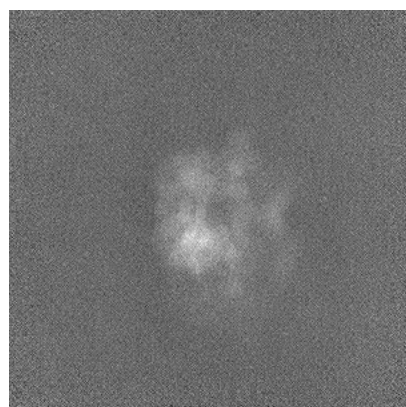


Y

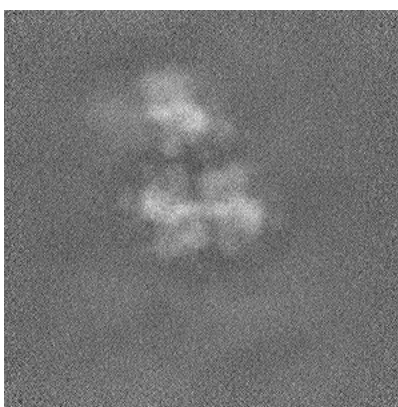


Z

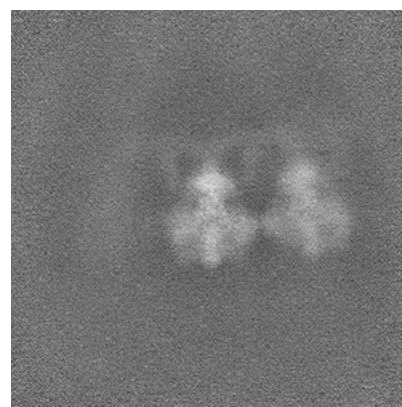
6.1.2 Raw map



X



Y

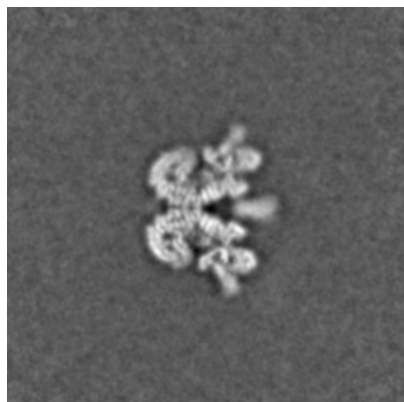


Z

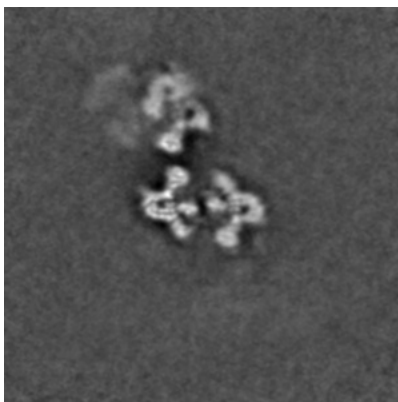
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

