



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:49 PM UTC

PDB ID : 9QMS / pdb_00009qms
EMDB ID : EMD-53237
Title : DNA-PK bound to 153 bp H2AX nucleosome with ATPyS
Authors : Hall, C.; Chaplin, A.K.
Deposited on : 2025-03-24
Resolution : 5.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

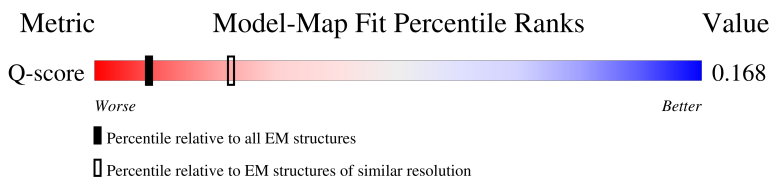
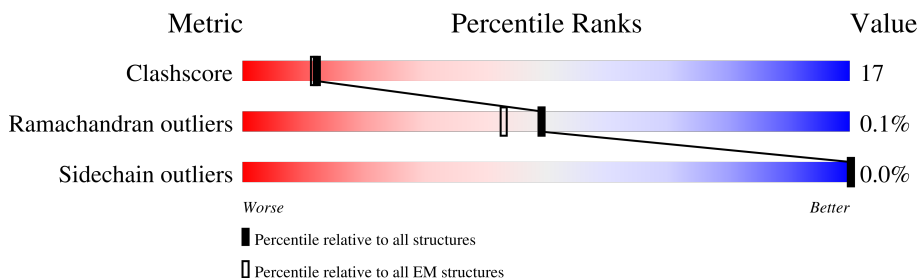
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 5.00 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.





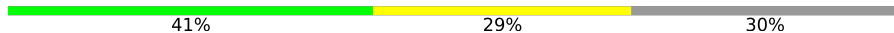




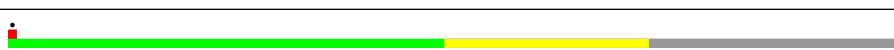
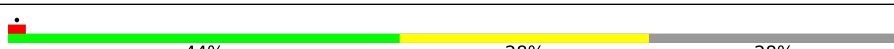

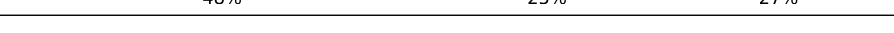
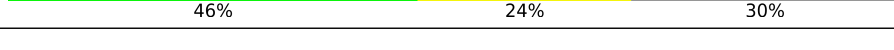
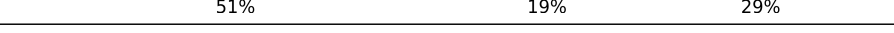
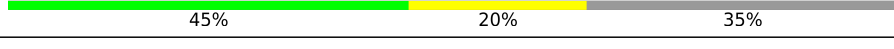
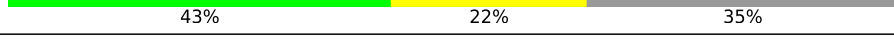



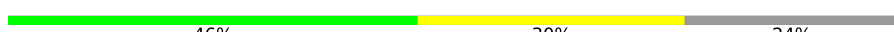




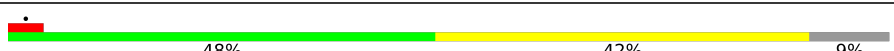

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 (4.50 - 5.50)

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	O	4128	
1	o	4128	
2	L	732	
2	N	732	

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Mol	Chain	Length	Quality of chain
2	l	732	
2	n	732	
3	C	143	
3	G	143	
3	c	143	
3	g	143	
4	D	126	
4	H	126	
4	d	126	
4	h	126	
5	A	136	
5	E	136	
5	a	136	
5	e	136	
6	B	103	
6	F	103	
6	b	103	
6	f	103	
7	K	609	
7	M	609	
7	k	609	
7	m	609	
8	I	153	
8	i	153	
9	J	153	

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Mol	Chain	Length	Quality of chain
9	j	153	 A horizontal bar chart showing the quality of chain j. The bar is divided into three segments: a green segment on the left labeled '30%', a yellow segment in the middle labeled '62%', and a grey segment on the right labeled '8%'. The segments are separated by thin black lines.

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 113260 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	3514	Total	C	N	O	S	0	0
			28053	18035	4713	5119	186		
1	o	3505	Total	C	N	O	S	0	0
			27969	17985	4707	5090	187		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	656	Total	C	N	O	S	0	0
			5240	3345	873	996	26		
2	N	640	Total	C	N	O	S	0	0
			5114	3270	850	968	26		
2	l	517	Total	C	N	O	S	0	0
			4117	2640	683	771	23		
2	n	517	Total	C	N	O	S	0	0
			4106	2630	684	769	23		

- Molecule 3 is a protein called Histone H2AX.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	100	Total	C	N	O	0	0
			767	485	149	133		
3	G	98	Total	C	N	O	0	0
			745	470	144	131		
3	c	102	Total	C	N	O	0	0
			779	491	153	135		
3	g	99	Total	C	N	O	0	0
			751	473	145	133		

