



## wwPDB EM Validation Summary Report ⓘ

Aug 8, 2023 – 03:20 pm BST

PDB ID : 8BOT  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

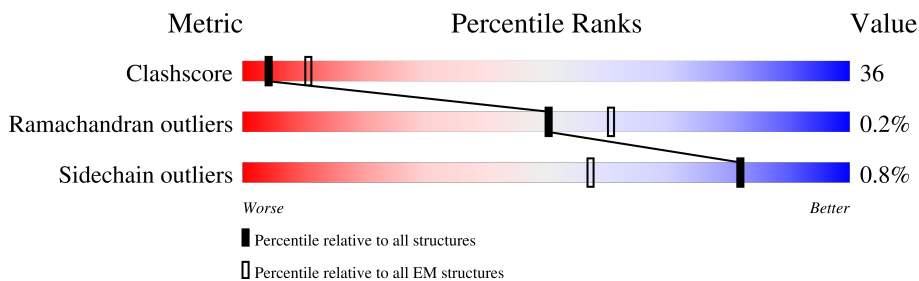
# 1 Overall quality at a glance i

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	K	336	
1	L	336	
1	N	336	
1	O	336	
2	M	911	
2	P	911	
3	Q	299	
3	R	299	

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Mol	Chain	Length	Quality of chain
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 [i](#)

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

- Molecule 2 is a protein called DNA ligase 4.

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

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

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

- 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
			Total	C	N	O	P		
9	D	24	493	238	92	139	24	0	0

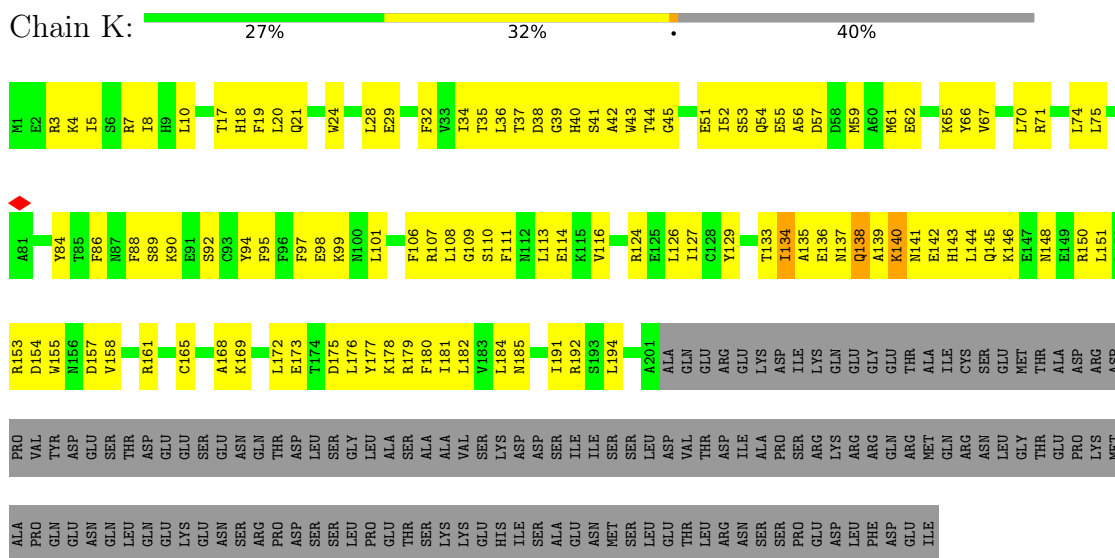
- Molecule 10 is a DNA chain called DNA (24-MER).

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

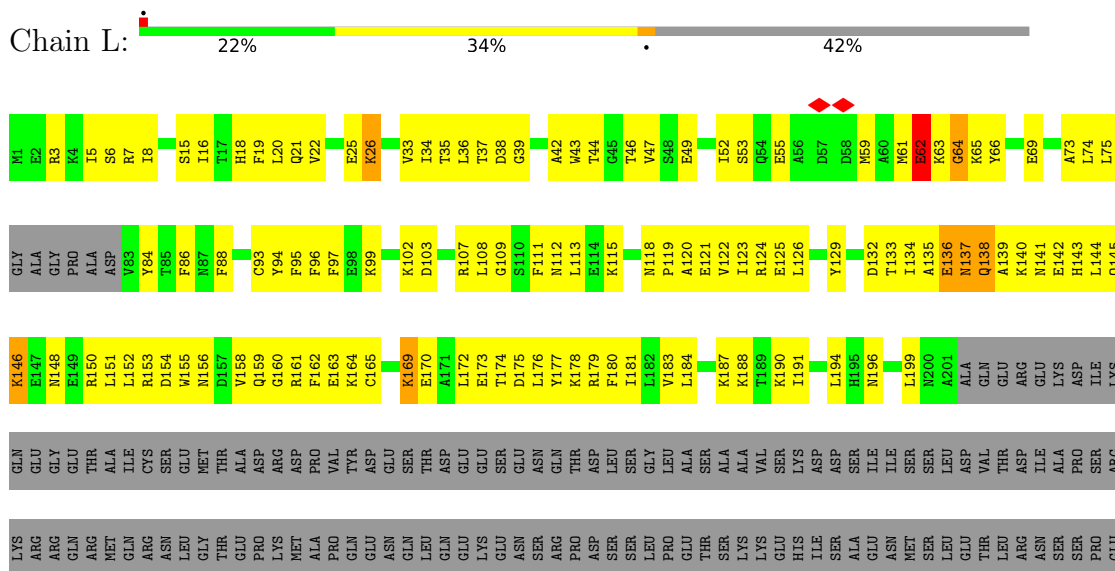
### 3 Residue-property plots

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

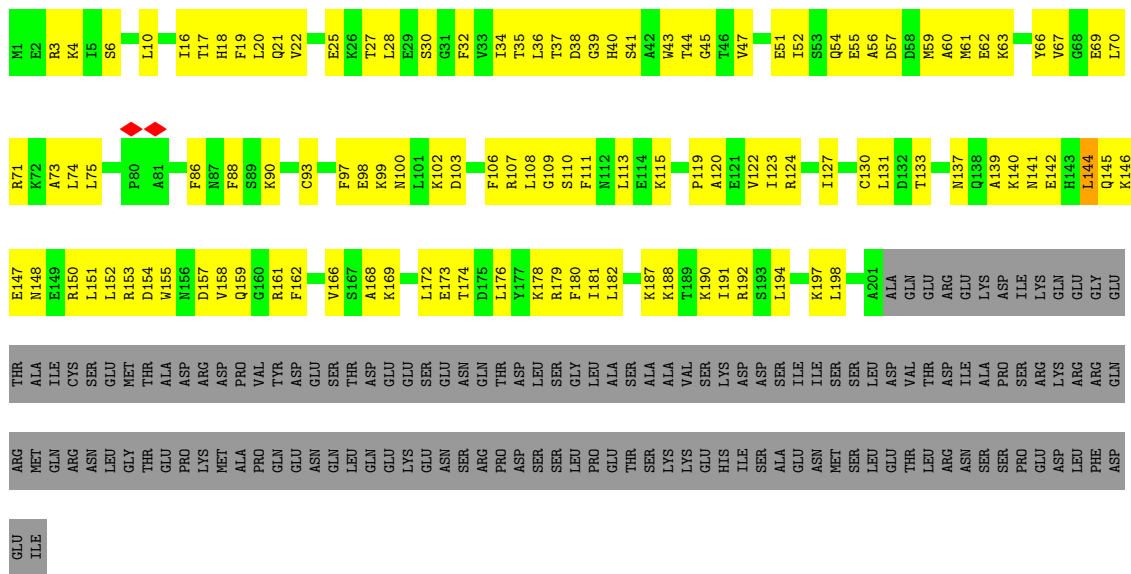
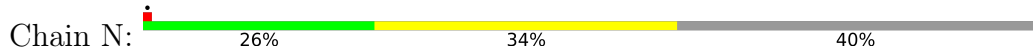


#### • Molecule 1: DNA repair protein XRCC4

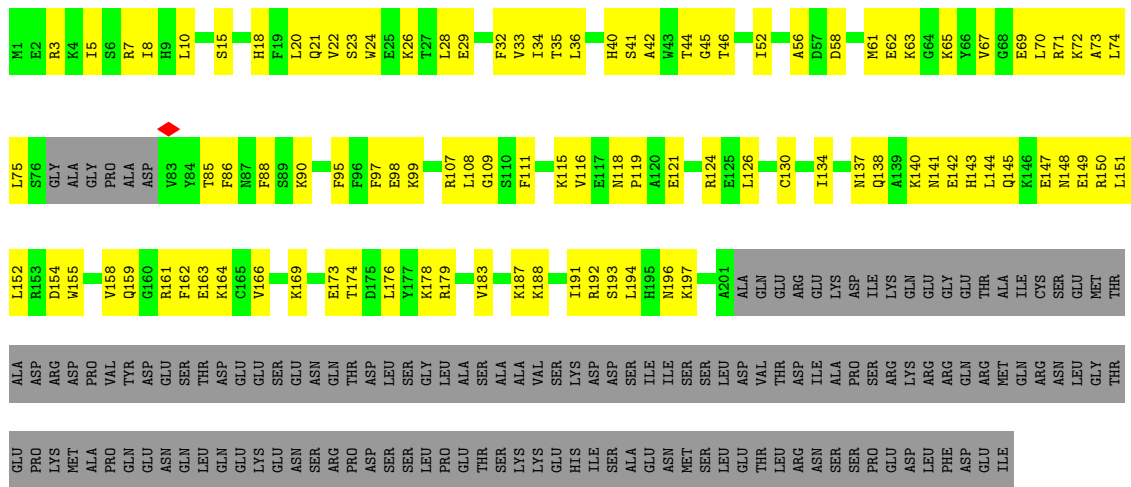
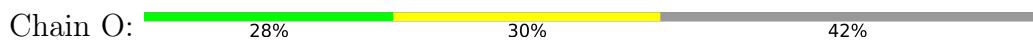


ASP  
LEU  
PHE  
ASP  
GLU  
ILE

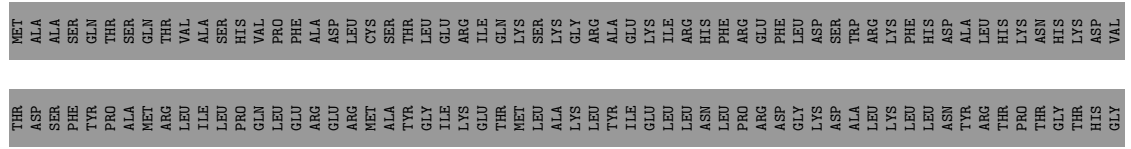
• Molecule 1: DNA repair protein XRCC4



• Molecule 1: DNA repair protein XRCC4

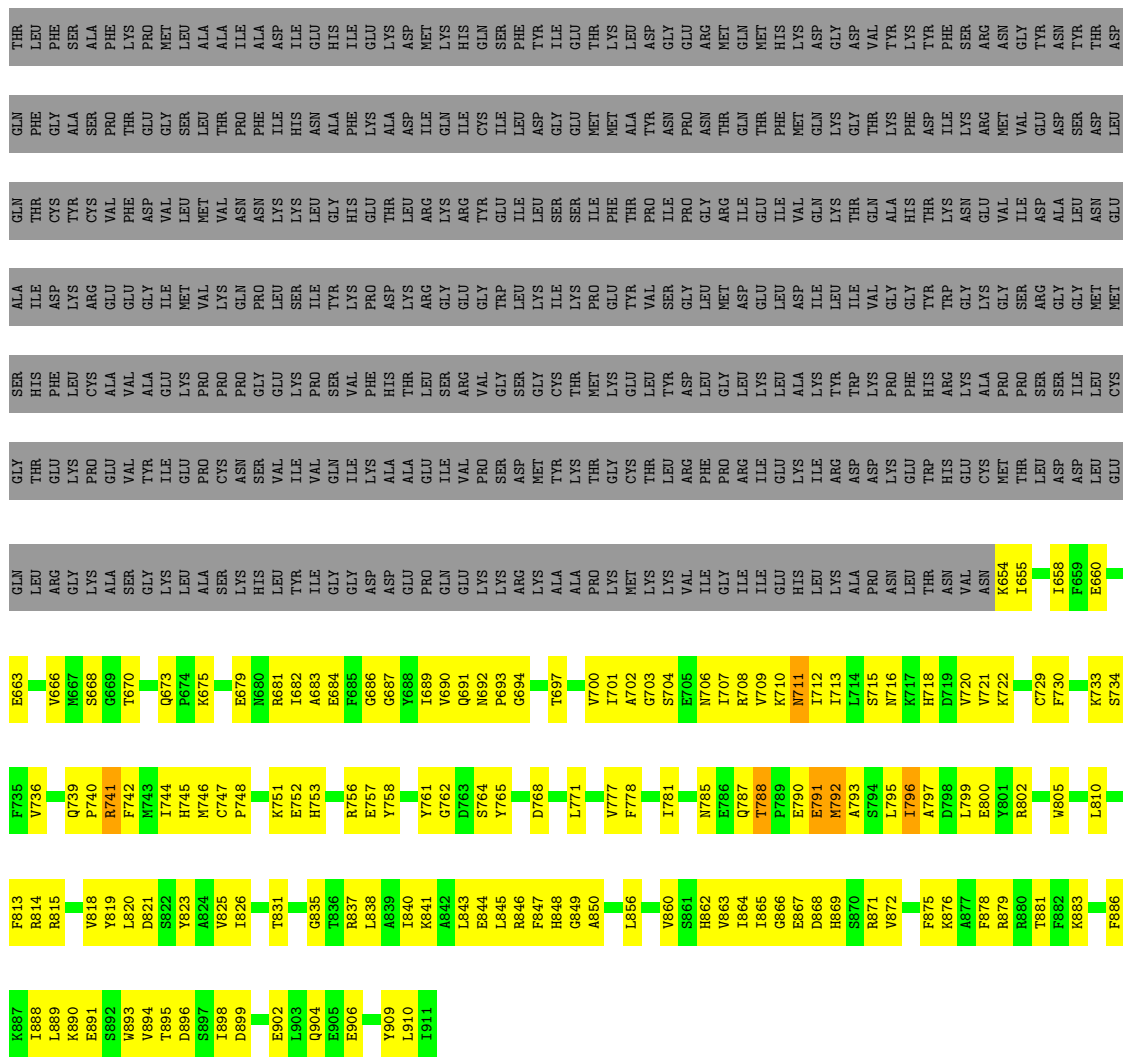


• Molecule 2: DNA ligase 4

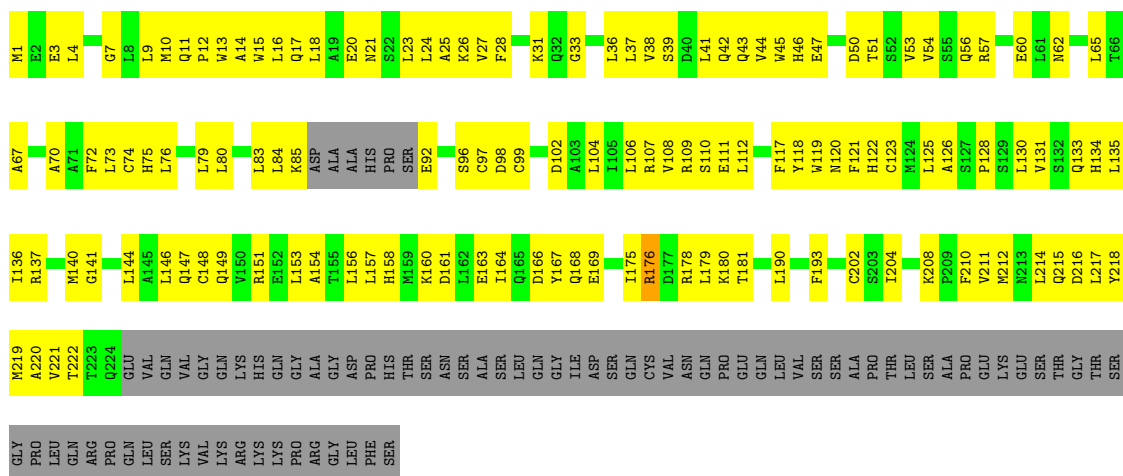




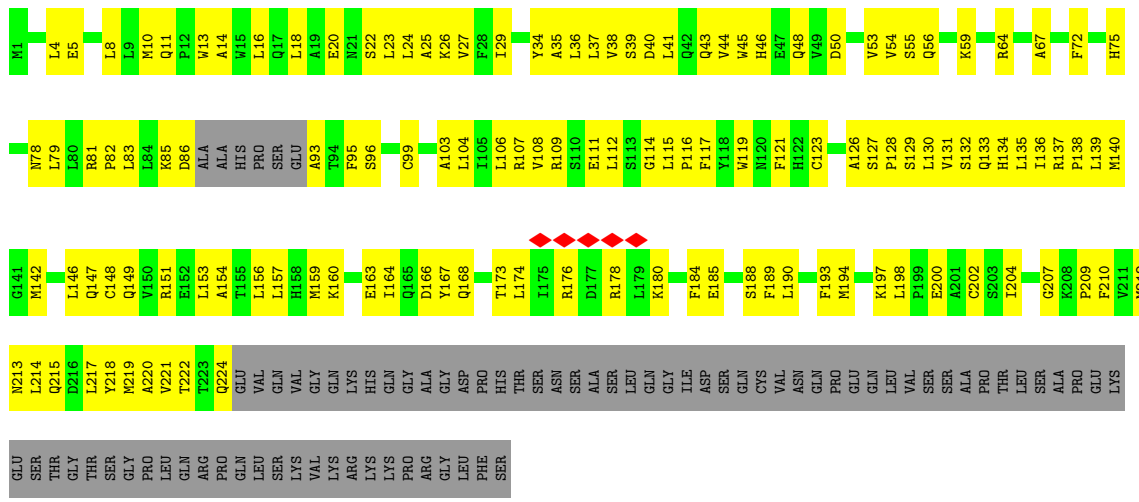
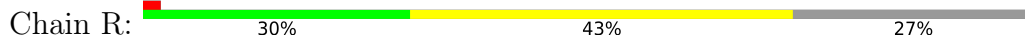