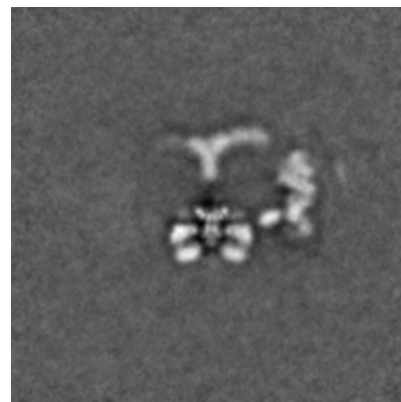
6.2.1 Primary map



X Index: 270

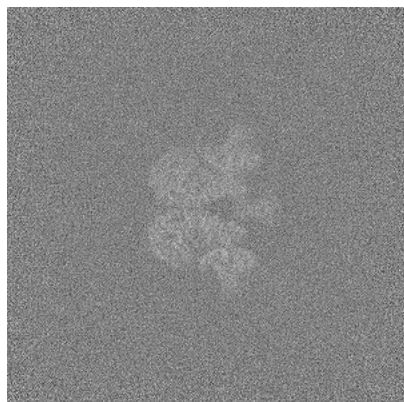


Y Index: 270

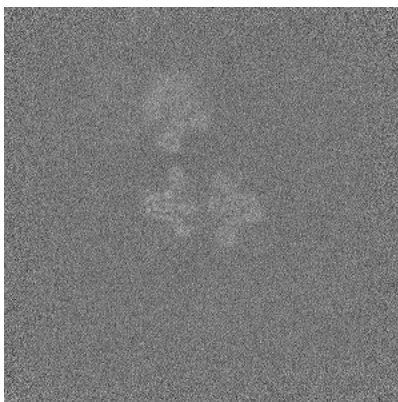


Z Index: 270

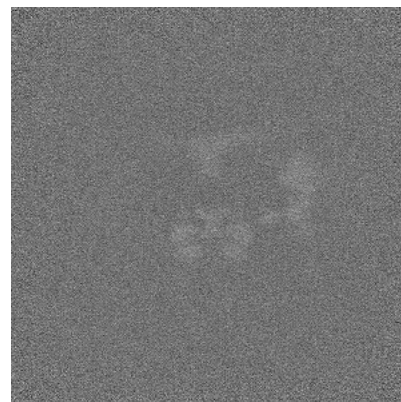
6.2.2 Raw map



X Index: 270



Y Index: 270

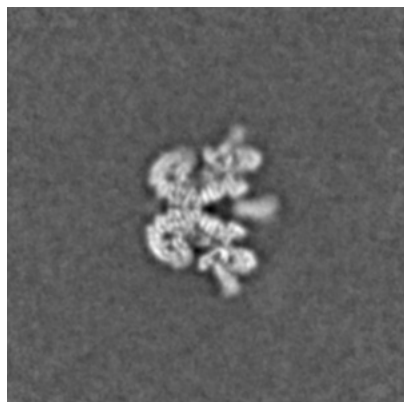


Z Index: 270

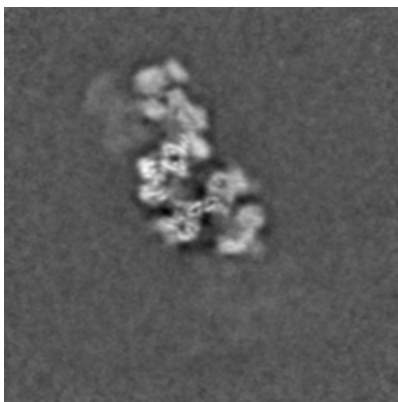
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

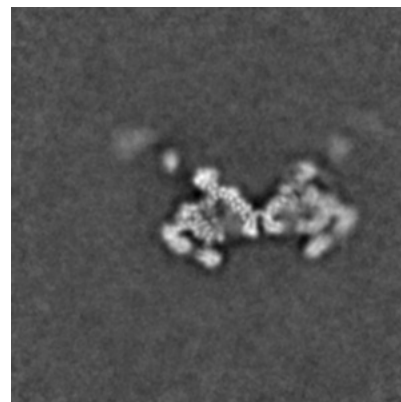
6.3.1 Primary map



X Index: 271

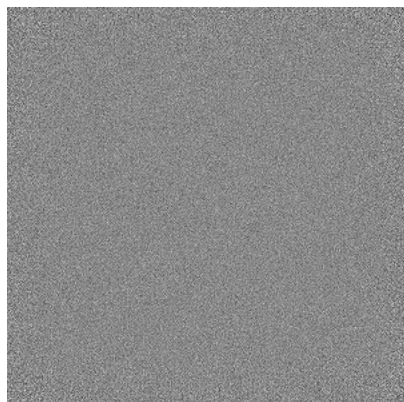


Y Index: 251

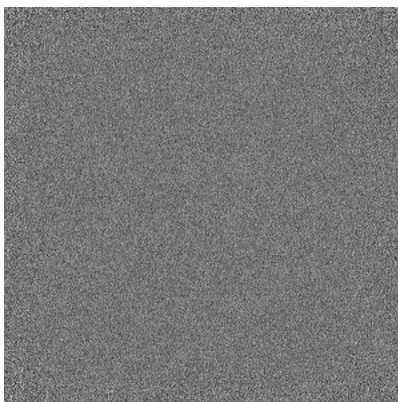


Z Index: 233

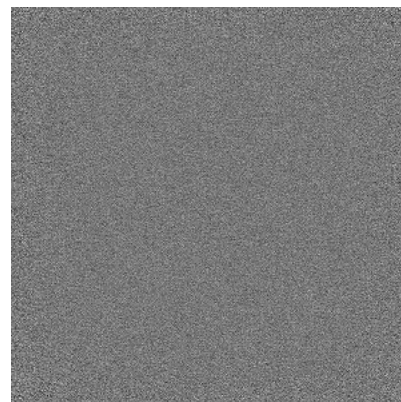
6.3.2 Raw map



X Index: 0



Y Index: 0

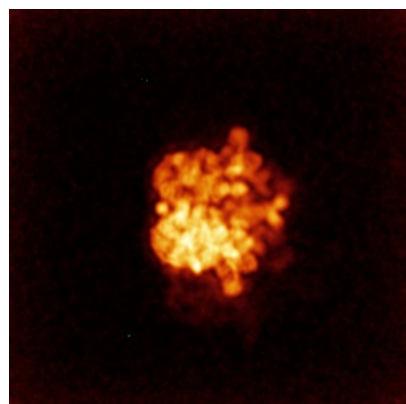


Z Index: 0

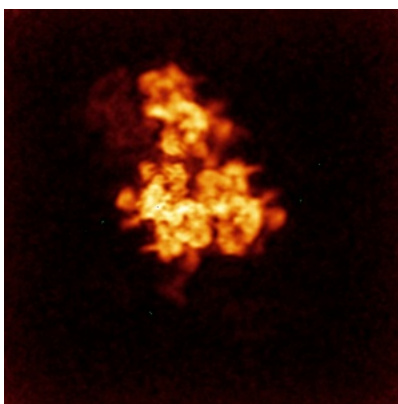
The images above show the largest variance slices of the map in three orthogonal directions.