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	92	Total	C	N	O	S	0	0
			706	444	126	134	2		
4	H	91	Total	C	N	O	S	0	0
			703	445	125	131	2		
4	d	91	Total	C	N	O	S	0	0
			708	447	125	134	2		
4	h	92	Total	C	N	O	S	0	0
			718	453	127	136	2		

- Molecule 5 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	95	Total	C	N	O	S	0	0
			778	491	148	135	4		
5	E	96	Total	C	N	O	S	0	0
			794	500	154	136	4		
5	a	88	Total	C	N	O	S	0	0
			717	454	134	125	4		
5	e	88	Total	C	N	O	S	0	0
			721	456	135	126	4		

- Molecule 6 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	79	Total	C	N	O	S	0	0
			631	400	121	109	1		
6	F	79	Total	C	N	O	S	0	0
			631	400	121	109	1		
6	b	78	Total	C	N	O	S	0	0
			620	393	120	106	1		
6	f	78	Total	C	N	O	S	0	0
			610	385	117	107	1		

- Molecule 7 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	493	Total	C	N	O	S	0	0
			3940	2528	658	736	18		
7	M	493	Total	C	N	O	S	0	0
			3970	2543	671	738	18		
7	k	493	Total	C	N	O	S	0	0
			3958	2538	666	736	18		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	m	489	Total	C	N	O	S	0	0
			3923	2514	660	732	17		

- Molecule 8 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	139	Total	C	N	O	P	0	0
			2829	1345	515	831	138		
8	i	141	Total	C	N	O	P	0	0
			2871	1364	520	846	141		

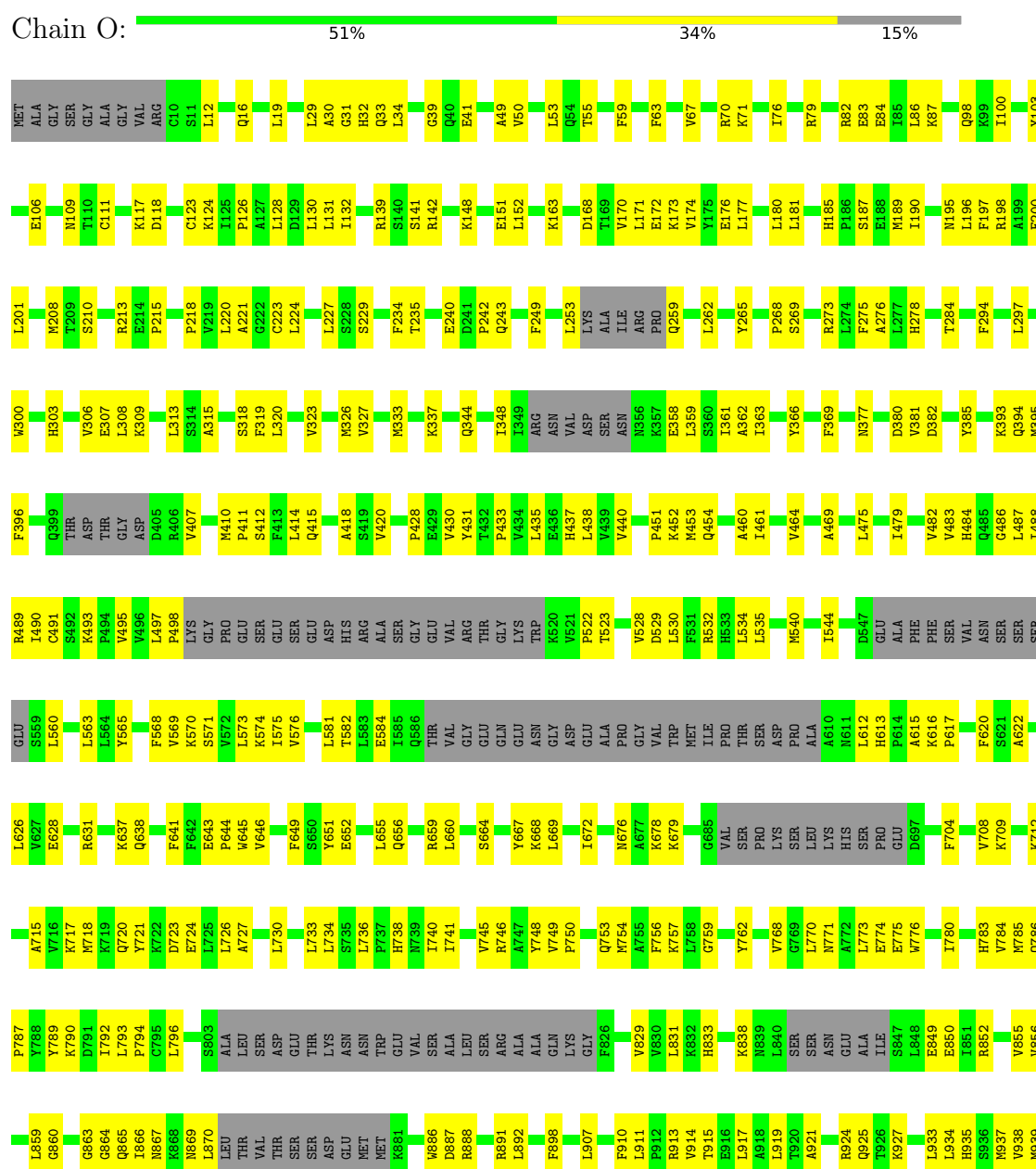
- Molecule 9 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	140	Total	C	N	O	P	0	0
			2886	1365	540	841	140		
9	j	141	Total	C	N	O	P	0	0
			2905	1375	542	847	141		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-dependent protein kinase catalytic subunit