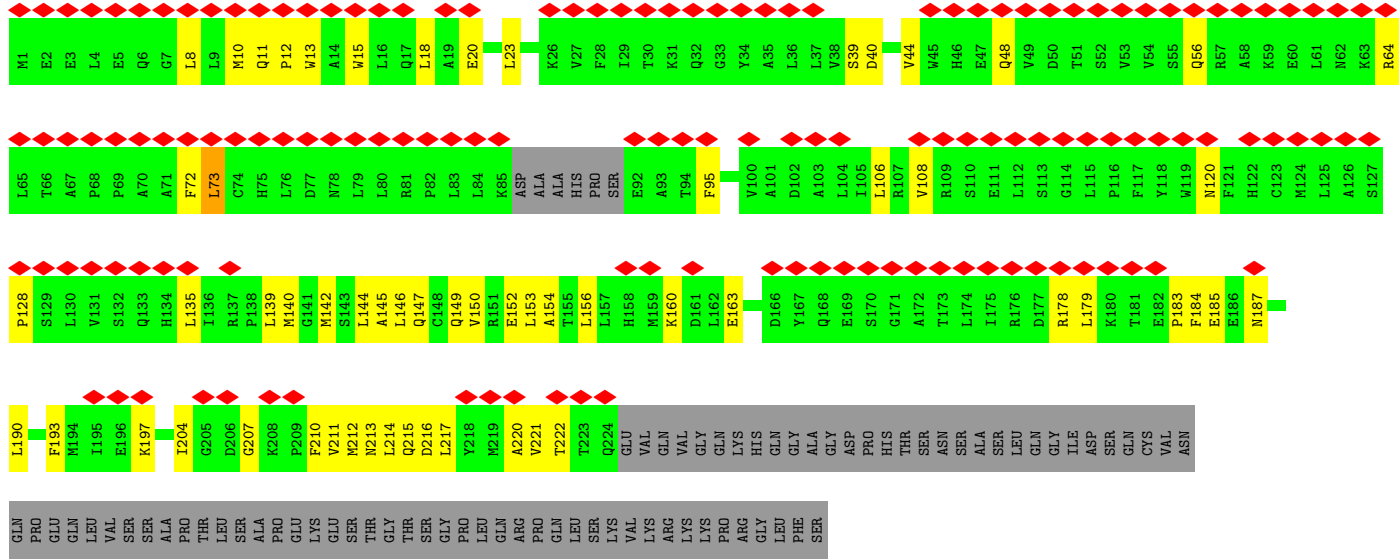
• Molecule 3: Non-homologous end-joining factor 1



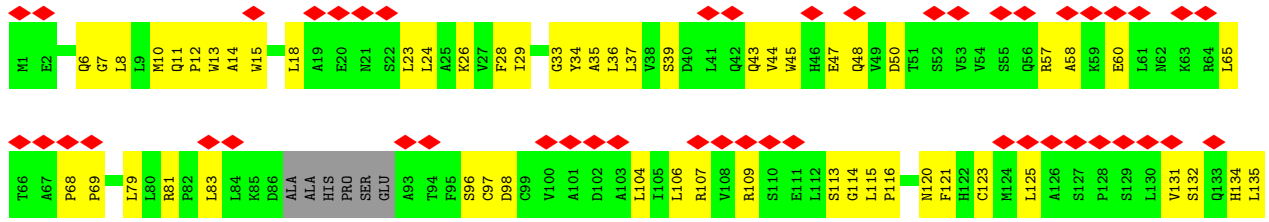
• Molecule 3: Non-homologous end-joining factor 1

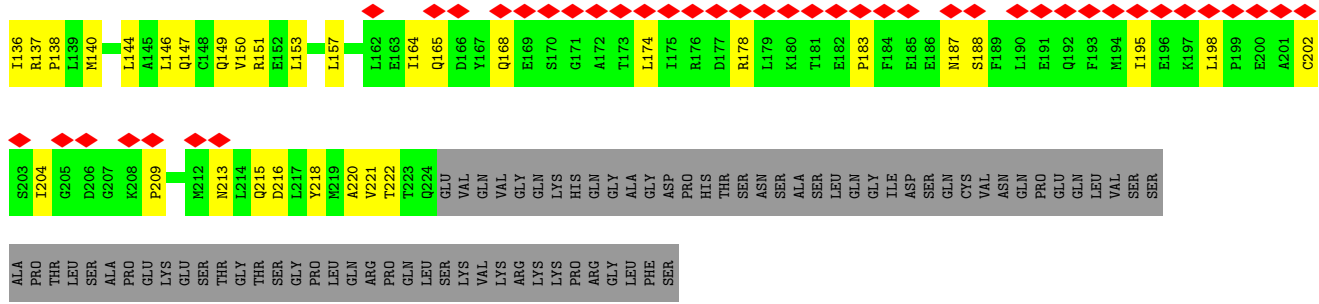


• Molecule 3: Non-homologous end-joining factor 1

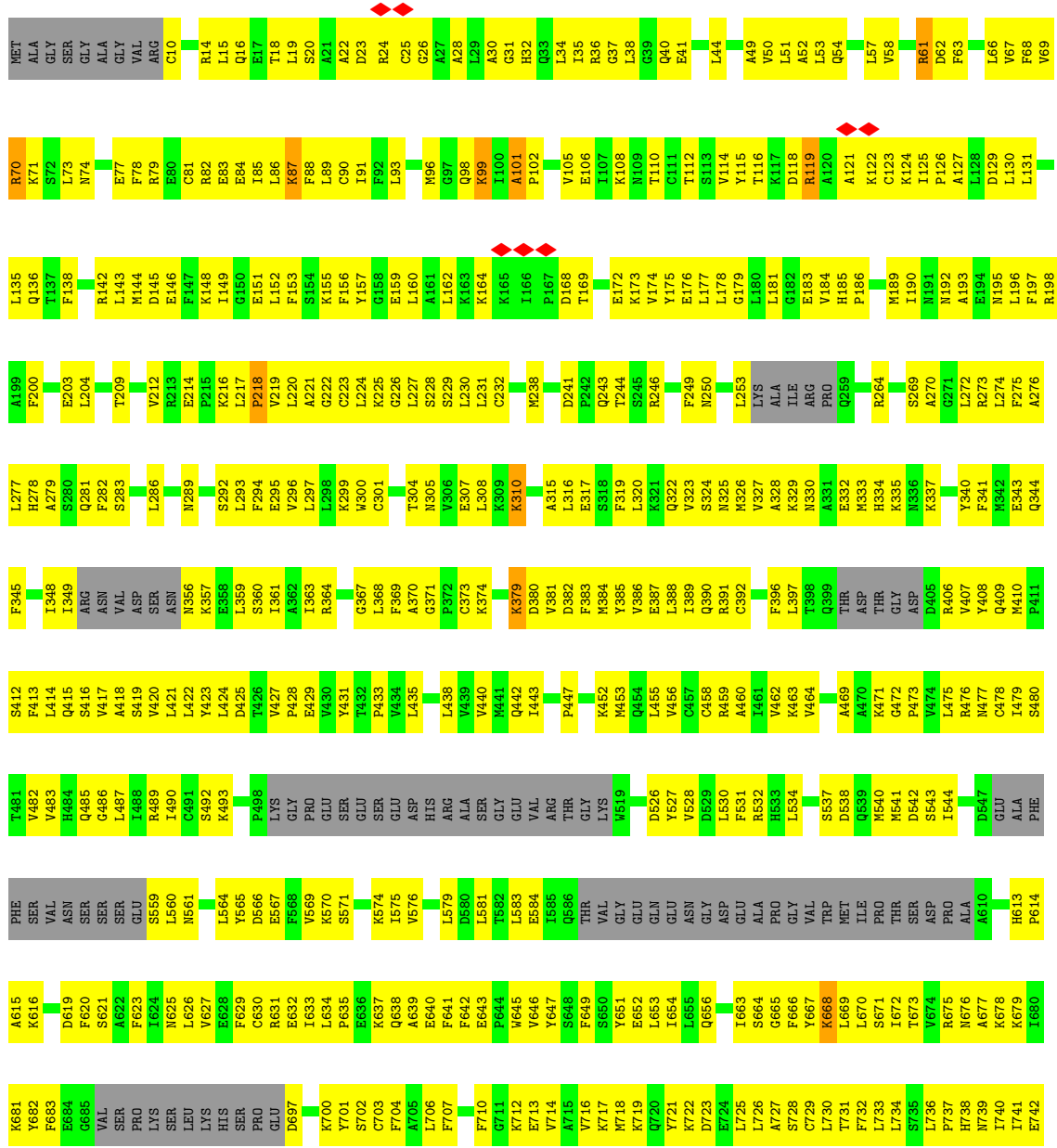


• Molecule 3: Non-homologous end-joining factor 1





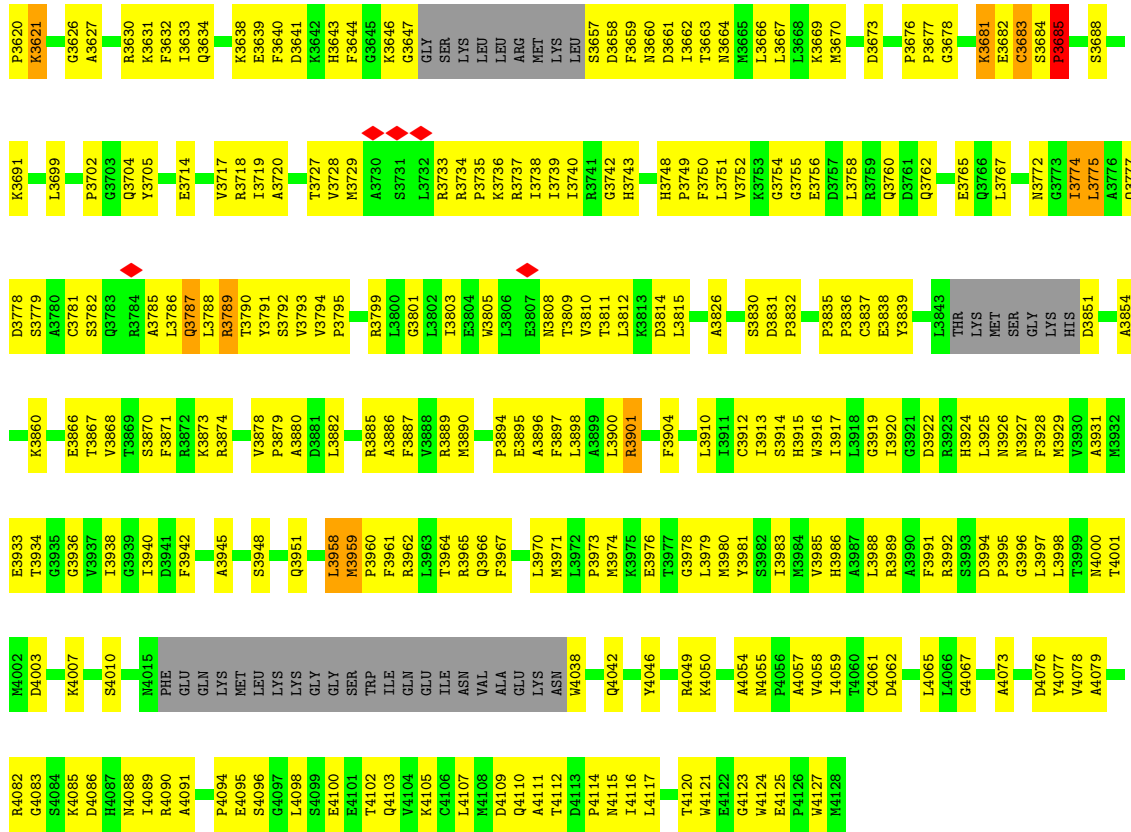
● Molecule 4: DNA-dependent protein kinase catalytic subunit