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

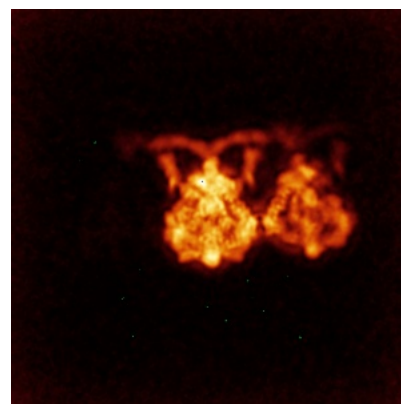
6.4.1 Primary map



X

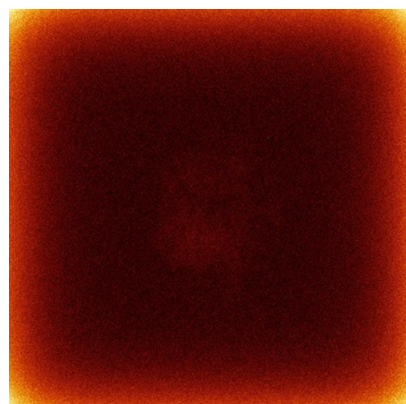


Y

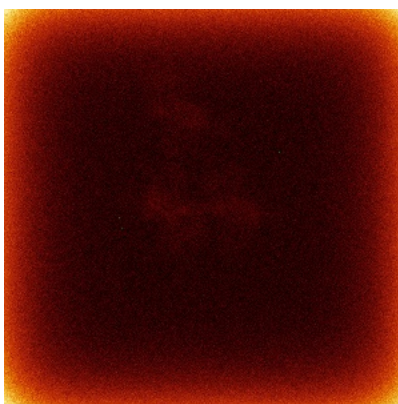


Z

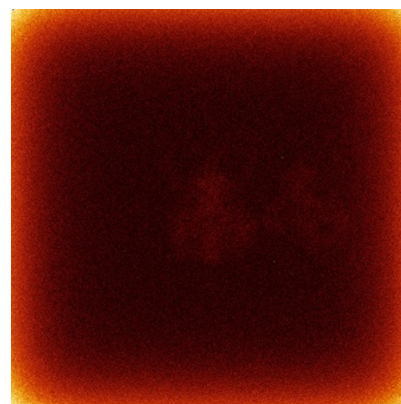
6.4.2 Raw map



X



Y

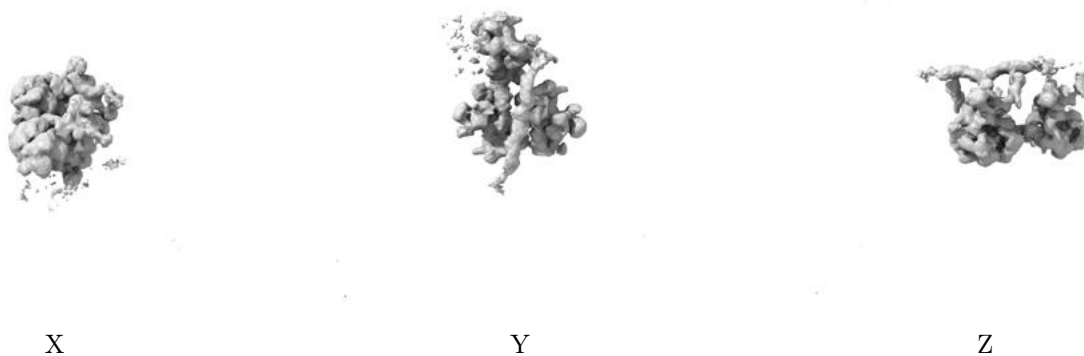


Z

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

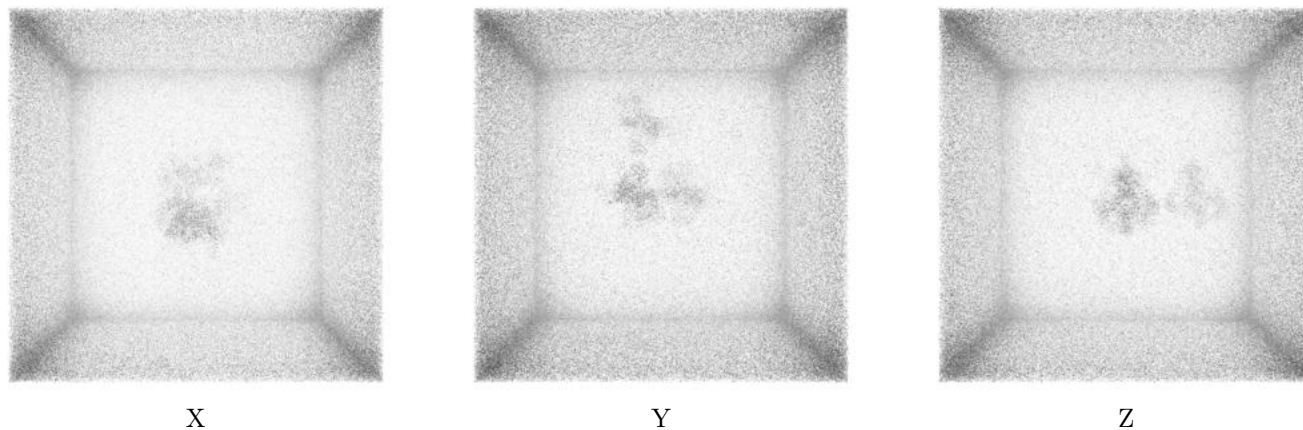
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.066. 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.