H2103	S2034	ASN	VAL	D1821	M1743	S1687	S1586	GLY	L1395	A1309	H1133	W1039	F940
H2104	T2035	LEU	PHE	R1822	K1744	F1688	M1589	ASP	P1396	E1310	L1134	W1039	H941
H2105	L2036	LEU	HIS	S1823	K1745	P1689	M1589	GLU	D1397	C1312	T1137	T1056	M948
L2106	M2040	PHE	SER	L1824	F1746	F1670	M1592	GLN	F1398	G1313	K1140	S1058	P949
L2107	Q2042	ASN	CYS	L1827	L1747	V1671	V1593	CYS	C1399	GLY	K1140	L1059	E950
L2108	L1828	ILE	ILE	L1828	L1750	T1674	V1596	LEU	V1400	THR	L1145	F1060	G952
L2109	W1829	THR	THR	W1829	P1756	Y1675	V1597	PRO	M1403	GLY	L1146	K1061	P957
L2110	H1830	ILE	GLU	H1830	M1757	L1676	L1597	S1502	K1404	ALA	N1146	R1062	M958
L2111	L1836	LEU	GLY	L1836	L1758	L1679	M1600	L1505	G1234	GLY	K1147	L1063	Y959
L2112	L1837	LEU	L1837	L1837	L1759	L1679	L1601	L1505	K1407	ASN	K1149	Y1064	O960
L2113	R1838	ARG	L1838	R1838	M1762	K1683	F1605	K1508	K1407	ARG	K1150	O960	L961
L2114	F1839	ARG	L1839	F1839	W1762	L1684	F1605	Q1589	Y1411	T1322	R1151	P1070	L962
L2115	F1840	TYR	L1840	D1685	C1767	D1685	R1608	L1510	K1412	S1323	L1152	A1072	K963
L2116	A1847	TYR	C1767	L1688	R1768	L1688	R1608	L1517	D1413	E1328	L1153	F1073	R964
L2117	I1848	PRO	R1768	K1689	H1772	K1689	Q1611	L1517	L1414	E1328	P1154	K1074	Y968
L2118	D1849	VAL	H1772	G1690	V1773	Q1691	K1612	L1524	L1415	R1329	R1155	R1075	
L2119	V1850	GLU	V1773	Q1691	M1774	Q1691	H1613	L1524	L1416	Y1330	G1156	L1076	
L2120	L1851	VAL	M1774	A1692	E1775	T1693	Q1614	R1527	E1417	M1331	F1157	G1077	
L2121	K1852	VAL	E1775	K1693	E1776	T1693	G1615	L1528	H1418	Y1332	L1165	F1082	
L2122	SER	PRO	E1776	L1694	L1777	L1695	K1617	L1531	K1422	S1333	L1166	C974	
L2123	ARG	ALA	L1777	L1695	F1778	L1696	L1618	L1532	I1423	S1249	D1167	I1085	
L2124	THR	GLY	Q1779	L1696	Q1779		A1619	L1532	T1424	L1250	L1168	Y1086	
L2125	LYS	GLU		F1699				A1536	A1425	L1250	V1169		
L2126	ASN	ARG	F1782	THR	F1782	THR	L1623	V1537	Q1426	PRO	L1170		
L2127	LEU	LEU	R1783	SER	R1783	SER	L1623	L1537	L1428	PHE	L1171	F1089	
L2128	ASN	ASN	R1784	GLU	R1784	GLU	V1626	L1538	I1428		L1172		
L2129	GLU	GLU	L1785	THR	L1785	THR	K1627	S1539	A1441		L1173	E1092	
L2130	SER	SER	GLY	GLY	GLY	GLY	K1628	ALA	G1355		P1179	L1095	
L2131	THR	THR	R1787	GLY	R1787	GLY	C1629	SER	W1356		Q1180	V1096	
L2132	LYS	LYS	S1790	SER	S1790	SER	D1630	LEU	A1263		C1183	E1097	
L2133	GLU	GLU		L1707			S1631	GLY	L1358		R1184	F1099	
L2134	LEU	LEU		L1707			W1632	SER	K1361		H1185	V1100	
L2135	ALA	ALA	T1793	V1713	V1713	V1713	W1633	SER	V1451		K1186	F1101	
L2136	GLU	GLU	Q1794	L1714	L1714	L1714	A1634	GLN	V1452		F1191	L1104	
L2137	ARG	ARG	V1795	E1715	E1715	E1715	K1635	GLY	C1455		P1196	I1105	
L2138	ASP	ASP	W1796	Q1716	Q1716	Q1716	D1636	SER	L1475		S1203	I1106	
L2139	VAL	VAL	L1797	L1717	L1717	L1717	S1637	VAL	L1475		P1199	Y1107	
L2140	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
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L2157	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2158	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2159	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2160	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2161	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2162	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
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L2180	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2181	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2182	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2183	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2184	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
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L2186	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2187	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2188	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
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L2190	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
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L2194	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2195	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2196	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2197	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2198	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2199	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2200	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2201	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2202	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2203	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2204	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2205	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2206	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2207	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2208	V1951	ALA	L1798	I1718	I1718	I1718	T1641	ILE	H1476		G1200	M1103	
L2209	V1951	ALA	L1798	I1718	I1718	I1718	T1641						