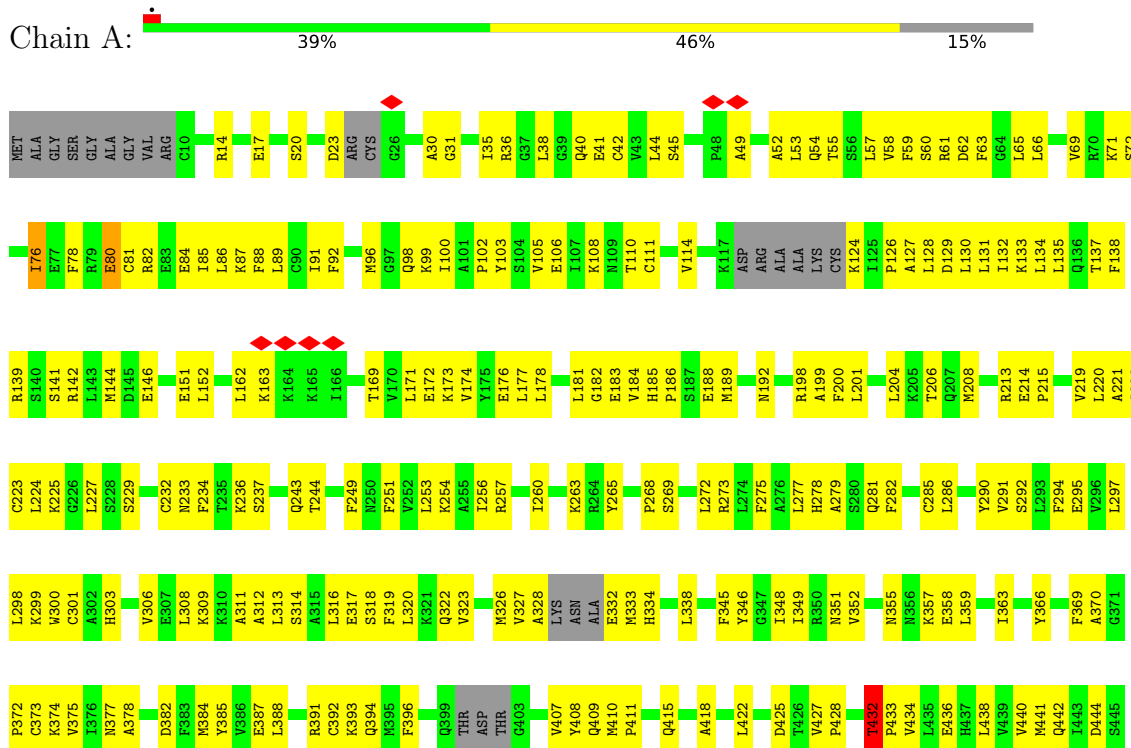
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F1559	Y1560	S1561	L1562	F1563	S1564	T1567	M1568	L1571	L1572	K1573	N1574	L1575	D1576	L1577	A1578	V1579	L1580	E1581	L1582	M1583	T1584	L1585	V1586	S1587	L1588	L1589	L1590	V1591	S1592	S1593	S1594	V1595	L1596	L1597	N1598	G1599	M1600	L1601	Q1611	K1612	H1613	L1616	K1617	L1618	A1619	T1620	T1621	I1622	L1623	Q1624	H1625	W1626	K1627	I1628	H1629	F1630	F1631	S1632	W1633	A1634	E1635	Y1636	L1637	THR	SER	LEU	THR	LEU	THR	GLY	GLY	ASP	GLU	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU
K1422	I1423	T1424	A1425	Q1426	S1427	E1430	L1431	V1434	N1435	L1436	Y1437	A1441	Q1442	V1443	D1444	R1445	S1446	R1447	L1448	A1449	A1450	Y1451	V1452	S1453	S1454	A1455	C1456	Q1457	L1458	H1459	A1460	A1461	G1462	L1463	L1464	H1465	N1466	I1467	L1468	P1469	Q1470	Q1471	L1476	H1477	H1478	H1479	T1481	G1490	I1491	A1492	PR0	GLY	H1418	L1419	R1420	ARG																									
GLN	CYS	PRO	SER	L1503	D1504	L1505	S1506	C1507	K1508	Q1509	L1510	A1511	S1512	G1513	L1514	L1515	E1516	L1517	A1518	F1519	A1520	F1521	L1524	E1525	F1526	R1527	L1528	V1529	S1530	L1531	L1532	M1533	M1534	F1535	A1536	V1537	L1538	S1539	T1540	ALA	SER	LEU	GLY	SER	GLN	GLY	SER	V1550	I1551	H1552	F1553	S1554	H1555	W1556	E1557	Y1558																									
F1559	Y1560	S1561	L1562	F1563	S1564	T1567	M1568	L1571	L1572	K1573	N1574	L1575	D1576	L1577	A1578	V1579	L1580	E1581	L1582	M1583	T1584	L1585	V1586	S1587	L1588	L1589	L1590	V1591	S1592	S1593	S1594	V1595	L1596	L1597	N1598	G1599	M1600	L1601	Q1611	K1612	H1613	L1616	K1617	L1618	A1619	T1620	T1621	I1622	L1623	Q1624	H1625	W1626	K1627	I1628	H1629	F1630	F1631	S1632	W1633	A1634	E1635	Y1636	L1637	THR	SER	LEU	THR	LEU	THR	GLY	GLY	ASP	GLU	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU
L1076	G1077	A1078	A1081	F1082	N1083	M1084	I1085	Y1086	R1087	E1088	F1089	R1090	E1091	E1092	L1095	V1096	F1099	V1100	F1101	E1102	A1103	L1104	V1105	I1106	Y1107	A1112	L1113	A1114	H1115	A1116	D1117	E1118	K1119	S1120	L1121	G1122	T1123	I1124	Q1125	Q1126	A1130	L1131	D1132	H1133	L1134	C1135	R1136	I1137	L1138	E1139	K1140	K1141	H1142	V1143																											
S1144	L1145	M1146	K1147	A1148	K1149	K1150	R1151	L1152	P1153	F1154	F1157	L1163	C1164	L1165	L1166	D1167	L1168	V1169	K1170	M1171	E1172	L1173	A1174	H1175	R1178	P1179	T1181	E1182	C1183	R1184	H1185	K1186	S1187	L1190	F1191	Y1192	L1193	G1194	V1195	L1198	R1202	S1203	P1204	M1205	L1206	K1209	D1210	K1213	L1220																																
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S1289	K1292	A1293	V1294	A1295	F1296	F1297	M1298	E1299	S1300	L1301	A1302	M1303	H1304	D1305	I1306	L1307	A1308	A1309	E1310	K1311	C1312	F1313	GLY	THR	GLY	ALA	GLY	ASN	ARG	T1322	S1323	E1326	G1327	E1328	R1329	S1333	L1402	M1403	K1404	A1405	L1406	K1407	M1408	S1409	P1410	E1411	K1412	D1413	I1414	L1415	A1416	T1417	H1418	L1419	R1420	ARG																									
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GLN	CYS	PRO	SER	L1503	D1504	L1505	S1506	C1507	K1508	Q1509	L1510	A1511	S1512	G1513	L1514	L1515	E1516	L1517	A1518	F1519	A1520	F1521	L1524	E1525	F1526	R1527	L1528	V1529	S1530	L1531	L1532	M1533	M1534	F1535	A1536	V1537	L1538	S1539	T1540	ALA	SER	LEU	GLY	SER	GLN	GLY	SER	V1550	I1551	H1552	F1553	S1554	H1555	W1556	E1557	Y1558																									
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VAL	SER	ALA	LEU	SER	ARC	ALA	ALA	GLN	LYS	GLY	F826	N827	K828	V829	V830	L831	K832	H833	L834	K835	K836	T837	K838	N839	L840	SER	SER	ASN	GLU	ALA	ILE	S847	L848	E849	E850	R851	R852	I853	R854	Q857	M858	L859	G860	S861	L862	G863	G864	I866	N867	L868	L869	L870	L871	THR	VAL	THR	THR	SER	SER	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU														
L743	D744	V745	R746	A747	Y748	V749	P750	A755	G759	Y762	L765	A766	E767	V768	G769	L770	M771	A772	T773	L774	E775	W776	I778	D781	H782	H783	W784	M785	Q786	P787	Y788	Y789	I792	D797	G798	Y799	L800	K801	T802	S803	ALA	LEU	SER	ASP	GLU	THR	LYS	ASN	ASN	TRP	GLU																														

T2603	PRO	E1708
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	PHE	L1710
	VAL	R1711
	GLU	R1712
	THR	V1713
	GLN	L1714
	ALA	S1781
	GLY	E1782
	SER	F1783
	GLM	L1717
	THR	R1784
	GLY	L1785
	LEU	A1788
	GLN	R1787
	GLY	R1788
	THR	F1789
	GLY	S1790
	THR	R1727
	GLY	E1728
	GLY	F1729
	GLY	P1730
	GLY	G1732
	GLY	T1733
	GLY	L1798
	GLY	E1799
	GLY	S1800
	GLY	F1736
	GLY	N1737
	GLY	N1738
	GLY	Y1739
	GLY	E1802
	GLY	E1803
	GLY	M1804
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V8555	A3556	L3416	A3338	L3273	GLY	Q8139	I3074	L3011	D2937	L2868	T9723	SER
A3557	R3557	F3419	D3354	V3274	ASP	E3140	K3075	E3012	V2936	L2869	L2803	THR
R3558	C3420	F3419	K3355	S3276	PRO	F3141	L3078	Y3013	L2804	L2871	L2804	ASP
K3559	D3421	C3420	A3356	W3275	SER	I3142	E3079	C3014	K2806	L2872	L2805	PRO
K3560	F3495	D3421	R3357	V3277	ARG	I3145	I3081	S3018	K2807	L2878	L2806	LEU
K3561	S3560	L3424	R3358	Q3278	ARG	S3146	F3082	I3019	L2808	R2731	L2808	VAL
L3562	R3561	R3425	I3359	S3279	MET	K3147	Y3082	D3020	L2809	V2876	L2809	ASP
L3563	L3562	E3428	L3360	Y3280	GLU	Q3148	S3083	S3021	F2810	F2733	F2810	HIS
Q3564	Q3564	E3428	E3361	C3281	VAL	G3149	E3084	A3022	S2811	M2734	M2733	THR
I3565	I3564	ASN	L3362	L3282	GLN	E3085	E3085	ASN	L2812	D2735	D2735	PRO
I3566	R3562	ALA	S3363	R3283	GLU	N3150	L3086	PRO	F2813	Q2736	Q2736	SER
I3567	R3563	SER	G3364	H3285	GLU	S3087	L3088	ASP	G2815	E2737	E2737	SER
I3568	D3570	SER	C3286	C3286	GLU	K3158	L3088	LEU	L2816	K2738	K2738	ASP
F3571	L3505	VAL	R3287	R3287	L3089	L3161	Y3090	ASN	L2817	L2739	L2739	SER
L3572	L3506	ILE	S3288	S3288	ASN	Y3090	Y3090	ASN	L2818	S2740	S2740	LEU
N3573	D3507	ASP	R3289	R3289	K3029	L3091	L3091	K3029	K2818	K2746	K2746	LEU
A3574	K3508	SER	R3290	R3290	Y3091	L3092	L3092	I2890	D2821	A2749	A2749	PHE
L3575	L3511	ALA	G3292	G3292	Y3092	I3093	I3093	R2891	D2822	E2750	E2750	ALA
Q3577	V3512	GLU	C3293	C3293	T3165	S3094	S3094	L2892	K2824	K2765	K2765	HIS
V3512	V3512	LEU	S3294	S3294	R3167	D3095	D3095	L2893	K2825	A2751	A2751	LYS
Q3515	Q3515	LEU	E3295	E3295	Y3168	Y3096	Y3096	E2894	L2826	R2763	R2763	ARG
H3516	H3516	A3441	Q3296	Q3296	P3169	D3097	D3097	E2894	L2826	E2764	E2764	SER
V3518	V3518	P3443	V3297	V3297	R3098	R3098	R3098	L2897	E2828	I2757	I2757	GLU
E3520	E3520	A3444	F3298	F3298	A3171	K3100	K3100	L2899	K2829	K2768	K2768	ARG
L3521	L3521	L3446	T3303	T3303	M3176	Y3101	Y3101	L2900	K2830	K2769	K2769	GLN
F3521	F3521	V3447	Q3383	Q3383	M3177	F3102	F3102	L2901	K2831	R2773	R2773	VAL
K3522	K3522	R3448	R3384	R3384	N3178	L3103	L3103	PRO	L2832	G2776	G2776	GLY
F3522	F3522	L3456	L3385	L3385	K3241	Q3042	Q3042	ALA	F2840	H2777	H2777	LYS
D3523	D3523	K3449	S3386	S3386	W3179	Q3043	Q3043	ALA	D2842	D2779	D2779	LYS
N3524	N3524	A3453	E3387	E3387	I3182	M3044	M3044	ARG	L2844	L2780	L2780	ARG
R3525	R3525	A3453	A3388	A3388	I3183	K3045	K3045	ARG	F2850	P2781	P2781	LEU
N3526	N3526	L3454	F3389	F3389	F3184	L3051	L3051	ARG	F2852	I2783	I2783	LEU
F3527	F3527	K3455	Q3390	Q3390	N3185	L3052	L3052	PRO	P2852	G2784	G2784	PRO
A3528	A3528	L3456	R3391	R3391	R3186	Q3053	Q3053	LYS	F2854	K2786	K2786	GLY
I3529	I3529	N3457	A3392	A3392	C3187	Q3054	Q3054	ARG	V2855	H2787	H2787	ASP
I3530	I3530	S3458	E3393	E3393	F3188	L3049	L3049	VAL	S2856	S2788	S2788	VAL
F3531	F3531	N3459	E3394	E3394	F3189	K3060	K3060	ARG	C2857	A2791	A2791	ASN
F3532	F3532	E3460	E3395	E3395	F3189	L3061	L3061	ARG	L2858	I2791	I2791	ASN
F3533	F3533	A3461	ALA	ALA	L3190	D3065	D3065	LYS	Q2864	T2792	T2792	LYS
L3534	L3534	R3462	GLN	GLN	S3191	L3066	L3066	LYS	Q2865	P2793	P2793	VAL
L3535	L3535	R3463	PRO	PRO	K3192	D3067	D3067	ARG	D2860	L2794	L2794	VAL
S3536	S3536	K3464	PRO	PRO	L3120	A2997	A2997	ARG	Y2930	Q2795	Q2795	GLY
S3537	S3537	K3464	PRO	PRO	L3121	L2999	L2999	ARG	Q2864	A2796	A2796	ALA
E3538	E3538	R3467	TRP	TRP	E3195	D3000	D3000	ARG	H2865	V2797	V2797	ALA
T3539	T3539	I3471	TRP	TRP	K3197	L3062	L3062	ARG	A2866	A2798	A2798	ALA
SER	SER	I3472	GLY	GLY	THR	F3064	F3064	ARG	L2925	Q2799	Q2799	ASP
PHE	PHE	ALA	ALA	ALA	LEU	I3065	I3065	ARG	L2926	L2930	L2930	ASP
LYS	LYS	E3476	ALA	ALA	PRO	I3066	I3066	ARG	L2926	L2930	L2930	ASP
ASP	ASP	T3479	R3407	R3407	GLU	I3067	I3067	ARG	L2926	L2930	L2930	ASP
T3545	T3545	T3479	G3408	G3408	GLU	I3068	I3068	ARG	L2926	L2930	L2930	ASP
H3549	H3549	L3480	G3408	G3408	ASP	D3068	D3068	ARG	L2926	L2930	L2930	ASP
Y3614	Y3614	S3481	G3331	G3331	ASN	Q3069	Q3069	ARG	L2926	L2930	L2930	ASP
A3615	A3615	L3482	T3332	T3332	SER	M3068	M3068	ARG	L2926	L2930	L2930	ASP
A3616	A3616	M3483	D3411	D3411	MET	K3134	K3134	ARG	L2926	L2930	L2930	ASP
L3617	L3617	T3484	K3412	K3412	ASN	L3135	L3135	ARG	L2926	L2930	L2930	ASP
G3618	G3618	K3485	Y3413	Y3413	VAL	E3071	E3071	ARG	L2926	L2930	L2930	ASP
D3619	D3619	S3489	I3336	I3336	ASP	G3072	G3072	ARG	L2926	L2930	L2930	ASP
			I3337	I3337	ASP	L3073	L3073	ARG	L2926	L2930	L2930	ASP



● Molecule 4: DNA-dependent protein kinase catalytic subunit







E2487	D2419	K2347	ASN	GLY	R2106	ASP	K1885	F1900	A1835	K1689	H1625	LEU	K1456
I2498	F2420	Q2348	SER	ILE	S2107	PHE	R1986	HIS	L1836	G1690	W1626	GLY	Q1457
L2501	V2421	L2349	LYS	THR	L2108	SER	R1986	GLY	R1837	Q1691	W1627	SER	L1458
V2505	V2423	Q2352	D2269	GLY	PRO	THR	TYR	CYS	E1838	V1765	K1628	SER	H1469
L2506	M2424	H2353	N2270	VAL	PRO	VAL	ASN	ILE	F1839	T1694	D1630	GLN	R1460
I2507	R2425	Q2353	S2271	GLN	GLN	GLN	PHE	THR	S1841	L1695	D1630	SER	L1464
L2510	R2426	M2356	L2277	SER	GLY	SER	PRO	GLY	T1842	L1696	W1633	VAL	L1468
L2511	R2427	E2357	A2282	TYR	TYR	VAL	VAL	GLY	I1843	P1697	D1636	ILE	L1488
D2512	D2428	D2358	T2192	SER	GLY	SER	GLU	GLU	V1844	F1698	D1637	HIS	S1470
E2513	D2429	K2359	L2193	TYR	ASP	VAL	VAL	TYR	V1845	F1699	S1637	S1553	S1471
M2514	E2430	F2360	S2194	SER	SER	SER	VAL	GLU	D1846	T1700	P1638	H1554	Q1471
P2515	Q2432	V2362	S2195	SER	VAL	SER	VAL	VAL	E1847	T1700	P1639	H1555	S1472
L2517	K2433	C2363	W2196	GLN	PRO	GLN	PRO	PRO	L1848	G1704	E1640	VAL	T1473
Q2518	L2436	R2364	L2199	ASP	ARG	ASP	MET	L1945	I1849	Q1707	T1641	ILE	D1474
R2522	L2439	G2365	L2200	PRO	ARG	PRO	GLU	L1918	V1850	L1707	K1642	ILE	L1475
N2523	Y2440	K2366	A2200	PRO	ARG	PRO	GLU	C1919	L1851	E1708	M1644	HIS	L1476
F2524	K2441	S2297	K2207	ARG	ARG	ARG	LYS	C1919	L1851	E1709	A1644	S1564	H1477
W2525	M2442	E2298	F2128	PHE	PHE	PHE	GLU	ALA	K1857	E1715	E1665	E1565	E1485
S2526	M2443	E2209	L2129	ARG	ARG	ARG	ILE	GLY	LEU	E1715	L1648	E1570	L1486
H2527	F2300	V2210	L2129	ARG	ARG	ARG	ILE	GLY	ASN	Q1716	A1650	L1571	V1487
E2528	V2210	V2210	L2129	ARG	ARG	ARG	LYS	GLU	E1860	L1717	K1651	L1572	Y1488
T2529	F2309	R2214	M2135	ARG	ARG	ARG	LYS	ASN	S1861	L1718	I1652	E1581	P1493
R2530	V2310	R2214	V2138	GLU	GLU	GLU	ALA	GLN	T1862	L1575	L1653	L1575	GLY
L2531	R2311	M2219	P2139	ALA	ALA	ALA	ALA	L1933	F1863	H1721	D1576	D1576	ASP
P2532	M2220	M2219	L2140	ARG	ARG	ARG	GLU	L1934	D1864	P1722	L1655	L1577	ASP
R2542	L2385	K2221	M2141	ASP	ASP	ASP	GLU	L1798	T1865	P1723	L1655	L1577	GLU
E2460	L2386	H2222	F2145	THR	THR	THR	ALA	L1939	T1866	Q1724	D1656	A1578	ARG
F2461	P2387	F2223	F2145	THR	THR	THR	ALA	L1939	I1867	Q1725	S1657	V1579	ARG
V2462	A2320	H2225	K2148	HIS	HIS	HIS	ASN	A1943	T1868	S1726	S1658	L1580	GLN
S2463	E2321	F2224	L2149	ASP	ASP	ASP	GLY	A1943	K1869	R1727	F1661	E1581	CYS
H2464	V2322	P2226	V2150	VAL	VAL	VAL	GLY	I1949	M1870	P1731	L1662	LEU	P1501
R2470	L2323	F2231	I2151	LEU	LEU	LEU	PRO	S1950	M1871	P1731	T1663	L1505	L1505
E2471	L2325	T2240	E2154	GLU	GLU	GLU	PRO	G1874	G1872	P1736	H1665	S1506	C1507
Q2472	L2325	L2241	E2155	LEU	LEU	LEU	PRO	Y1874	Y1874	R1735	G1666	C1507	C1507
M2473	L2396	L2241	V2156	TYR	TYR	TYR	PRO	K1875	K1875	R1735	S1667	V1593	V1593
Y2474	C2397	L2241	F2157	MET	MET	MET	TYR	I1876	I1876	F1736	F1668	L1601	L1510
W2475	Y2329	C2244	R2158	SER	SER	SER	SER	C1954	L1877	N1737	P1669	Q1602	L1510
E2548	VAL	W2245	F2159	SER	SER	SER	LEU	V1955	D1878	Q1817	E1670	Q1603	E1516
K2549	NET	C2248	F2159	LEU	LEU	LEU	LEU	PHE	V1879	S1818	E1671	S1604	E1516
L2550	GLU	C2248	Y2160	SER	SER	SER	SER	ASN	M1880	F1819	F1672	F1605	F1519
E2551	ARG	C2248	A2161	TYR	TYR	TYR	TYR	GLU	Y1882	C1742	T1673	E1607	A1520
H2552	LYS	Y2253	A2161	TYR	TYR	TYR	TYR	L1959	S1882	K1745	I1676	R1608	F1521
F2553	LYS	R2254	W2164	LEU	LEU	LEU	ALA	Q1963	R1883	F1746	I1676	E1526	E1526
F2554	ILE	L2255	M2094	ASP	ASP	ASP	ASP	Q1963	LEU	L1747	S1677	R1527	R1527
W2408	LEU	I2256	A2095	SER	SER	SER	SER	F1987	PRO	D1748	L1678	L1528	L1528
L2411	F2257	F2257	T2098	THR	THR	THR	THR	SER	D1887	L1750	A1680	Q1611	V1529
L2412	E2339	E2339	A2099	SER	SER	SER	SER	GLU	D1888	L1827	D1681	K1617	S1530
L2413	S2340	K2259	S2174	LEU	LEU	LEU	LEU	GLU	L1824	E1751	L1682	K1617	S1530
L2414	L2341	F2260	E2175	GLU	GLU	GLU	GLU	P1971	L1825	L1752	T1682	L1618	A1536
Q2414	C2342	SER	W2176	GLU	GLU	GLU	GLU	P1971	L1825	S1753	L1683	L1618	A1536
L2415	E2343	GLY	K2102	NET	NET	NET	NET	L1975	H1890	Q1754	H1830	A1613	A1536
K2416	L2344	LYS	H2103	SER	SER	SER	SER	K1895	S1894	M1757	D1685	T1622	S1539
S2417	V2345	ASP	M2104	GLY	GLY	GLY	GLY	F1978	K1895	L1832	L1686	L1623	THR
K2418	A2346	PRO	H2105	GLU	GLU	GLU	PHE	E1979	I1896	E1760	L1688	Q1624	SER