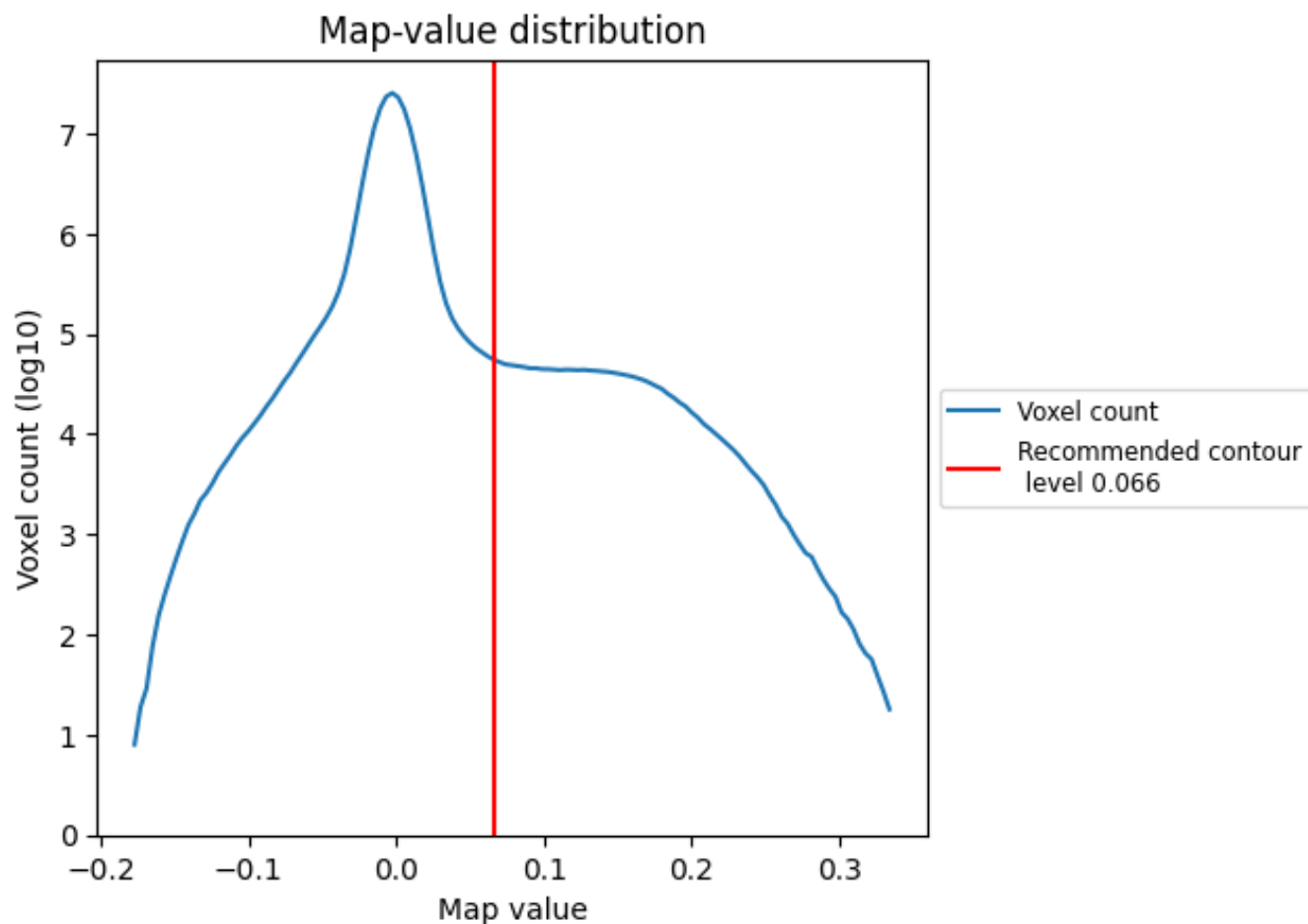
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