L3480	E3582	L3767	L3857	R3965	V4038	R4119
K3483	W3588	V3770	K3858	Q3966	Y4039	T4120
I3487	V3592	I3774	K3860	F3967	R4040	W4124
K3493	A3597	L3788	T3867	I3968	R4041	E4125
Q3494	LYS	E3700	V3868	N3969	Q4042	P4126
F3495	THR	I3701	T3869	L3970	I4043	W4127
I3496	PRO	Q3704	T3870	M3971	I4044	M4128
S3497	V3601	Q3707	F3871	L3972	A4047	
W3498	V3606	R3708	K3872	M3974	R4048	
I3499	I3606	G3707	K3873	K3975	A4054	
S3500	E3607	R3708	K3874	E3976		
V3503	K3608	K3710	E3875	L3977	V4058	
A3504	M3609	G3709	S3876	M3983	I4059	
L3505	A3510	W3805	K3877	M3984	V4064	
L3506	E3611	L3816	L3882	V3985	L4064	
D3509	L3617	I3719	R3889	H3986	H4068	
Q3510	P3623	A3720	P3894	A3987	P4072	
A3511	G3624	F3722	L3898	L3988	Y4077	
V3512	L3625	V3726	A3905	R3989	Y4078	
A3513	G3626		A3909	N4000	A4079	
N3524	R3629	M3729	A3912	M4002	V4080	
Q3527	K3631	S3731	C3912	V4004	A4081	
F3533	G3647	L3732	C3913	V4006	G4082	
S3536	GLY	R3734	S3914	K4008	S4084	
S3537	SER	R3735	H3915	P4009	K4085	
E3538	LYS	K3736	G3919	S4010	H4087	
S3539	LEU	R3737	L3918	D4011	M4088	
TVR	ARG	I3738	I3920	W4013	I4089	
SER	MET	R3741	H3924	K4014	R4090	
PHE	LYS	G3742	L3925	Y4015	A4091	
LYS	LEU	D3744	N3926	PHE	Q4092	
ASP	ASP	E3745	N3927	GLU	E4093	
T3546	T3546	R3746	K3928	GLN	P4094	
T3547	T3547	E3747	MET	LYS	E4095	
G3548	M3665	H3748	K3929	LEU	S4096	
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F3553	K3669	V3752	D3941	GLY	K4105	
F3554	M3670	E3756	F3946	TRP	G4106	
R3557	N3671			ILE	L4107	
V3567	K3672			ILE	M4108	
L3572	L3680	R3759		ASN	D4109	
A3574	K3681	D3760		VAL	Q4110	
	E3682	Q3762		ALA	D4113	
	G3683	R3763		GLU	P4114	
	P3685	V3764		LYS	L4117	
		E3766		ASN	G4118	

● Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain o:  49% 35% 15%

MET	P92	I166	Q243	K626	M410
ALA	I93	P167	T244	V327	P411
GLY	E94	D168	S245		S412
SER	K95	T169	R246		F413
GLY	N96	V170	E247		L414
ALA	G97	L171	I248		V417
GLY	Q98	E172	F249		A418
VAL	K99	Y175	N250		S419
ARG	I100	E176	F251		V420
C10	Y103	L177	V252		F341
L13	S104	L181	LYS		P428
R14	V105		ALA		T432
L15			ILE		T435
L19	K108	V184	ARG		L435
T110	M109	H185	PRO		V436
D23	T110	P186	Q259		H437
R24	C111	S187	I260		L438
S113	T112	E188	D261		Q442
V114	S113	M189	L262		F446
Y115	V114	I190	K263		P447
T116	Y115	N191	R264		Q448
K117	T116	N192	Y265		Y449
A120	K117	A193	A266		S450
A121	A120	E194	V267		M453
K122	I121	N195	P268		Q454
C123	C123	L196	S269		L455
L38	K124	F197	A270		R459
G39	I125	L201	L274		A460
Q40	I125	F275	F275		V464
E41	L128	L204	T284		L468
C42	D129	C285	C285		A469
S45	L130	Q207	L286		P473
A49	L131	S210	L287		V474
A52	K132	A213	Y290		L475
F59	L134	V212	V296		R476
L66	Q136	K216	K299		N477
V67	R139	V219	H303		C478
R70	R142	L220	E307		I479
K71	D145	C223	L308		H484
N74	F147	L227	K309		Q485
S75	K148	L230	K310		G486
I76	E151	L231	L313		L487
F78	L152	C232	S314		I488
R79	E159	N233	A315		K493
E80	E159	F234	L316		F498
L162	E162	T235	S318		LYS
L163	L162	E240	F319		GLY
K164	K164	D241	L320		PRO
K165	K165	P242	V323		