V2565	M2566	M2567	M2568	P2569	D2571	Y2572	P2573	M2574	P2575	M2576	F2577	P2580	L2581	S2583	C2584	E2585	F2586	L2591	D2592	M2595	ARG																																				
PRO	VAL	ALA	GLY	GLN	LYS	ILE	VAL	GLY	THR	GLN	HIS	ASP	PHE	ARG	THR	LEU	ALA	GLY	ASP	GLY	VAL	ARG																																			
ARG	ALA	PRO	VAL	GLN	LYS	ILE	VAL	GLY	THR	GLN	HIS	ASP	PHE	ARG	THR	LEU	ALA	GLY	ASP	GLY	VAL	ARG																																			
GLU	GLN	LYS	ARG	GLU	LYS	ILE	GLU	ILE	LYS	GLN	MET	LYS	LYS	LYS	GLN	GLN	ASP	VAL	VAL	GLY	VAL	ARG																																			
V2769	V2770	L2771	Y2772	R2773	S2774	Y2775	G2778	L2779	D2780	L2781	D2782	L2783	Q2784	L2785	K2786	H2787	S2788	S2789	L2790	L2791	L2792	P2793	L2794	Q2795	A2796	L2803	L2804	A2805	K2806	Q2807	L2808	F2809	F2813																								
GLU	GLN	LYS	ARG	GLU	LYS	ILE	GLU	ILE	LYS	GLN	MET	LYS	LYS	LYS	GLN	GLN	ASP	VAL	VAL	GLY	VAL	ARG	GLU	GLY	VAL	ARG	THR	LEU	ALA	GLN	MET	TVR	ALA	ARG	LYS	GLY	VAL	ALA																			
S2814	G2815	L2816	L2817	K2818	L2819	M2820	D2821	K2824	T2825	L2826	S2827	E2828	K2829	M2830	W2831	L2832	K2835	L2836	D2839	F2840	M2841	F2842	F2843	L2844	W2845	L2846	L2847	F2848	L2783	Q2784	L2785	K2786	H2787	S2788	Q2859	D2860	L2861	S2862	H2865	A2866	L2868	L2869	S2870	L2871	D2872	P2873	A2874	A2875	C2880	L2884	Q2885	Q2886	P2887				
V2888	G2889	L2890	R2891	L2892	L2893	E2894	E2895	A2896	L2897	L2898	R2899	LEU	LEU	PRO	ALA	GLU	LEU	ALA	PRO	LYS	VAL	VAL	ARG	ARG	ARG	ARG	PRO	D2918	D2919	V2920	L2921	R2922	W2923	V2924	E2925	L2926	A2927	K2928	L2929	Y2930	R2931	S2932	L2933	G2934	E2935	Y2936	D2937	V2938	L2939	R2940	G2941	G2942	F2943	L2944	S2945	E2946	L2947
G2948	L2952	A2959	R2962	S2963	E2967	L2968	A2969	K2970	Q2971	L2976	Q2979	D2980	W2981	E2985	P2986	K2991	F2993	W2994	E2995	L2996	A2997	D3000	M3003	H3004	K3009	S3010	Y3013	C3014	S3015	S3018	L3019	F3024	L3027	W3031	F3034	G3035	Y3036	Q3037	E3038	L3039	Y3040																
L3041	M3044	R3046	K3060	Q3064	GLY	GLU	ALA	ASP	Q3069	L3061	L3062	I3065	D3066	M3069	H3070	G3071	E3072	L3073	A3076	I3077	L3078	E3079	H3081	Y3082	S3083	L3086	S3087	L3088	L3089	Y3090	L3091	L3092	Q3093	R3098	A3099	K3100	Y3101	I3102	I3103	Q3104	N3105	G3106	Q3108	M3111	Q3112	N3113											
I3117	S3124	K3128	V3132	Q3133	L3135	L3136	E3137	L3138	F3141	L3142	S3143	S3146	K3147	N3150	L3151	S3152	S3153	Q3154	V3155	F3156	L3157	K3158	R3159	L3160	L3161	N3162	T3163	T3165	N3166	R3167	F3168	P3169	D3170	A3171	K3172	D3174	P3175	M3176	R3177	I3178	W3179	D3180	R3186	F3189	L3190	S3191	K3192	L3193									
E3194	E3195	K3196	L3197	PRO	LEU	PRO	GLU	ASP	ASN	GLN	ASP	GLY	ASP	PRO	SER	ASP	ARG	MET	GLU	VAL	GLN	GLU	GLU	GLU	D3226	R3232	S3233	K3235	F3236	S3237	M3238	K3239	M3240	K3241	M3242	I3243	D3244	S3245	A3246	M3251	L3254	A3255	M3256	K3257	L3258	L3259	K3260	E3261									
L3262	E3265	T3268	R3269	D3270	D3271	W3272	L3273	V3274	S3275	Q3278	F3279	Y3280	L3282	C3281	R3282	L3283	S3284	H3285	S3288	R3289	S3290	Q3291	G3292	C3293	V3297	L3301	K3302	L3306	LEU	ASP	GLU	ASN	ASN	V3312	Y3315	L3316	A3322	Q3326	L3330	G3331	T3332	L3333	R3335	L3336	I3337	A3338	N3339										
E3344	C3347	L3348	I3351	E3352	E3353	A3356	I3359	L3360	E3361	L3362	S3363	G3364	S3365	S3366	S3367	K3372	V3373	I3374	A3375	G3376	L3377	Q3378	R3380	A3381	F3382	Q3383	H3384	R3385	V3389	E3394	ALA	ALA	GLN	PRO	PRO	SER	TRP	ALA	G3408	V3409	Y3413	M3414	T3415	A3416	L3416												
D3418	F3419	C3420	D3421	Q3422	R3425	F3429	ASN	ALA	SER	VAL	ILE	SER	ALA	VAL	L3439	L3445	V3446	V3447	F3448	K3449	R3450	L3454	Q3378	R3380	A3381	F3382	Q3383	H3384	R3462	L3463	F3464	F3465	R3466	R3467	L3468	L3469	Q3470	L3471	L3472	Y3475	E3478	T3479	L3480	S3481	L3482	R3483	T3484	R3485	F3486	L3487							
V3490	P3491	C3492	W3493	Q3494	F3495	L3496	S3497	W3498	L3499	S3500	H3501	M3502	V3503	A3504	L3505	K3508	A3511	V3512	Q3515	V3518	E3519	E3520	N3524	Y3525	F3526	A3528	L3529	V3530	Y3531	P3532	F3533	I3534	L3535	S3536	S3537	E3538	S3539	Y3540	F3542	K3543	D3544	T3545	S3546	T3547	G3548	H3549	K3550	F3554	L3558								
L3562	ASP	GLN	GLY	G3566	V3567	I3568	S3569	D3570	F3571	L3572	N3573	A3574	L3575	D3576	Q3577	P3581	L3584	F3585	W3588	S3589	Y3592	E3593	L3596	A3597	K3598	THR	PRO	VAL	ASN	K3603	I3606	M3609	Y3610	E3611	R3612	M3613	L3617	A3622	P3623	G3624	G3626	A3627	F3628	R3629	R3630	K3631	F3632	I3633									













K129	D201	L267	F340	R404	Y473	GLY
R130	L202	V268	D341	N405	R474	SER
F131	M203	I269	D342	I406	S475	ARG
Q132	H204	S270	P343	P407	D476	LYS
D133	L205	V271	G344	P408	S477	PRO
M134	K206	Q272	L345	Y409	F478	PRO
M135	K207	I273	M346	F410	E479	VAL
G136	F211	Y274	L347	V411	M480	GLU
H137	D212	M275	M348	A412	P481	TYR
G138	I213	L276	G349	L413	V482	TYR
S139	I214	L277	F350	V414	L483	SER
D140	S214	Q278	K351	Q415	Q484	GLU
D141	Y141	L281	P352	Q416	Q485	GLU
S142	R218	L282	L353	E417	H486	LEU
L143	S222	P283	V354	E419	F487	LYS
E145	I144	P283	L355	E419	R488	THR
E146	A147	K287	K357	Q423	L489	I148
L147	ALA	L288	Y361	K424	L493	SER
C150	GLU	Y289	H360	I425	L493	LYS
L153	ASP	R290	Y361	Q426	M498	GLY
F154	ASP	E291	L362	V427	E499	THR
S155	LEU	T292	R363	T428	P500	GLU
D156	ARG	E294	P364	P429	P500	LYS
V157	VAL	P295	S365	P430	E512	PHE
K160	HIS	V295	L366	Q431	A513	THR
M161	PHE	K297	F367	F432	M514	THR
S162	SER	T300	V368	Q433	M514	VAL
H163	S237	R301	E372	L434	K516	PRO
K164	K238	R301	S373	P436	R517	LEU
R165	K239	R301	L374	L437	L518	LYS
I166	E240	R301	V375	A440	D523	GLU
M167	D241	R301	I376	D441	E524	ALA
F168	L242	R301	G377	D442	F525	CYS
F169	L243	R301	S378	K443	K526	ARG
T170	R244	R301	S379	R444	E527	ALA
M171	K245	R301	T380	K445	L528	TYR
E172	V246	R301	L381	M446	P531	GLY
D173	R247	R301	F382	M453	P532	LYS
M174	A248	R301	A384	A454	D533	SER
A183	K249	R301	L385	E457	Y534	GLY
R187	R252	R301	L386	Q458	ASN	LYS
K189	K253	R301	I387	V459	PRO	LYS
A190	A254	R301	C389	V459	GLU	GLN
G191	L256	R301	K392	K461	GLY	GLN
D192	S257	R301	E393	M462	VAL	LEU
L193	R258	R301	V394	K463	THR	GLU
R194	L259	R301	L397	A464	ALA	ALA
D195	K260	R301	E333	V465	LYS	GLU
T196	L261	R301	E334	V466	ARG	LEU
G197	K262	R301	R399	E467	LYS	THR
L198	L263	R301	Y400	K468	HIS	LYS
F199	K264	R301	L469	L469	ASP	PHE
L200	D266	R301	R401	R470	ASN	ASN
		R301	P402	F471	GLU	GLY
		R301	R403	T472	SER	ASP

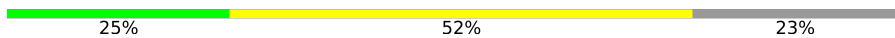
• Molecule 5: X-ray repair cross-complementing protein 6