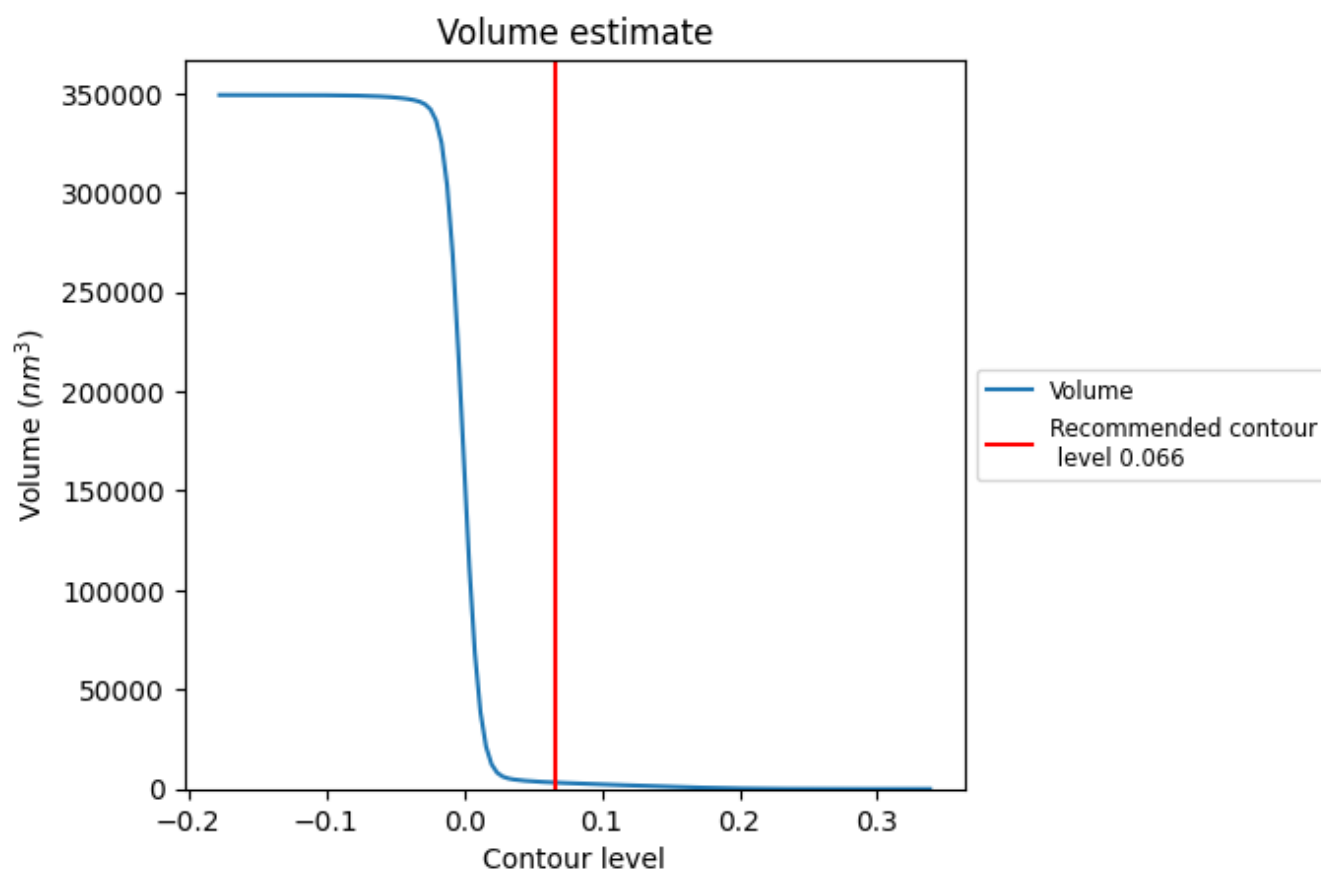
This section contains the results of statistical analysis of the map.

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.

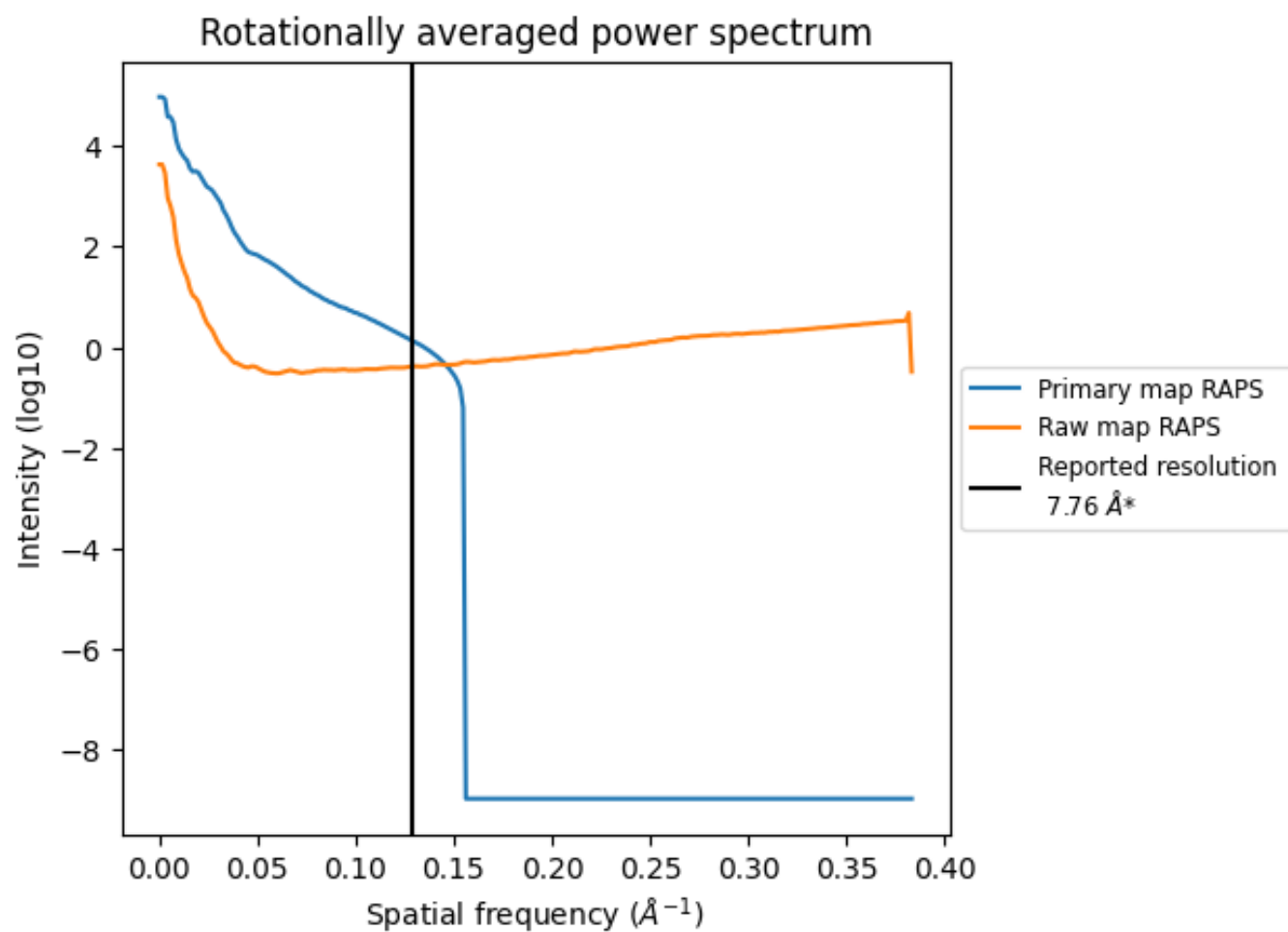
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3218 nm^3 ; this corresponds to an approximate mass of 2907 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 ⓘ