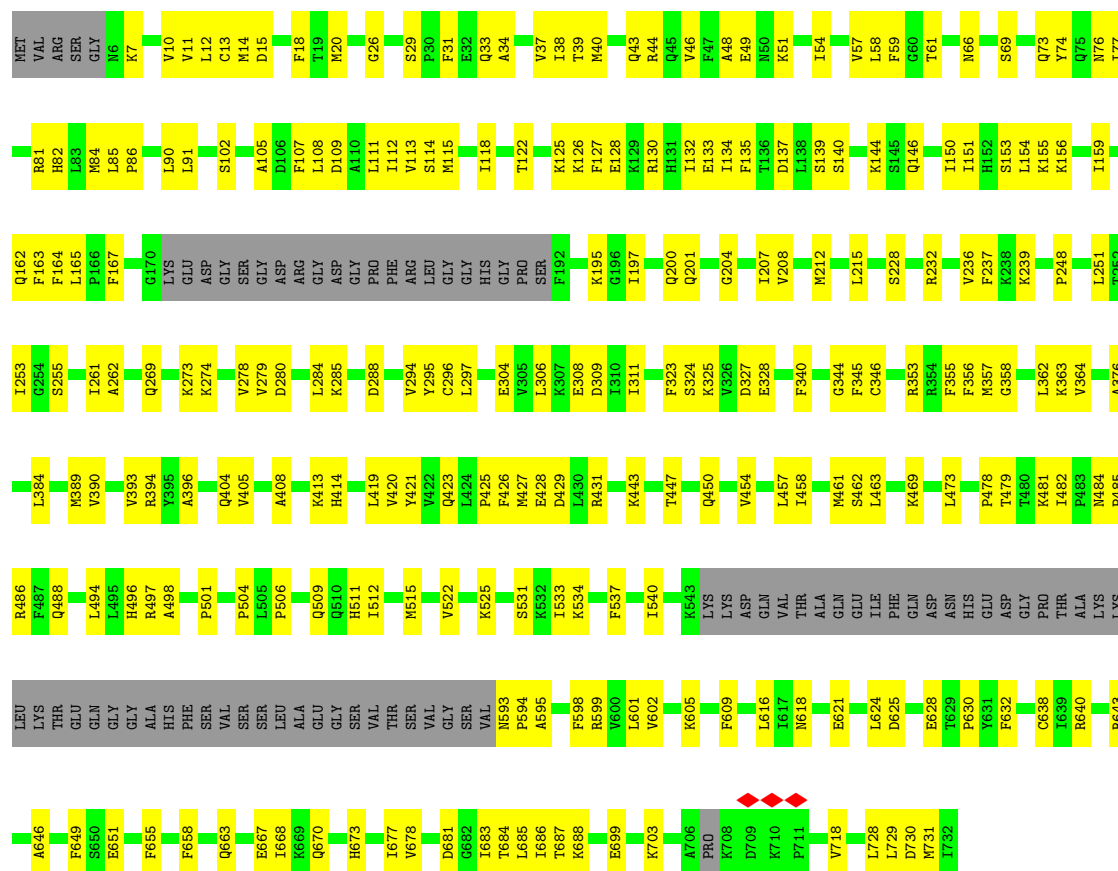


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S2856	R2773	E2564	Q2472	K2394	Y2316	L2235	N2141	ARG	GLU	GLN	F1863	G1768
I2858		M2565	Y2473	T2395	L2396	L2236	R2142	GLU	ARG	LEU	D1864	I1768
I2861	R2776	L2568	L2476	C2397	A2318	I2238	L2144	GLN	LYS	LYS	Q1866	C1790
S2862	G2778	M2568	L2477	L2398	A2319	L2241	F2145	ASP	ALA	Y1940	I1867	S1791
C2863	D2779	M2576	M2478	E2399	A2320	L2242	L2146	PRO	ARG	C1947	T1868	Q1794
Q2864	L2780	F2577		R2404	E2321	V2242	A2147	THR	ALA	A1948	K1869	L1797
H2865			D2482		T2326	C2244	I2151	VAL	ALA	I1949	M1870	G1872
A2866	L2783	L2581	R2485	Y2412	L2327	W2245	V2156	ASP	ASN	I1952	R1806	L1806
A2867	Q2784		D2486	K2418	R2328	K2246		ASP	GLY	C1953	LYS	ASP
L2868		C2584	PRO		E2338		P2159	VAL	ASP	C1954	ASP	ASP
		E2585	GLU	F2420	M2331	L2249	Y2160	LEU	SER	L1959	V1879	
P2873		F2586	SER	D2426	E2332	L2249	A2161	GLU	ASP	K1960	M1880	PRO
		Q2587	TRP	R2427	R2333	Y2253		LEU	GLY		Y1881	ARG
		E2588	GLU	V2423	L2337	F2257	W2164	GLU	PRO	Q1963	S1882	LEU
		T2600	T2491	M2424	L2341	F2267	A2172	MET	SER	GLY	R1883	SER
		T2603	D2494	H2425	E2338	F2280	S2166	GLU	TYR	PHE	L1884	P1885
			S2495	H2426	L2341	F2280	P2167	ASP	MET	PHE	T1815	
			Q2496	D2428	L2344	K2263	L2171	ASN	SER	PHE	R1816	LYS
			E2497	R2428	L2344	D2264	A2172	ASP	LEU	SER	Q1817	ASP