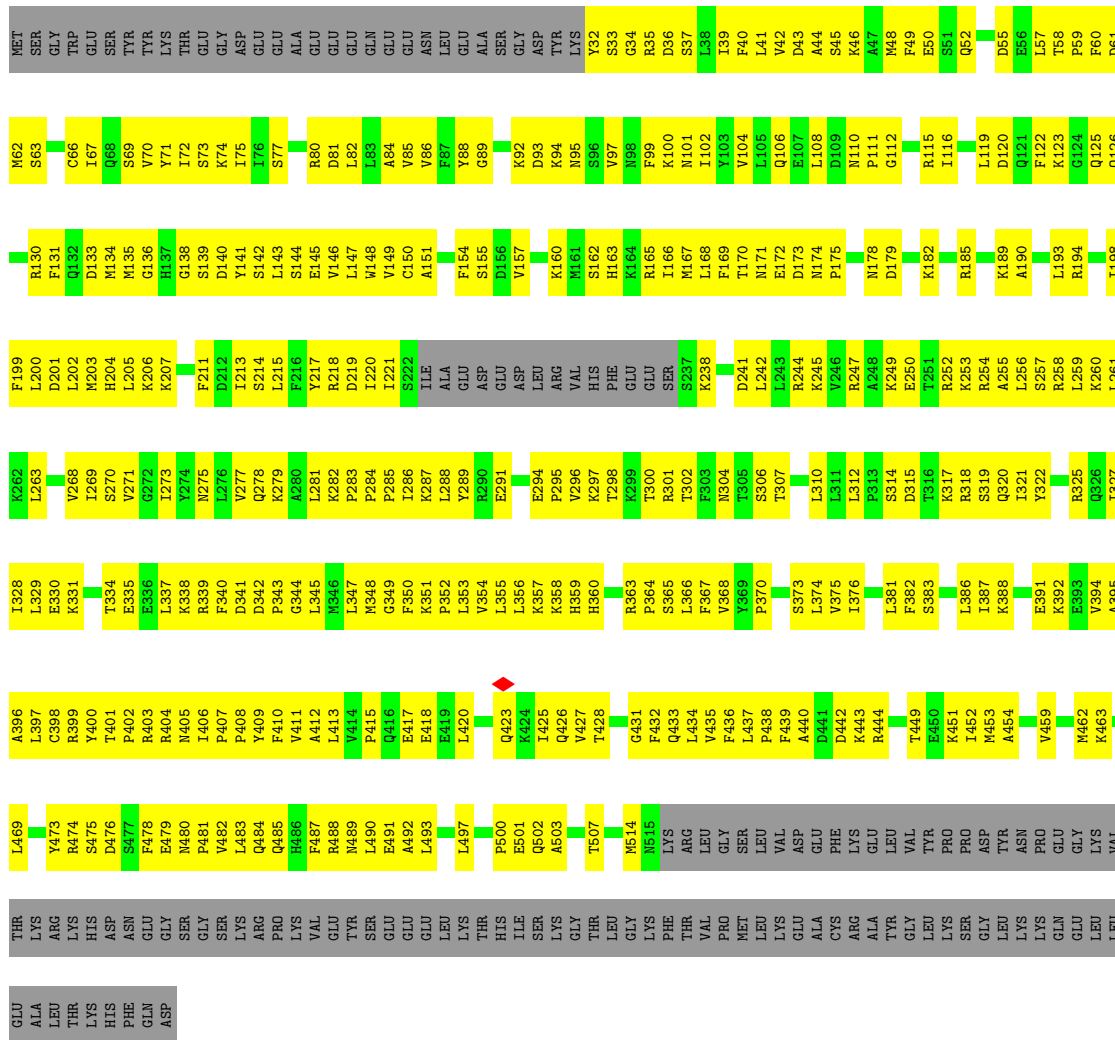


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SER	K74	S156	D156	E294	Y361	V427	D505
GLY	I75	D156	W157	P295	R362	T428	L506
TRP	I76	Q157	W158	V296	P363	P429	T507
GLU	S77	Q158	W159	K297	S364	P430	L508
LYS	S78	Q158	F159	T298	P365	Q433	P509
VAL	D79	K160	K160	K299	L366	L434	K510
TYR	R80	M161	V161	T300	F367	L434	V511
LYS	R80	M161	V161	T302	V368	V435	V512
THR	D81	H163	H163	F303	Y369	F436	E512
GLU	L82	PHE	PHE	N304	P370	L437	L518
GLY	L83	K164	K164	N304	E371	P438	M515
ASP	A84	H165	H165	T305	E372	F439	K516
GLU	V85	I166	I166	S396	S373	A440	R517
LEU	Y88	M167	L168	T307	L374	D442	L518
GLU	O89	F169	L168	G308	V375	D442	G519
LYS	O89	F169	L168	G309	V375	D442	G519
ALA	D93	T170	T170	L310	I376	K443	S520
GLU	K94	M171	M171	L311	G377	R444	L521
GLN	N95	E172	E172	L312	S378	K445	V522
GLU	N95	E172	E172	L312	S378	M446	D523
GLU	N98	P175	P175	L313	L381	E524	E524
LEU	F99	HIS	GLY	K100	GLY	I452	K526
GLY	N101	ASN	ASN	K100	ASN	T455	E527
ALA	I102	SER	SER	N101	ASP	T455	Y530
GLY	Y103	ASP	ASP	I102	ASP	P456	P531
TYR	V104	A181	A181	Y103	SER	Q458	P532
PRO	L105	K182	K182	V104	L256	V459	D533
LEU	Q106	A183	A183	Q106	L256	G460	Y534
LYS	E107	S184	S184	Q106	L259	K461	ASN
LYS	L108	R185	R185	Q107	K262	M462	PRO
GLU	P111	A186	A186	L108	K262	M462	PRO
ALA	G112	R187	R187	S33	L263	K463	GLU
ALA	G112	R187	R187	G34	L263	K463	GLU
TYR	L119	K189	K189	R35	M264	L469	LYS
GLY	D120	I198	I198	D36	D266	R470	VAL
LEU	Q121	F199	F199	F40	D267	P401	THR
LYS	F122	L200	L200	A44	L267	P402	LYS
ARG	K123	D201	D201	S45	V268	R403	ARG
GLY	G124	L202	L202	K46	I269	R404	ARG
LEU	Q125	M203	M203	M48	S270	M405	LYS
LYS	Q126	H204	H204	F49	V271	N406	HIS
LYS	Q126	H204	H204	F49	G272	I406	HIS
LYS	Q127	L205	L205	E50	T273	P407	ASP
GLN	Q128	K206	K206	SER	Y274	P408	ASN
GLY	K129	LYS	LYS	SER	M275	V411	GLY
VAL	R130	PRO	PRO	SER	L276	A412	SER
LEU	F131	GLY	GLY	GLY	V277	G344	SER
GLU	G138	GLY	GLY	GLY	Q278	L413	LYS
GLU	Y141	L143	L143	GLU	K279	V414	ARG
THR	S142	S144	S144	GLU	P283	P415	PRO
ASP	F60	R218	R218	ASP	P284	Q416	PRO
ASN	I64	D219	D219	GLU	P285	E417	LYS
GLY	Q65	V146	V146	GLU	P286	E418	LYS
SER	C66	L147	L147	GLU	K287	E419	VAL
				GLU	L288	F419	GLU
				GLU	R289	L420	TYR
				GLU	Y290	L353	SER
				GLU	R290	V354	ARG
				GLU	R290	M348	PRO
				GLU	R290	K351	LYS
				GLU	R290	P352	LYS
				GLU	R290	L353	VAL
				GLU	R290	L420	GLU
				GLU	R290	D421	GLU
				GLU	R290	D422	GLU
				GLU	R290	K357	GLU
				GLU	R290	K358	GLU
				GLU	R290	K424	GLU
				GLU	R290	L425	LEU
				GLU	R290	P500	LEU

LYS	THR	GLY	HIS	ILE	SER	GLU	LYS	GLY	THR	LEU	LEU	GLY	LYS	THR	THR	PRO	MET	ALA	LEU	LYS	LYS	GLU	GLY	GLU	GLU	ALA	ALA	CYS	ARG	ALA	ASN	ALA	TYR	TYR	GLY	GLY	LEU	LEU	LYS	LYS	GLN	GLU	G34	G34	R35	D36	S37	L38	I39	F40	L41	L42	L43	D44	S45	K46	A47	M48	F49	E50	S51	Q52	D55	E56	L57	T58	F59	F60	D61
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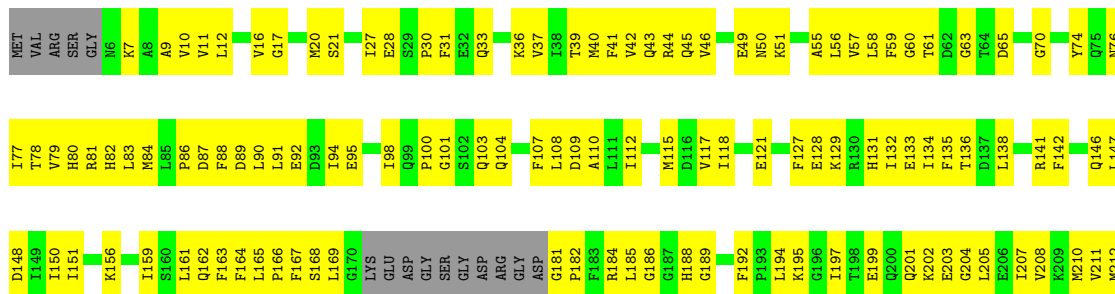
• Molecule 5: X-ray repair cross-complementing protein 6

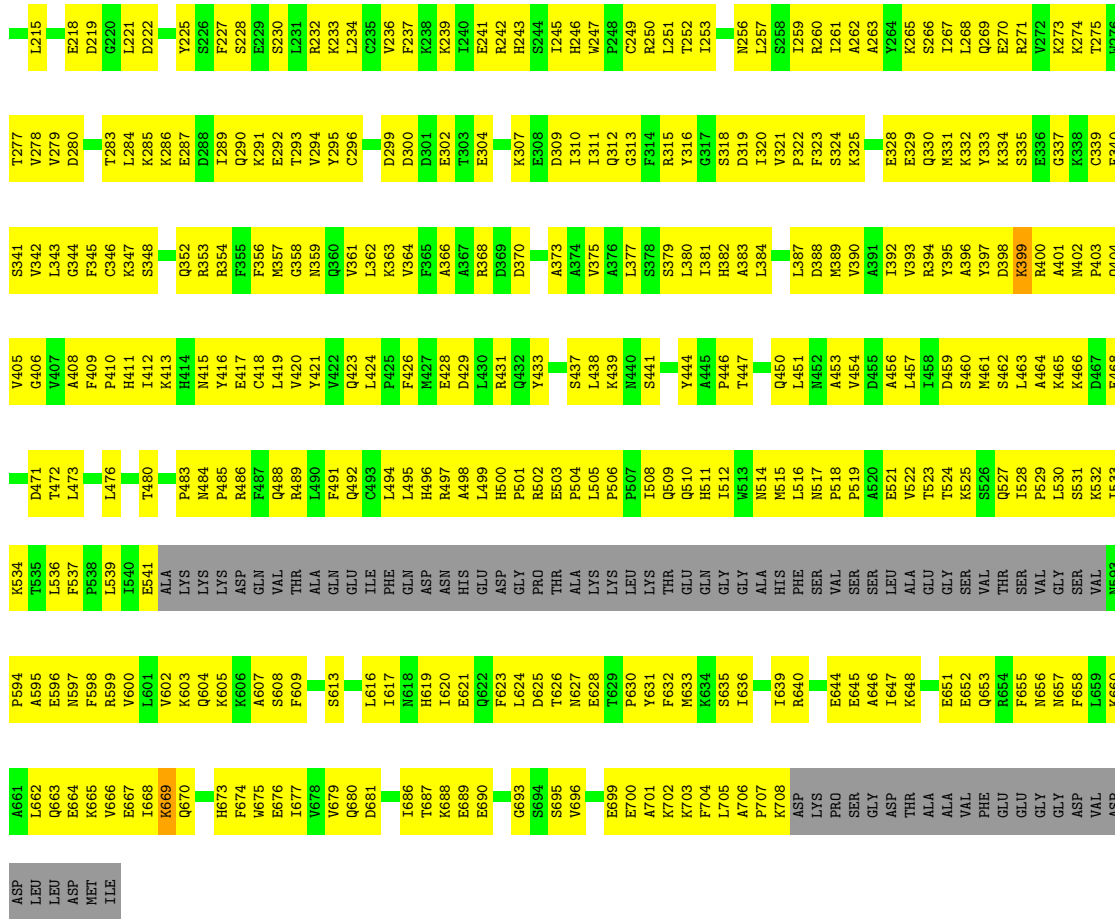
Chain T: 



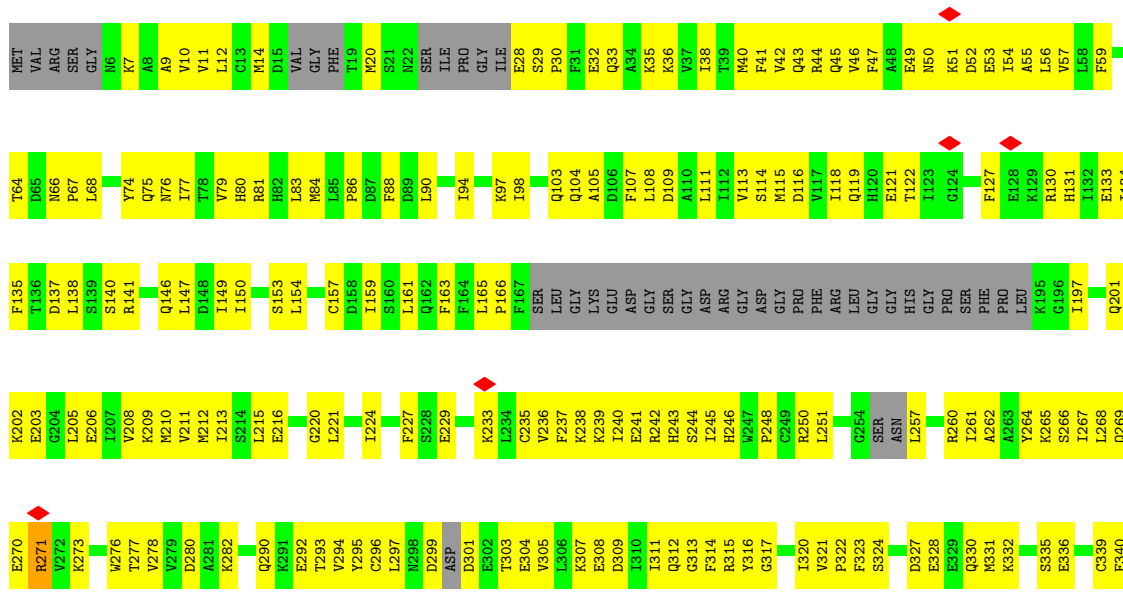
• Molecule 6: X-ray repair cross-complementing protein 5

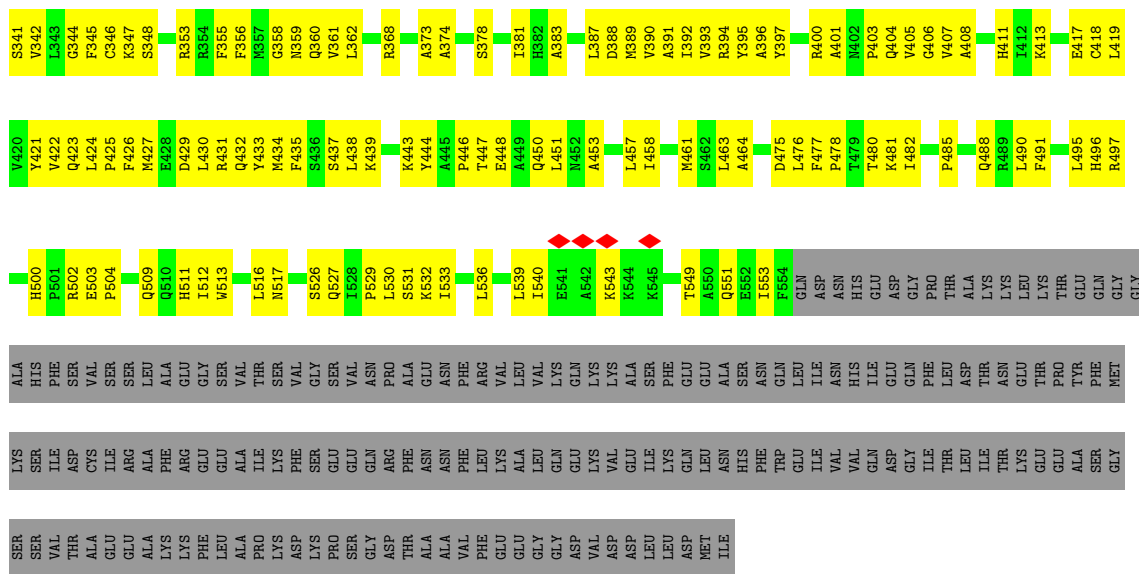
Chain H: 





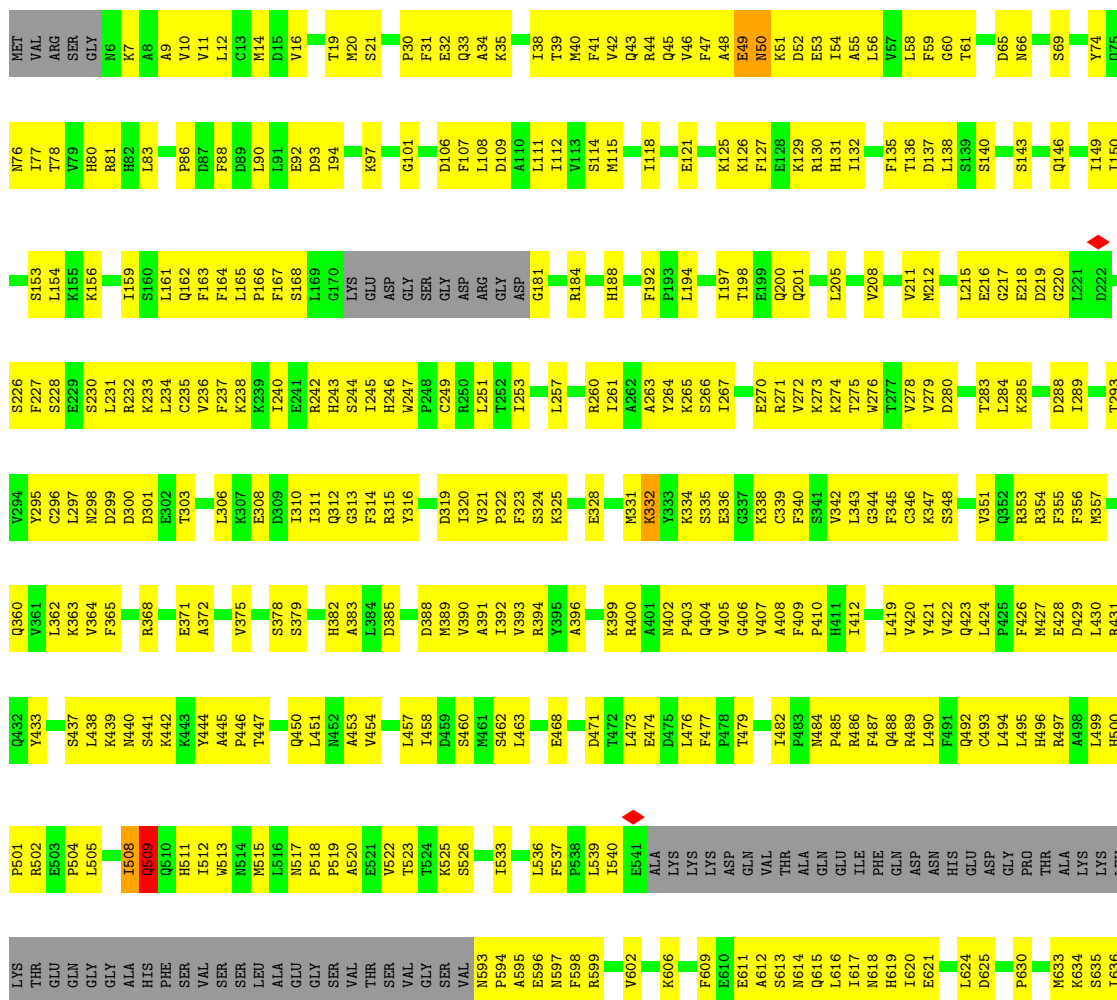
• Molecule 6: X-ray repair cross-complementing protein 5