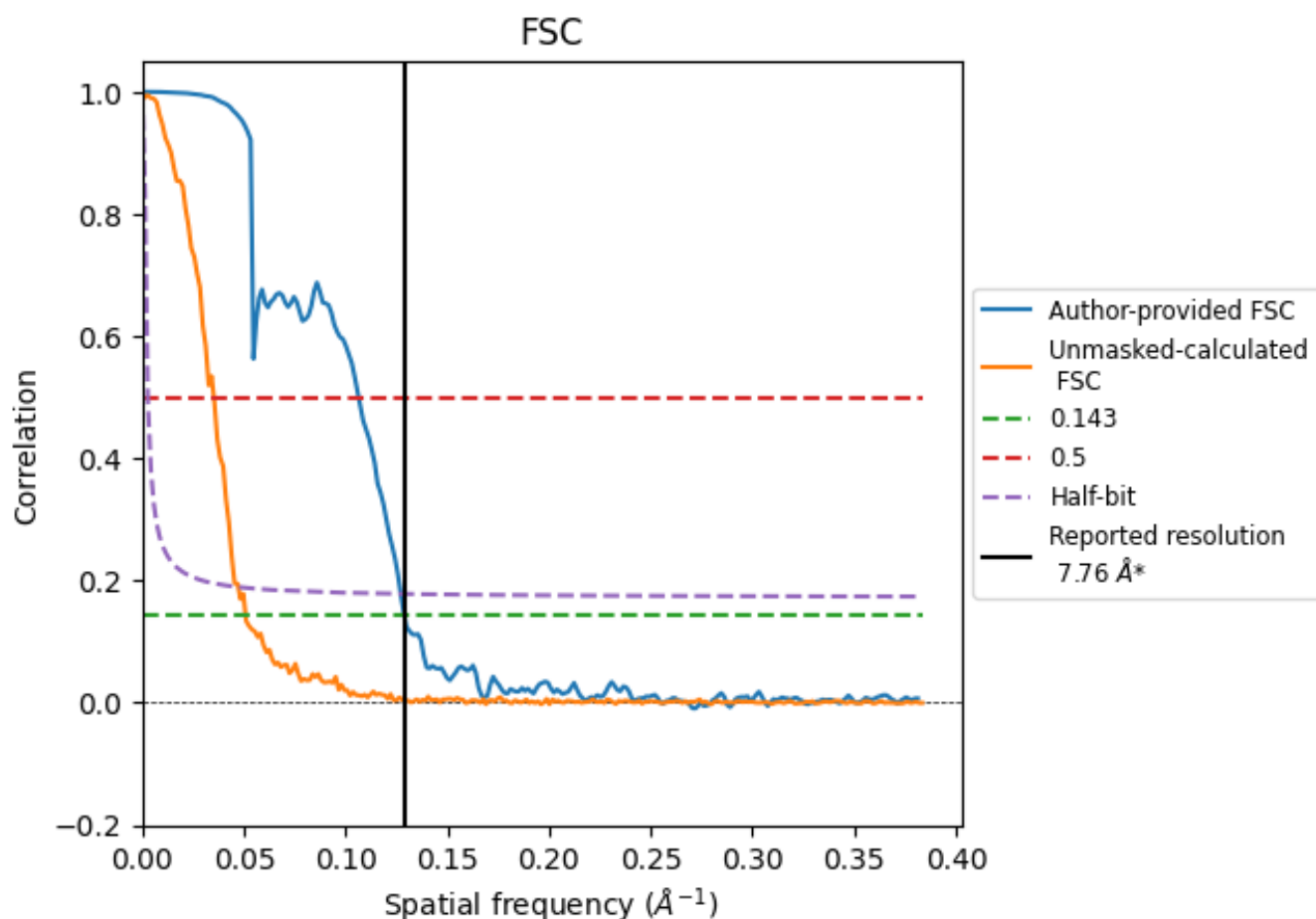


*Reported resolution corresponds to spatial frequency of 0.129 $\text{\AA}^{-1}$

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 0.129 Å⁻¹

8.2 Resolution estimates [i](#)

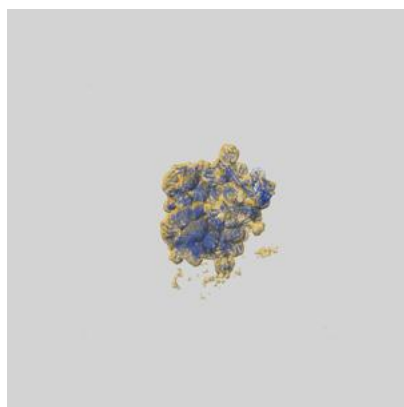
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.76	-	-
Author-provided FSC curve	7.76	9.40	7.87
Unmasked-calculated*	19.69	28.41	21.19