			I2498	D2429	L2344	D2265	A2173	GLU	TYR	GLU	S1818	VAL
				E2430	K2347	W2286		ASP	LYS	LYS	F1819	V1820
			L2501	R2431	Q2348	S2287	N2176	GLU	ALA	LEU	D1821	LYS
			A2502	Q2452	Q2348	S2287	ASN	GLU	ALA	ILE	L2036	LEU
			K2503	K2433	L2349	K2268	G2179	ASP	ASP	ILE	S2037	LEU
			D2504	W2434	K2350	D2269		GLY	GLY	PHE	C1831	GLN
			V2505	C2435	Q2351	N2270		LYS	ASP	ASN	S1832	VAL
			L2506	L2436	H2352	S2271		ASN	ASN	ASN	L1824	GLY
			I2507	D2437	Q2353	V2272		LEU	LEU	ASN	L1835	LEU
				I2438		D2273		LEU	LEU	ASN	L1836	GLY
			L2510	Y2440	M2356	Q2274		LEU	LEU	ASN	F1839	ASP
			N2514	K2441	K2359	Q2275		GLY	GLY	ASN	F1840	ILE
			L2517	M2442	F2360	Q2276		GLN	GLN	ASN	S1841	THR
			T2521	M2443	I2361	D2284		GLY	GLY	ASN	T1842	GLY
			R2522	P2444	V2362	L2285		GLY	GLY	ASN	T1843	GLY
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			L2540		A2541			GLY	GLY	ASN	L1919	VAL
			E2541	H2464	L2384			GLY	GLY	ASN	L1920	VAL
			A2542	P2465	L2385			GLY	GLY	ASN	L1921	VAL
			M2543	S2466	L2386			GLY	GLY	ASN	L1922	VAL
				T2467	F2387			GLY	GLY	ASN	L1923	VAL
				T2468	L2388			GLY	GLY	ASN	L1924	VAL
			Y2546	C2469	F2389			GLY	GLY	ASN	L1925	VAL
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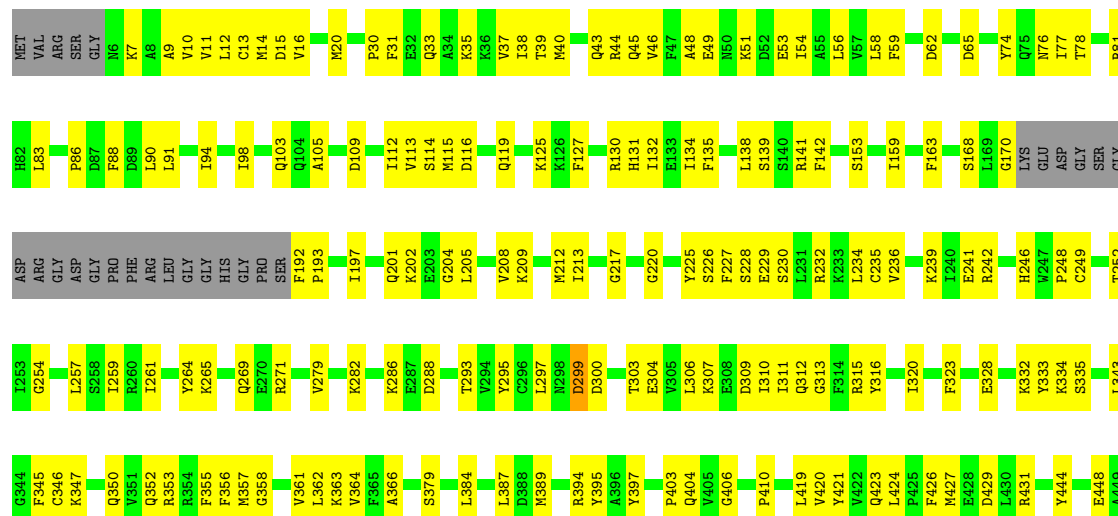
• Molecule 2: X-ray repair cross-complementing protein 5