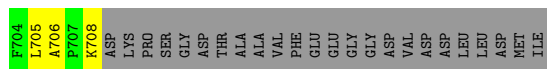




● Molecule 6: X-ray repair cross-complementing protein 5

Chain U: 34% 53% 12%

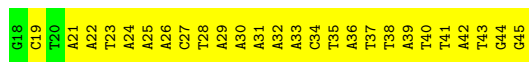




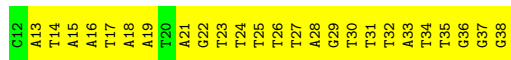
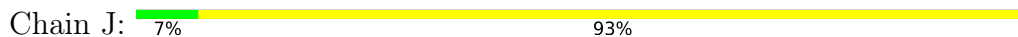
• Molecule 7: DNA (28-MER)



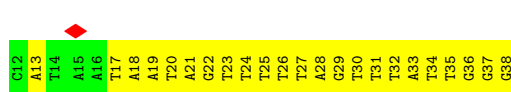
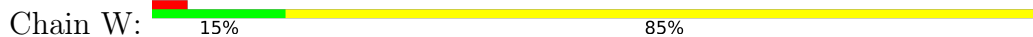
• Molecule 7: DNA (28-MER)



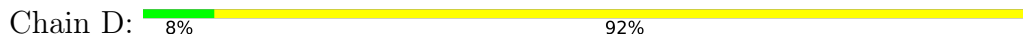
• Molecule 8: DNA (27-MER)



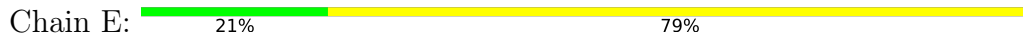
• Molecule 8: DNA (27-MER)



• 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 ( $\text{\AA}$ )	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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	0.29	0/1647	0.55	0/2215
1	L	0.29	0/1605	0.55	0/2155
1	N	0.27	0/1654	0.51	0/2224
1	O	0.25	0/1603	0.51	0/2154
2	M	0.26	0/2135	0.50	0/2883
2	P	0.30	0/2140	0.50	0/2890
3	Q	0.26	0/1755	0.54	0/2377
3	R	0.26	0/1773	0.53	0/2402
3	X	0.27	0/1766	0.51	0/2392
3	Y	0.24	0/1773	0.49	0/2402
4	A	0.27	0/27902	0.50	0/37795
4	F	0.31	0/28192	0.54	1/38135 (0.0%)
4	S	0.27	0/28373	0.51	1/38372 (0.0%)
5	B	0.28	0/3712	0.52	0/5018
5	G	0.30	0/4000	0.55	0/5388
5	T	0.27	0/3833	0.56	0/5160
6	C	0.26	0/4039	0.50	0/5457
6	H	0.28	0/5232	0.52	0/7057
6	U	0.27	0/5246	0.54	0/7075
7	I	0.69	1/647 (0.2%)	1.06	3/996 (0.3%)
7	V	0.51	0/647	0.95	0/996
8	J	0.68	0/623	1.11	0/961
8	W	0.54	0/623	1.01	0/961
9	D	0.63	0/554	0.94	0/852
10	E	0.57	0/552	1.10	0/851
All	All	0.29	1/132026 (0.0%)	0.54	5/179168 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	42	DA	O3'-P	5.67	1.68	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	25	DA	P-O3'-C3'	-8.62	109.36	119.70
7	I	26	DA	P-O3'-C3'	-7.91	110.21	119.70
7	I	24	DA	P-O3'-C3'	-7.13	111.14	119.70
4	S	956	PRO	N-CA-CB	6.08	110.60	103.30
4	F	3685	PRO	N-CA-CB	-5.38	96.68	102.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1618	0	1597	156	0
1	L	1579	0	1564	147	0
1	N	1625	0	1611	129	0
1	O	1577	0	1557	109	0
2	M	2087	0	2036	192	0
2	P	2091	0	2042	166	0
3	Q	1723	0	1733	161	0
3	R	1739	0	1754	166	0
3	X	1733	0	1749	58	0
3	Y	1739	0	1754	79	0
4	A	27365	0	26865	1703	0
4	F	27665	0	27584	2153	0
4	S	27830	0	27817	1924	0
5	B	3646	0	3608	304	0
5	G	3924	0	3997	405	0
5	T	3764	0	3852	411	0
6	C	3968	0	3876	296	0
6	H	5128	0	5128	500	0
6	U	5143	0	5166	489	0
7	I	576	0	318	69	0
7	V	576	0	318	67	0
8	J	557	0	311	59	0
8	W	557	0	311	65	0
9	D	493	0	273	46	0
10	E	494	0	278	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	129197	0	127099	9101	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 36.

The worst 5 of 9101 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%)	15	55
1	L	191/336 (57%)	169 (88%)	19 (10%)	3 (2%)	9	44
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%)	34	72
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Y	214/299 (72%)	198 (92%)	16 (8%)	0	100	100
4	A	3448/4128 (84%)	3149 (91%)	294 (8%)	5 (0%)	51	86
4	F	3463/4128 (84%)	3030 (88%)	419 (12%)	14 (0%)	34	72
4	S	3464/4128 (84%)	3094 (89%)	361 (10%)	9 (0%)	41	77
5	B	463/609 (76%)	403 (87%)	59 (13%)	1 (0%)	47	81
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%)	34	72
6	H	636/732 (87%)	549 (86%)	87 (14%)	0	100	100
6	U	636/732 (87%)	552 (87%)	82 (13%)	2 (0%)	41	77
All	All	15708/20769 (76%)	14007 (89%)	1662 (11%)	39 (0%)	50	81

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 [i](#)

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%)	174 (99%)	2 (1%)	73	84
1	L	173/303 (57%)	165 (95%)	8 (5%)	27	52
1	N	179/303 (59%)	176 (98%)	3 (2%)	60	78
1	O	173/303 (57%)	173 (100%)	0	100	100
2	M	232/808 (29%)	231 (100%)	1 (0%)	91	94
2	P	233/808 (29%)	226 (97%)	7 (3%)	41	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	191/262 (73%)	190 (100%)	1 (0%)	88	93
3	R	194/262 (74%)	193 (100%)	1 (0%)	88	93
3	X	193/262 (74%)	189 (98%)	4 (2%)	53	72
3	Y	194/262 (74%)	193 (100%)	1 (0%)	88	93
4	A	2916/3671 (79%)	2899 (99%)	17 (1%)	86	92
4	F	2987/3671 (81%)	2949 (99%)	38 (1%)	69	81
4	S	3020/3671 (82%)	3001 (99%)	19 (1%)	86	92
5	B	387/548 (71%)	386 (100%)	1 (0%)	92	95
5	G	436/548 (80%)	435 (100%)	1 (0%)	93	96
5	T	422/548 (77%)	422 (100%)	0	100	100
6	C	426/649 (66%)	423 (99%)	3 (1%)	84	90
6	H	567/649 (87%)	562 (99%)	5 (1%)	78	87
6	U	573/649 (88%)	569 (99%)	4 (1%)	84	90
All	All	13672/18480 (74%)	13556 (99%)	116 (1%)	82	89

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	3901	ARG
6	U	509	GLN
4	A	891	ARG
6	U	508	ILE
4	S	2369	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	510	GLN
4	A	3422	GLN
3	Y	11	GLN
4	A	753	GLN
4	A	2859	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

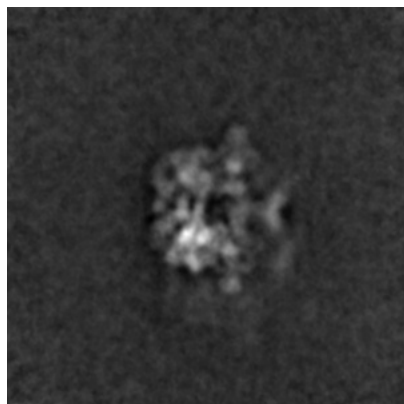
## 6 Map visualisation [i](#)

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.

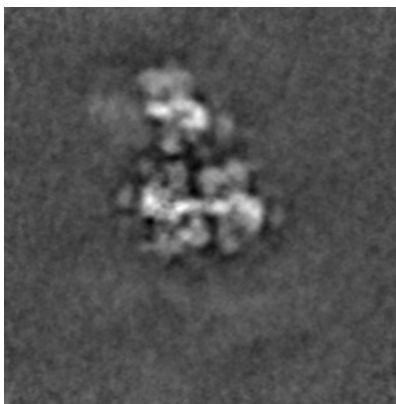
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

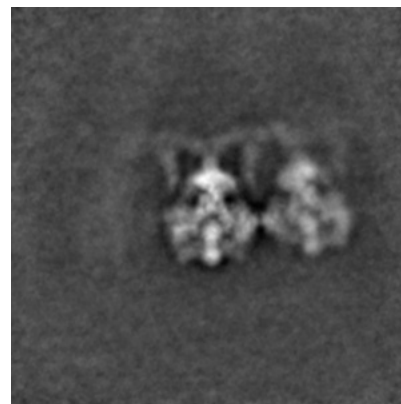
#### 6.1.1 Primary map



X

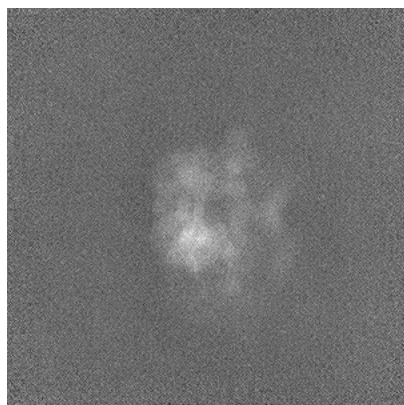


Y

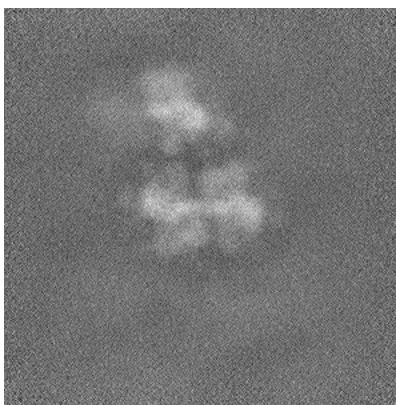


Z

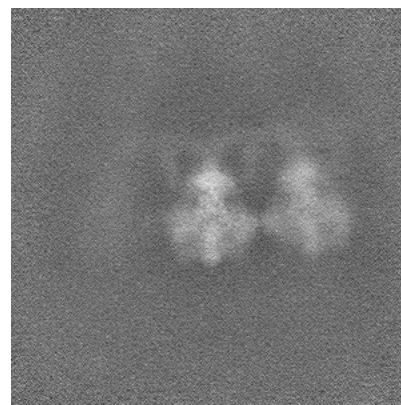
#### 6.1.2 Raw map



X



Y

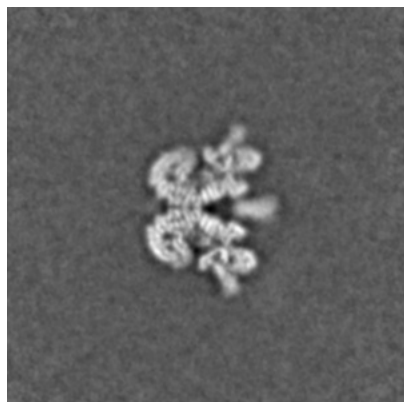


Z

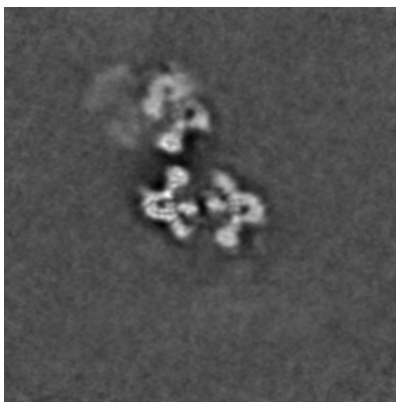
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

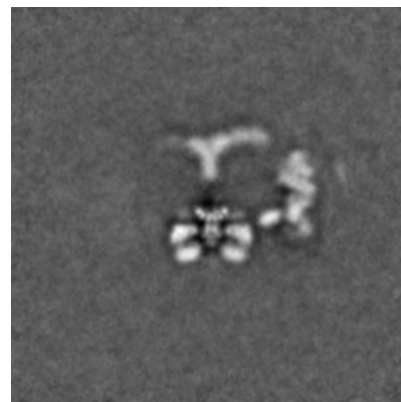
### 6.2.1 Primary map



X Index: 270

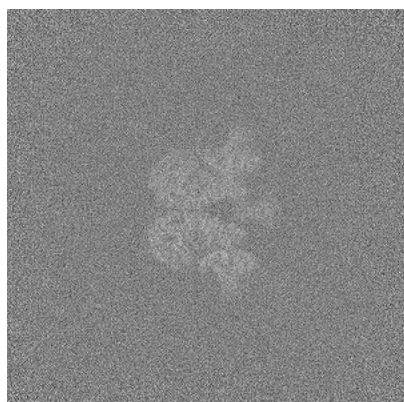


Y Index: 270

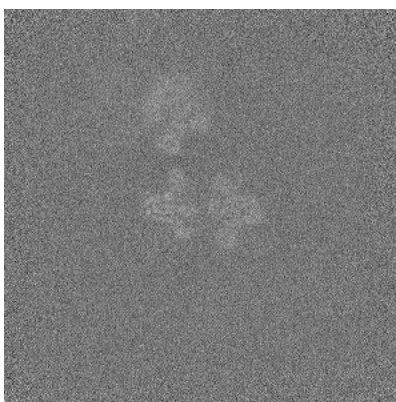


Z Index: 270

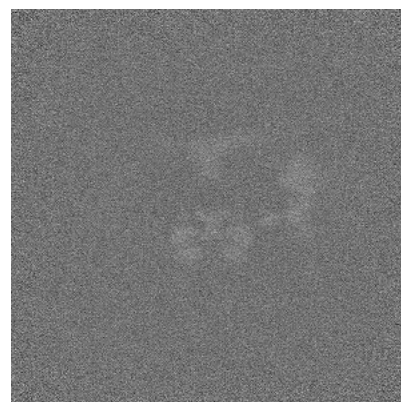
### 6.2.2 Raw map



X Index: 270



Y Index: 270

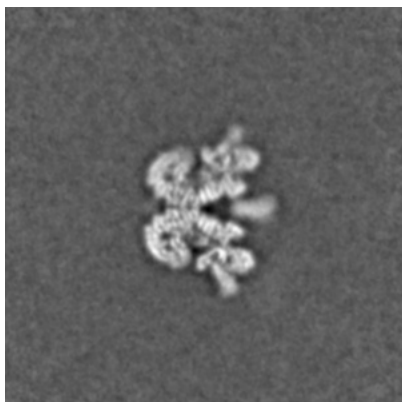


Z Index: 270

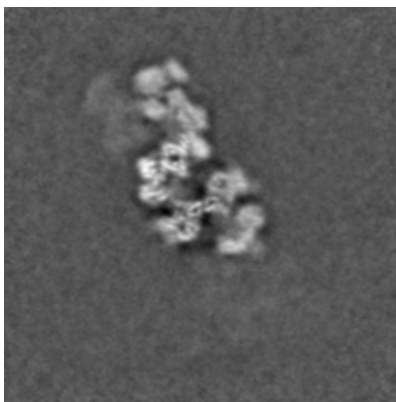
The images above show central slices of the map in three orthogonal directions.