*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 19.69 differs from the reported value 7.76 by more than 10 %

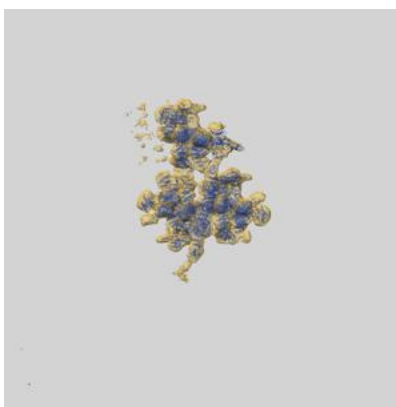
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16145 and PDB model 8BOT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

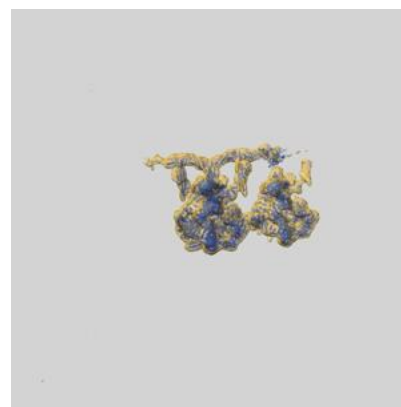
9.1 Map-model overlay [i](#)



X



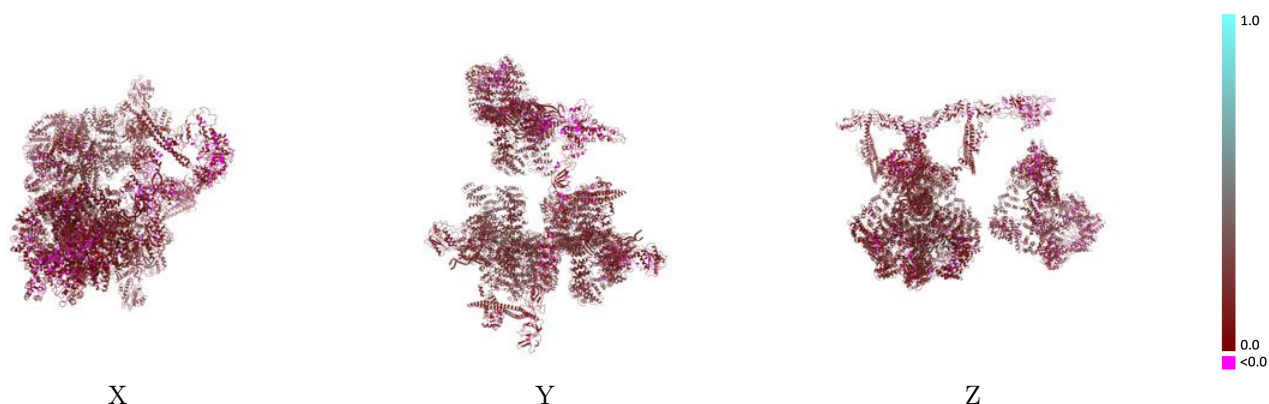
Y



Z

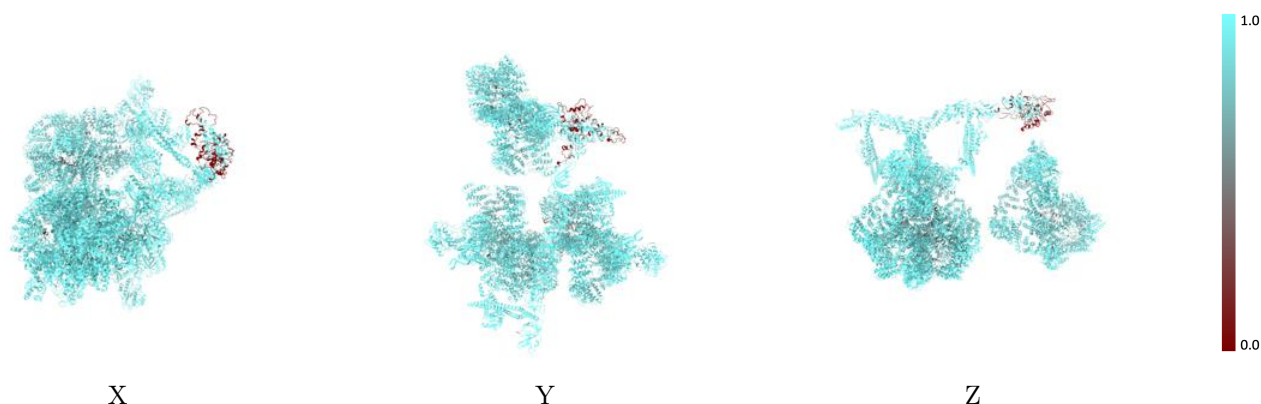
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