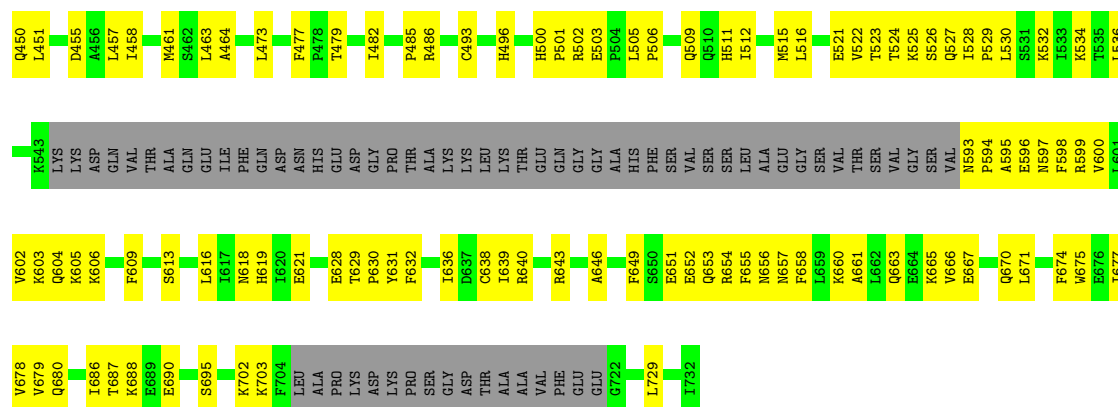
Chain L:  57% 33% 10%



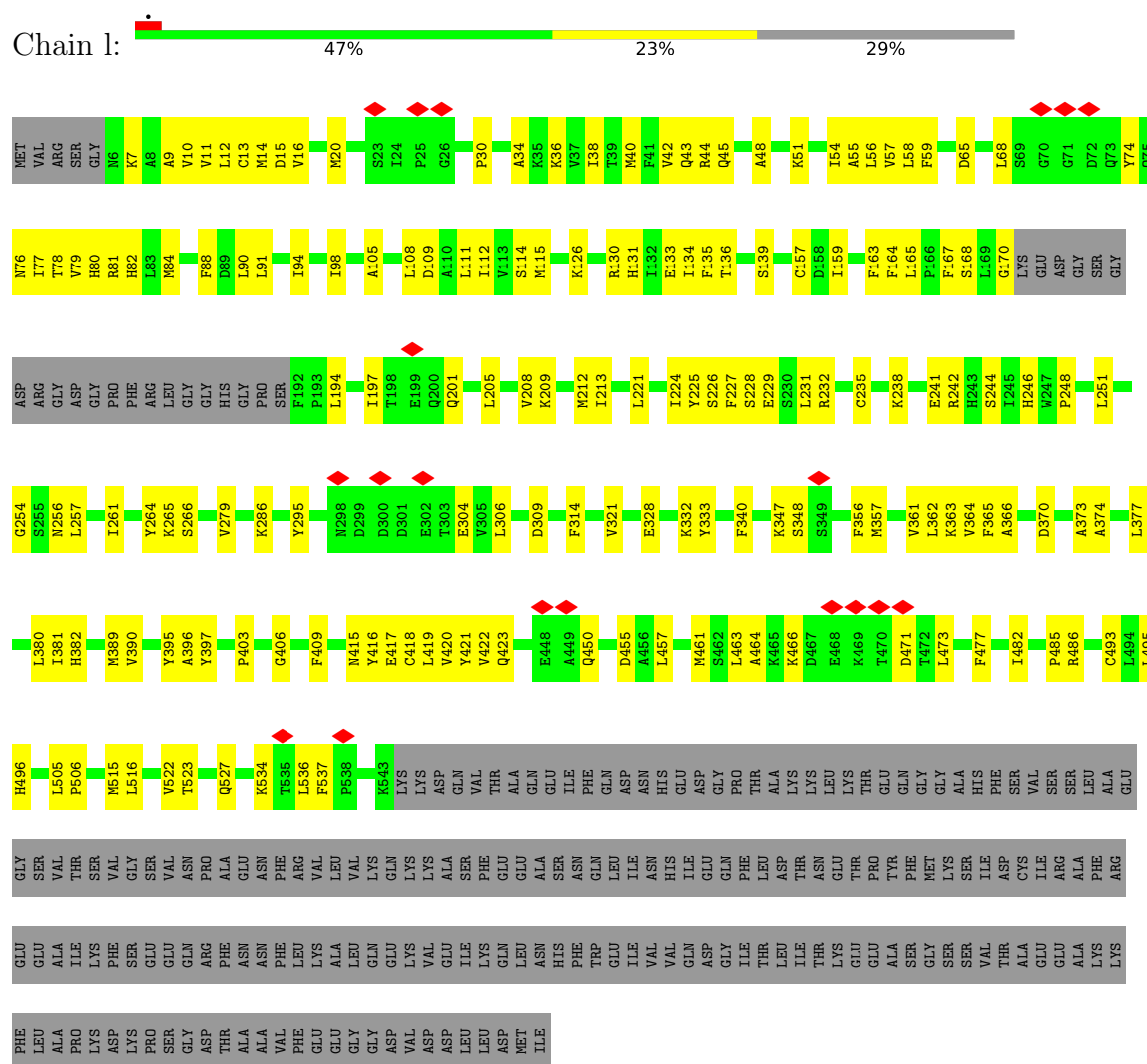
• Molecule 2: X-ray repair cross-complementing protein 5