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

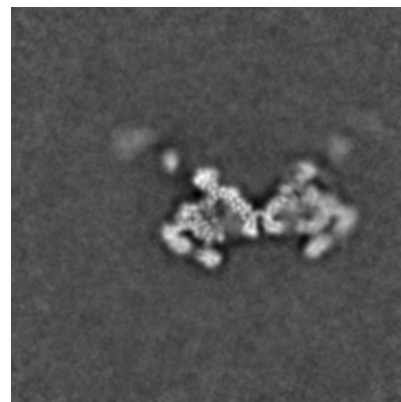
### 6.3.1 Primary map



X Index: 271

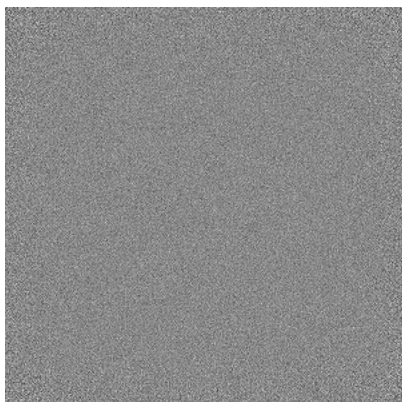


Y Index: 251

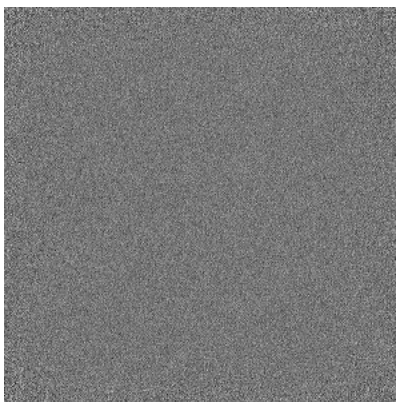


Z Index: 233

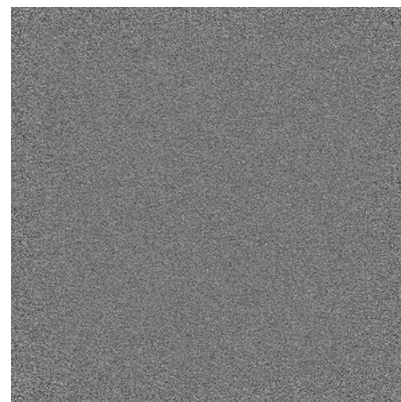
### 6.3.2 Raw map



X Index: 0



Y Index: 0

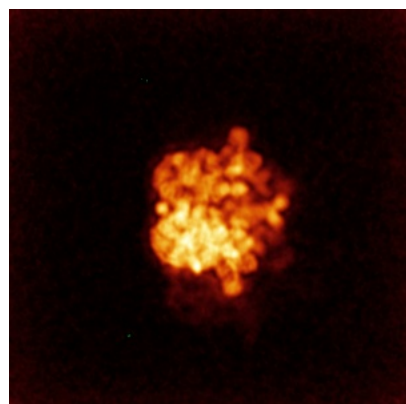


Z Index: 0

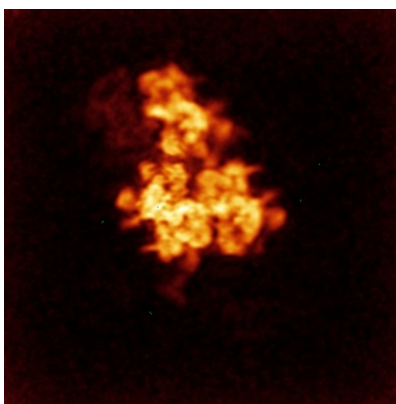
The images above show the largest variance slices of the map in three orthogonal directions.

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

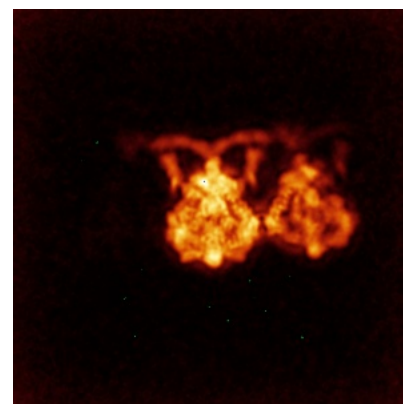
### 6.4.1 Primary map



X

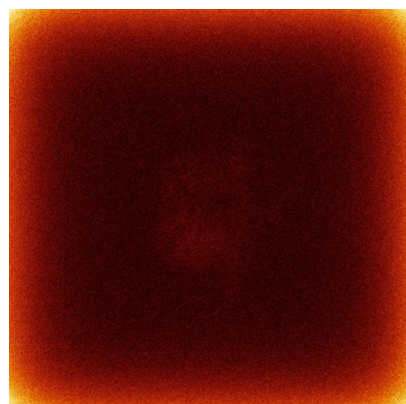


Y

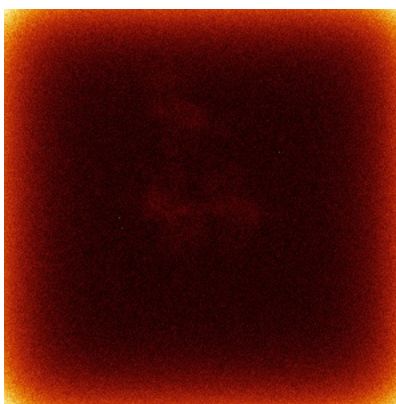


Z

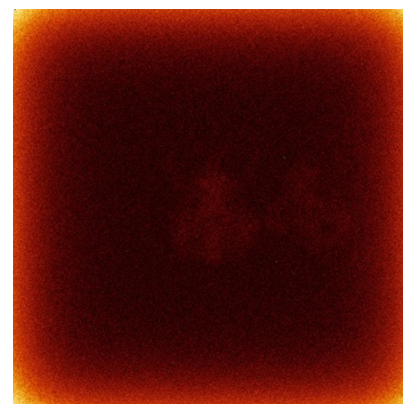
### 6.4.2 Raw map



X



Y



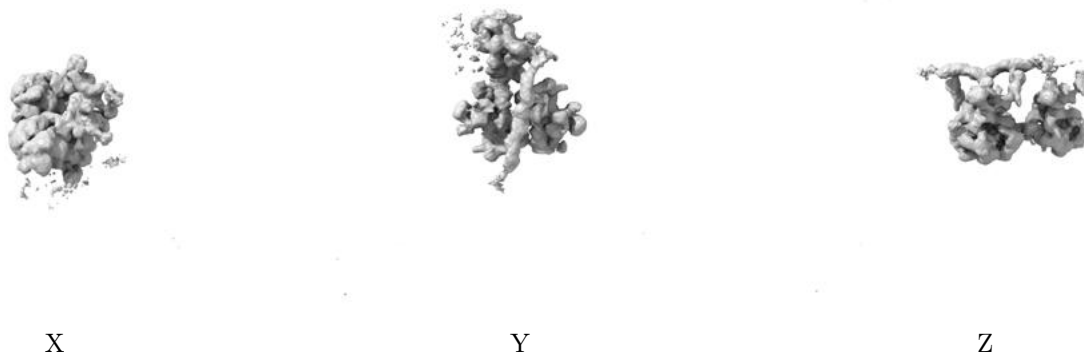
Z

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.



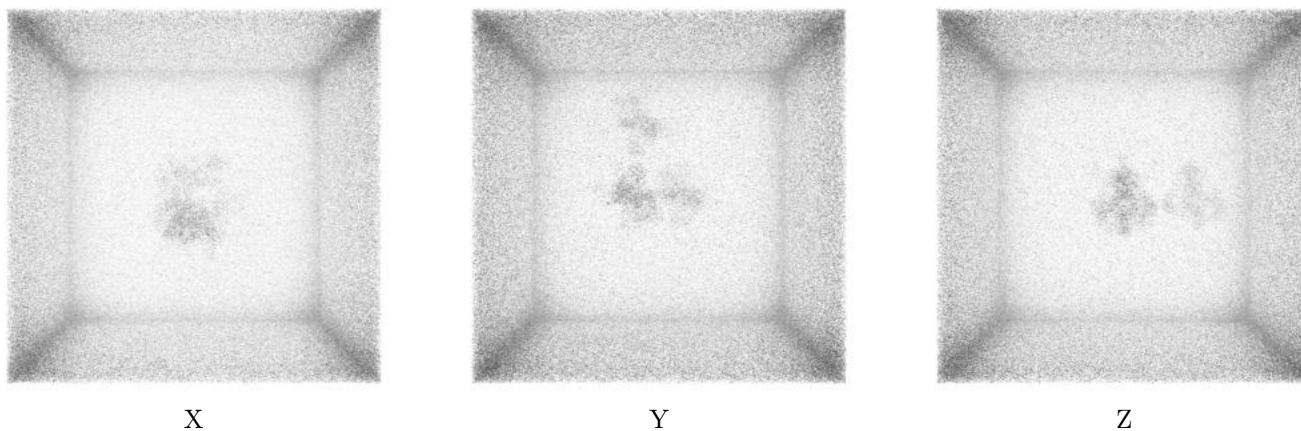
## 6.5 Orthogonal surface views [i](#)

### 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.

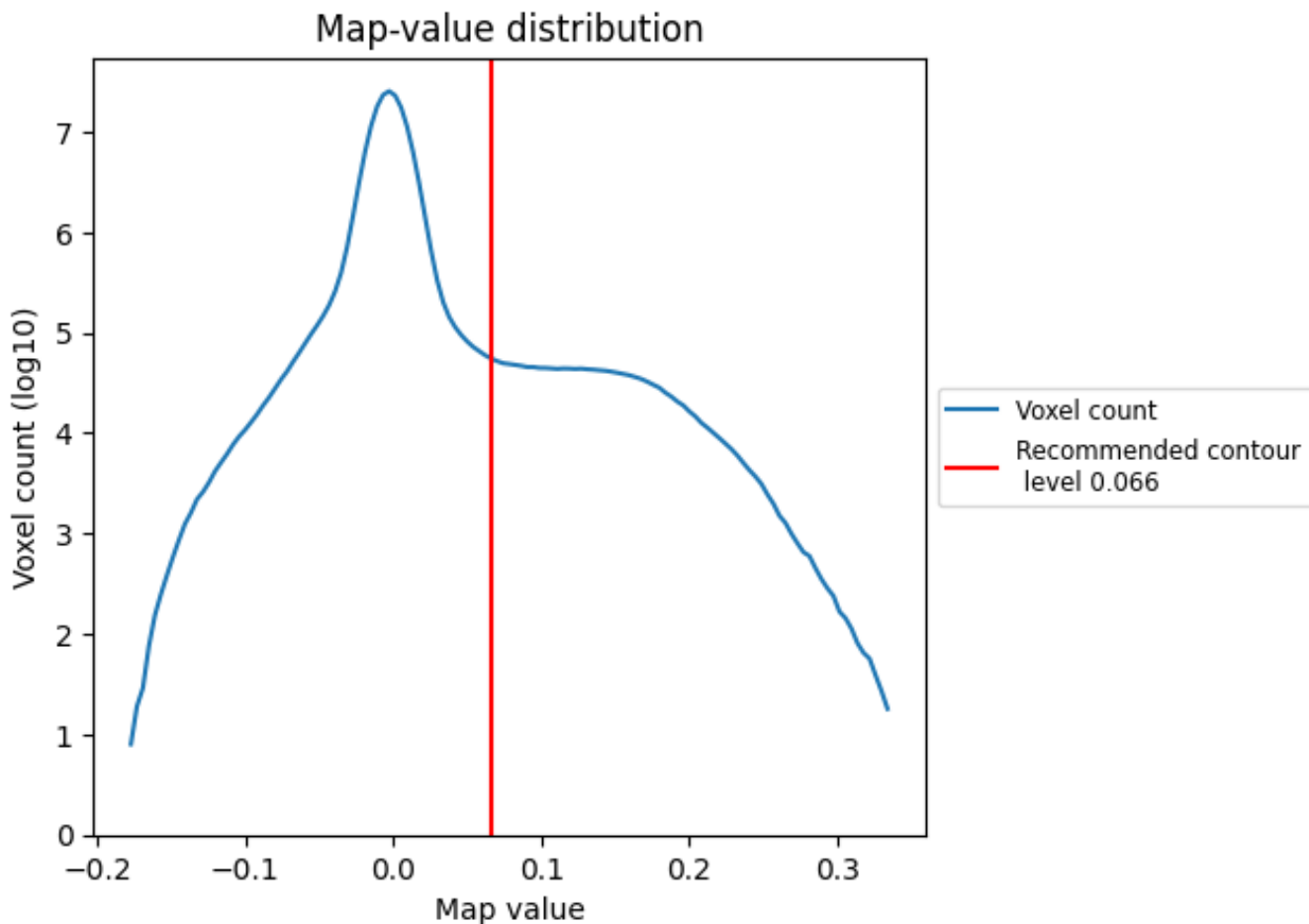
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

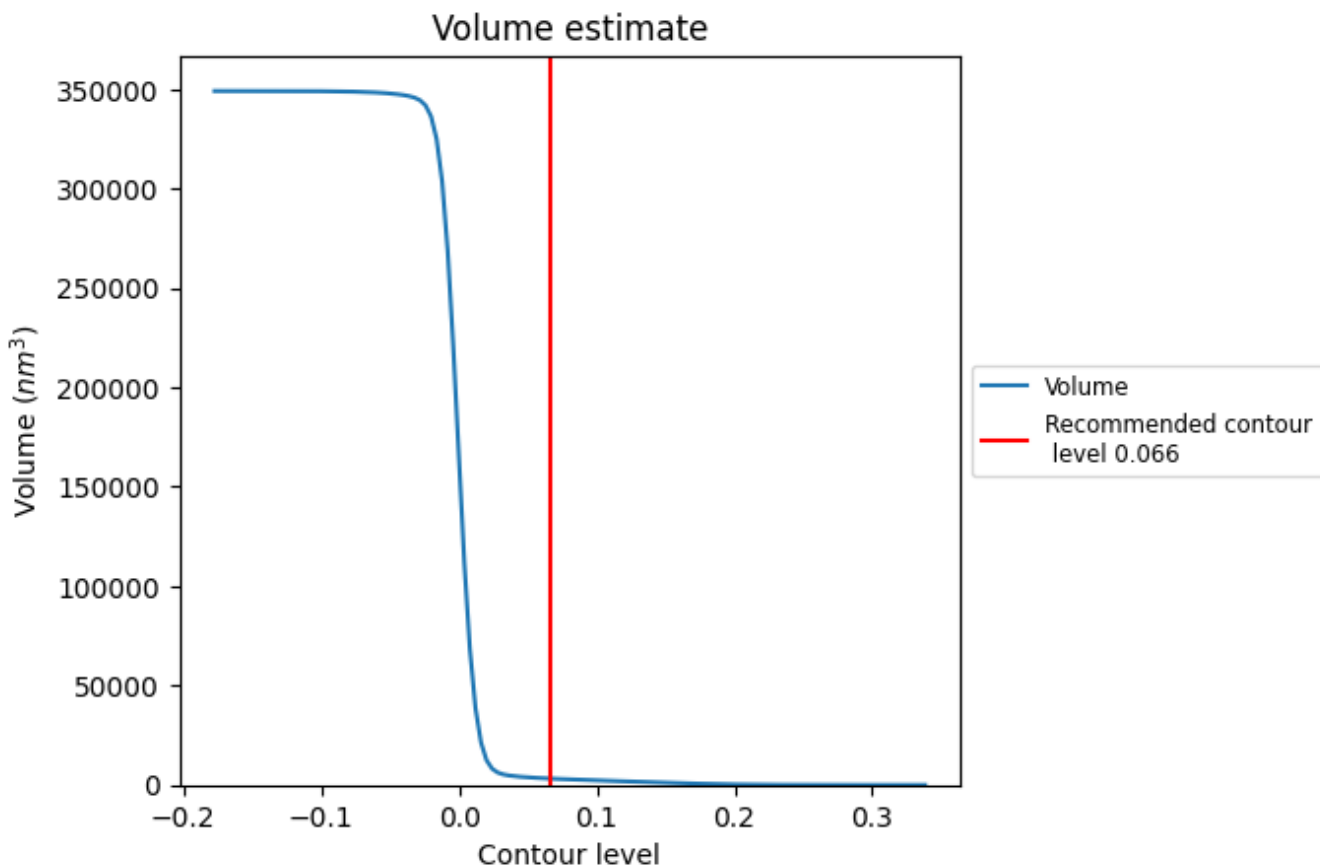
This section contains the results of statistical analysis of the map.