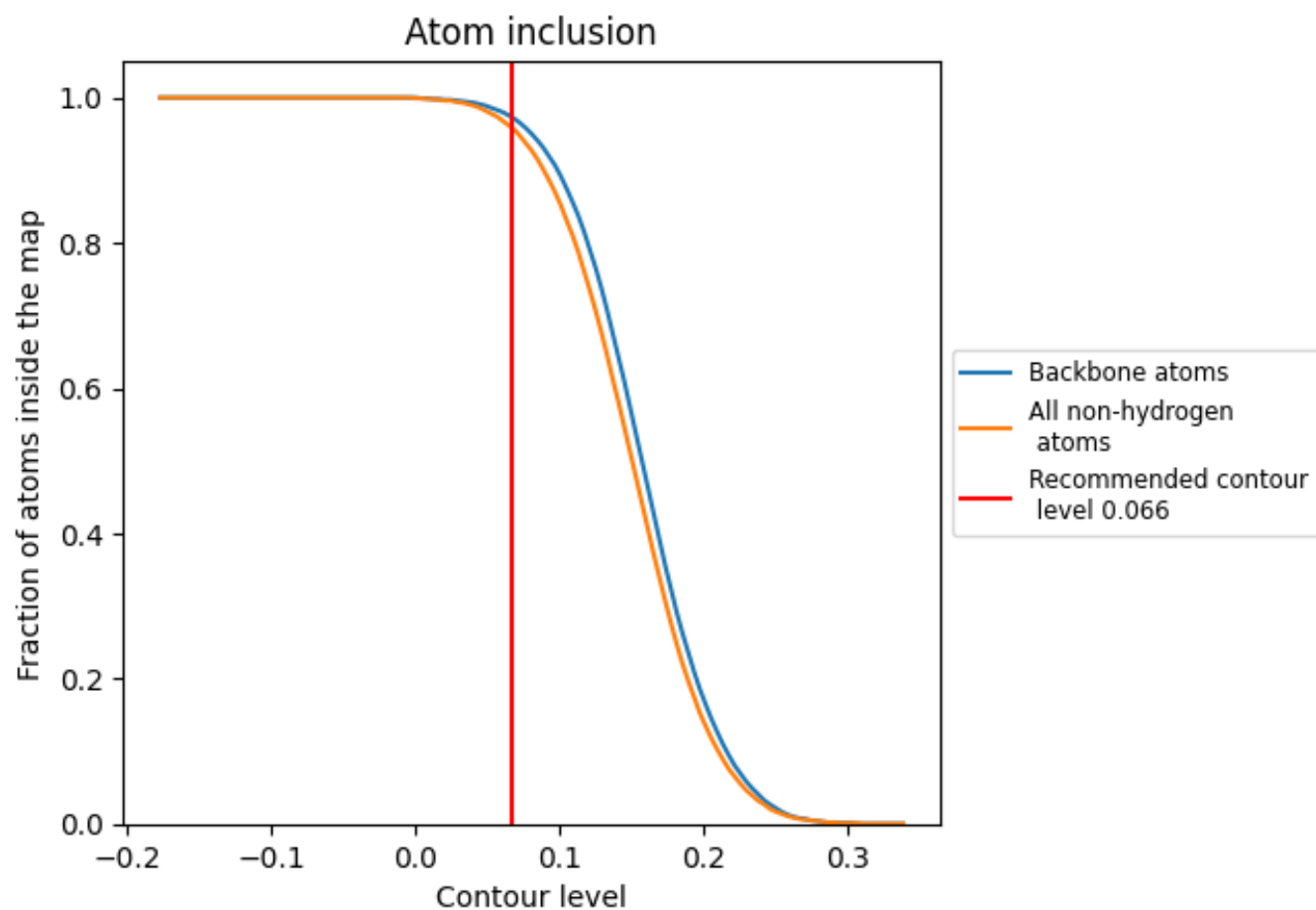
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.066).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.066) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.1280
A	 0.9590	 0.1310
B	 0.9880	 0.1210
C	 0.9700	 0.1010
D	 0.9960	 0.1890
E	 0.9840	 0.1540
F	 0.9720	 0.1730
G	 0.9840	 0.1610
H	 0.9910	 0.1450
I	 0.9950	 0.1790
J	 1.0000	 0.1930
K	 0.9820	 0.1000
L	 0.9670	 0.1010
M	 0.9960	 0.1020
N	 0.9790	 0.1060
O	 0.9830	 0.1110
P	 1.0000	 0.1230
Q	 0.9930	 0.0770
R	 0.9700	 0.0840
S	 0.9730	 0.1100
T	 0.9880	 0.0830
U	 0.9900	 0.0810
V	 1.0000	 0.1270
W	 0.9770	 0.1250
X	 0.3270	 0.0590
Y	 0.5760	 0.0680