### 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.

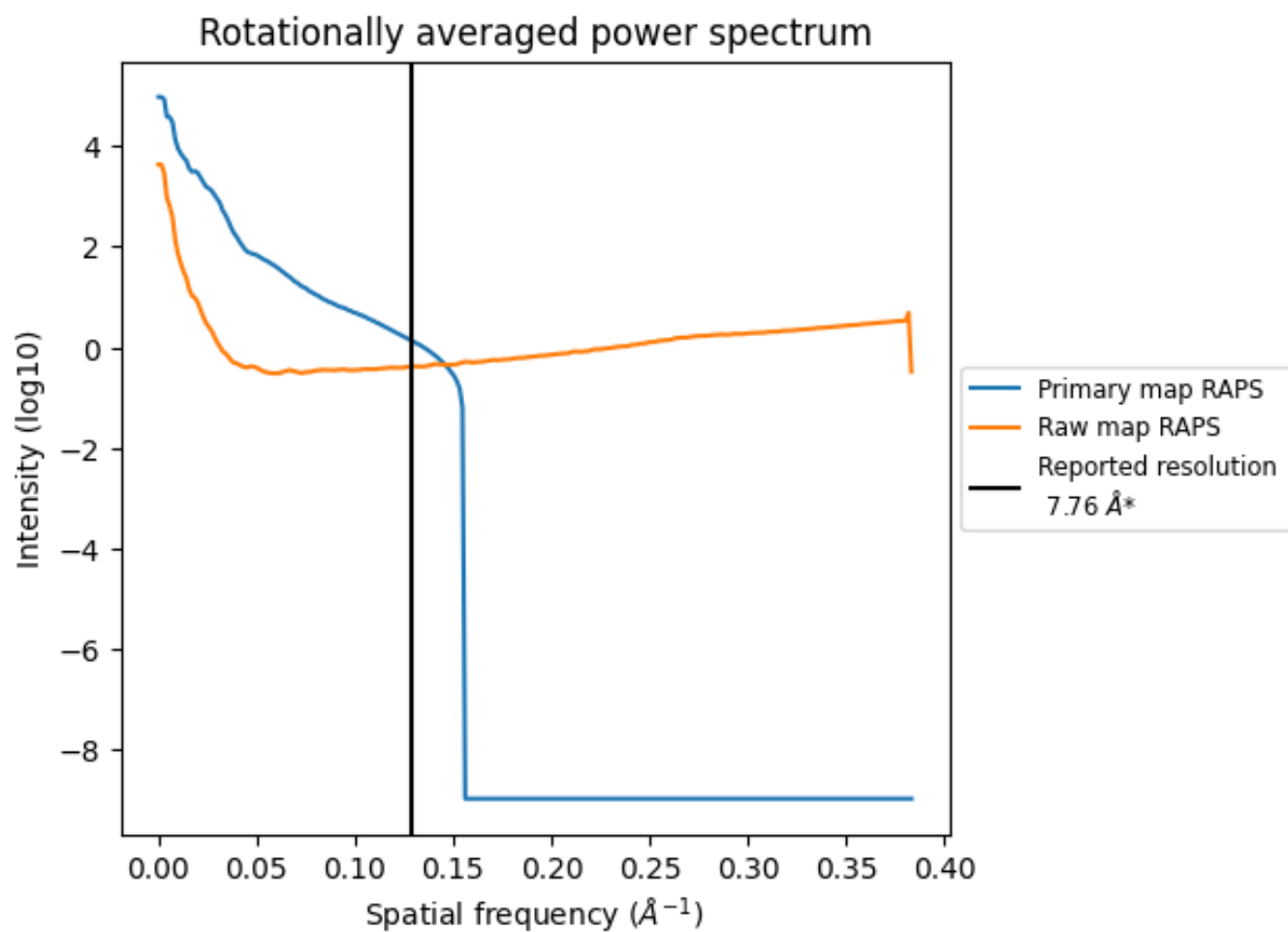
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3218 nm<sup>3</sup>; 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 [i](#)

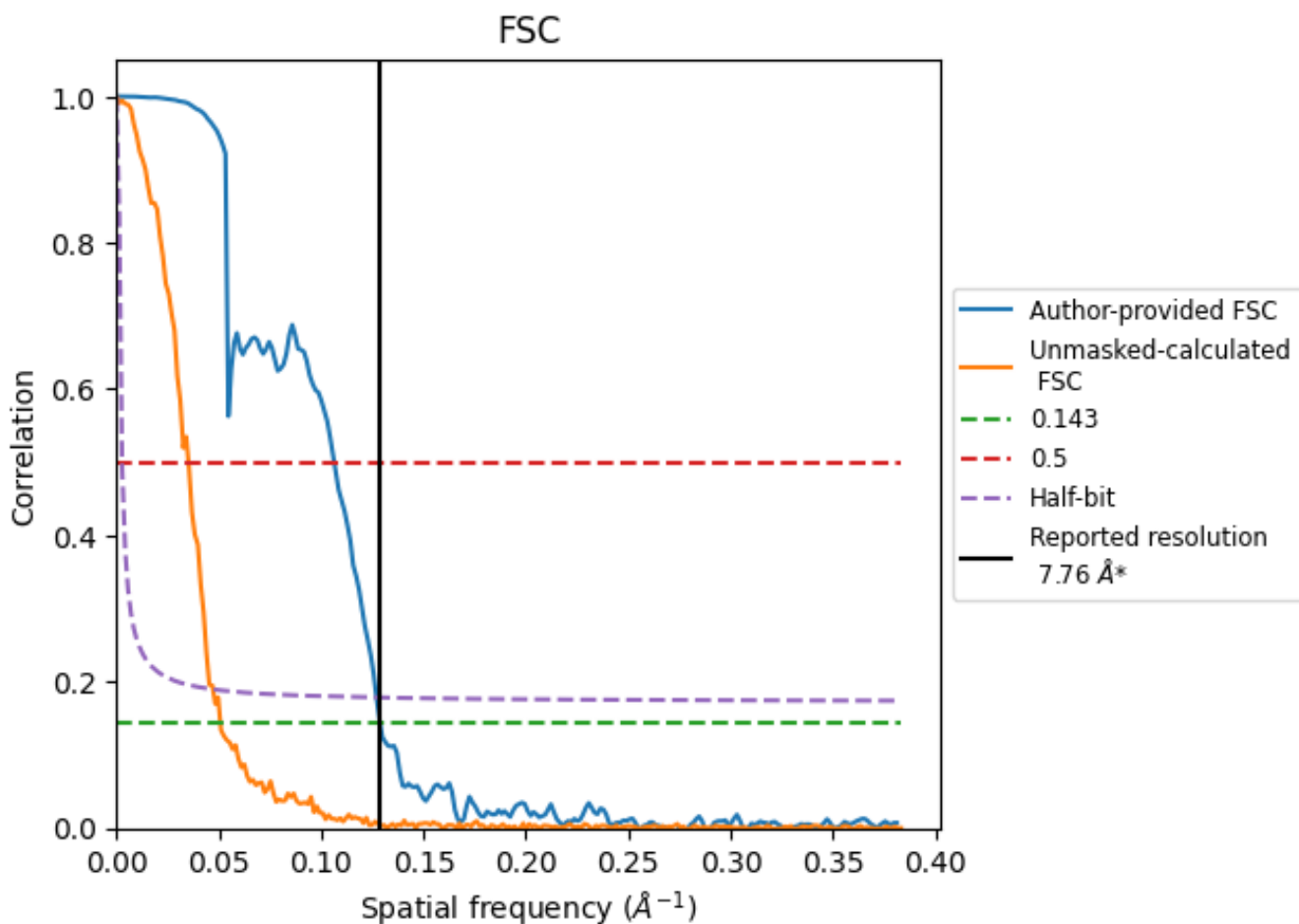


\*Reported resolution corresponds to spatial frequency of 0.129 Å<sup>-1</sup>

## 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  $0.129 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

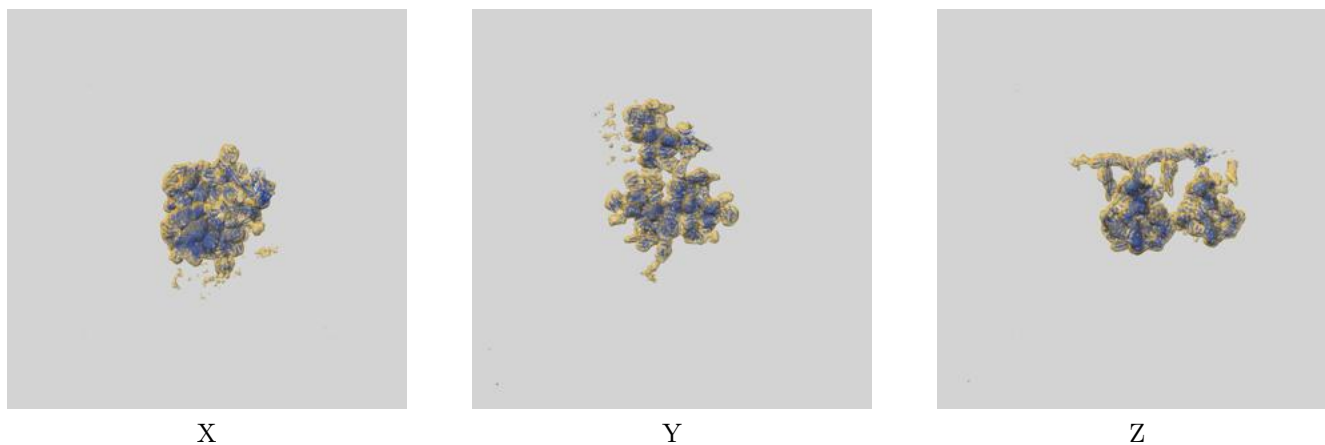
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.76	-	-
Author-provided FSC curve	7.76	9.40	7.87
Unmasked-calculated*	19.69	28.41	21.19

\*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](#)

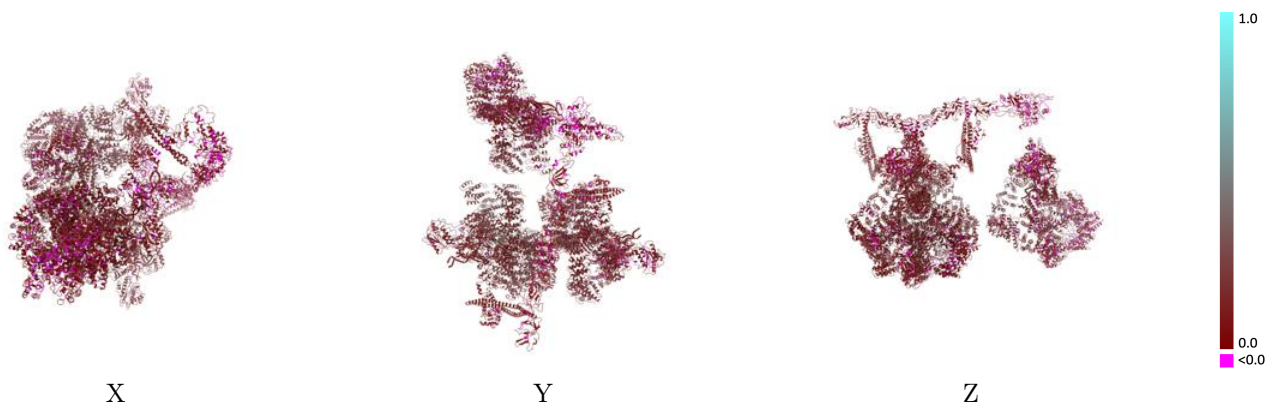
This section contains information regarding the fit between EMDB map EMD-16145 and PDB model 8BOT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



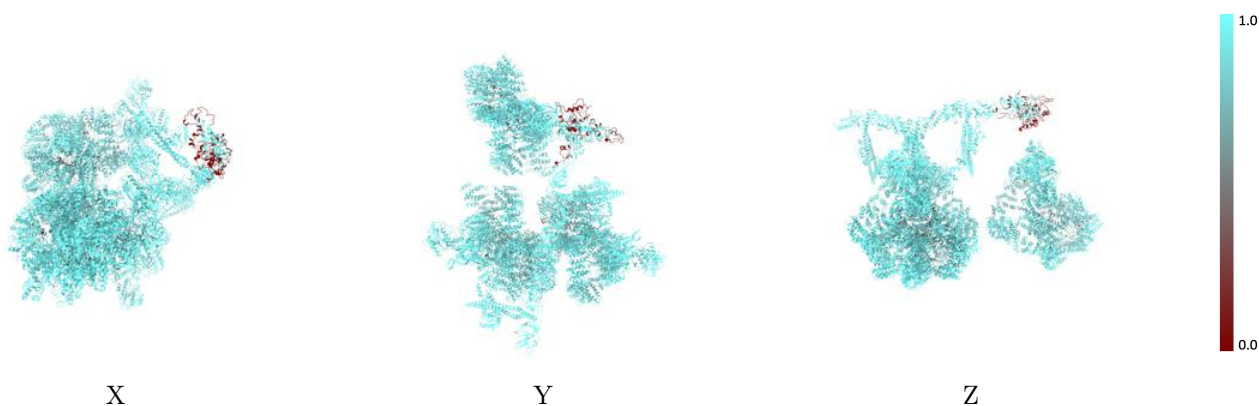
The images above show the 3D surface view of the map at the recommended contour level 0.066 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

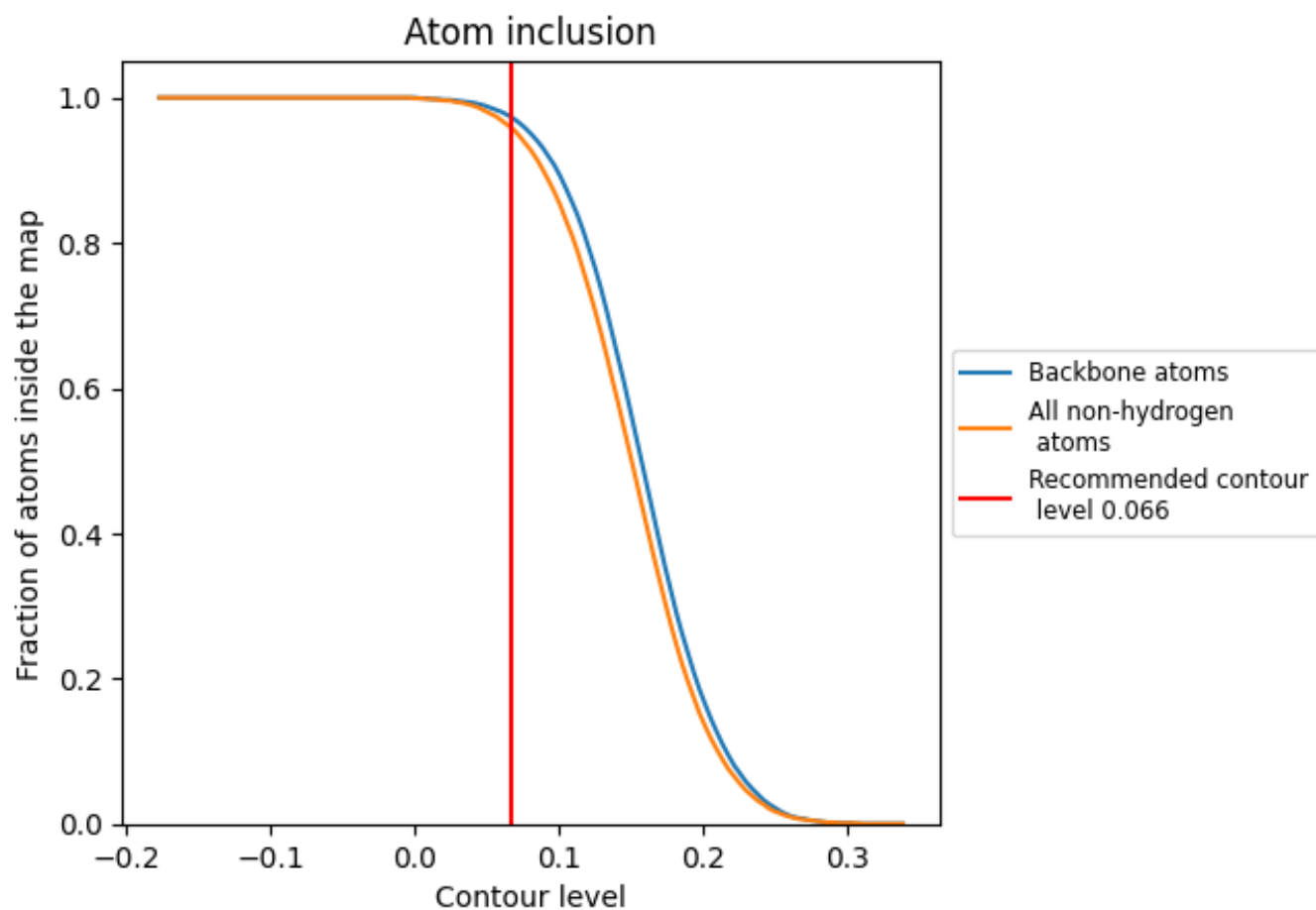
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.066).























































## 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