Chain N:  50% 37% 13%





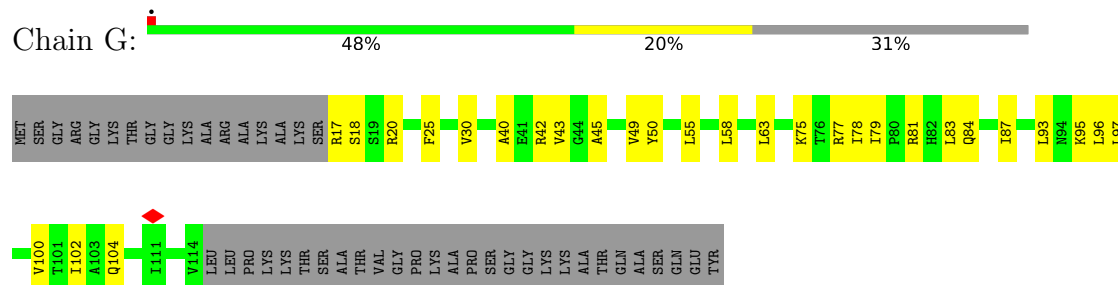
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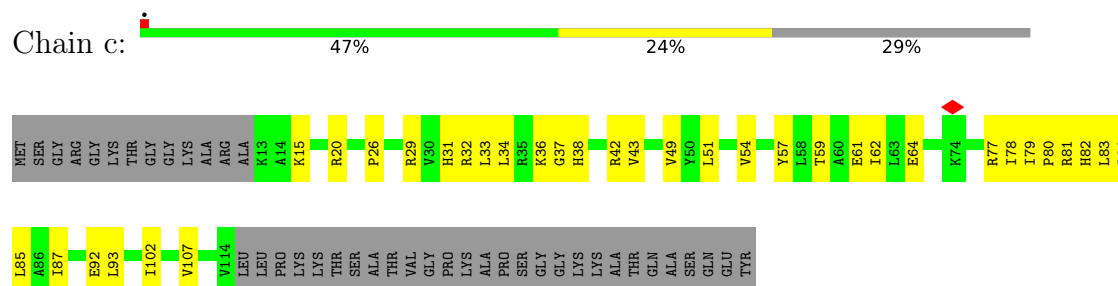
• Molecule 2: X-ray repair cross-complementing protein 5



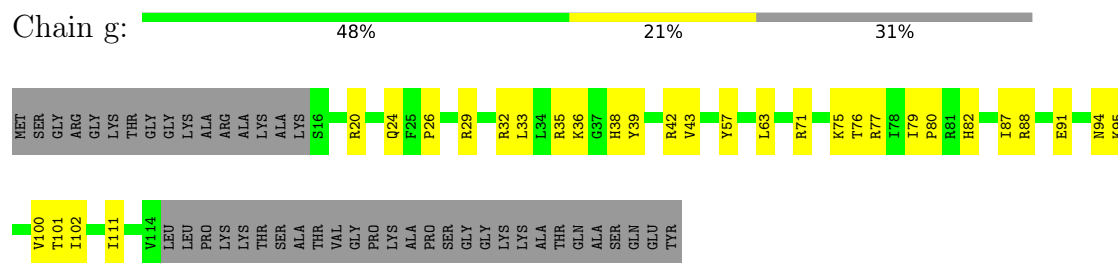
- Molecule 3: Histone H2AX



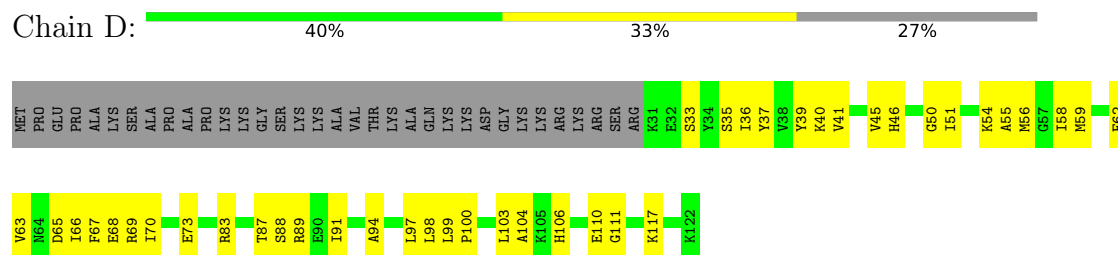
- Molecule 3: Histone H2AX



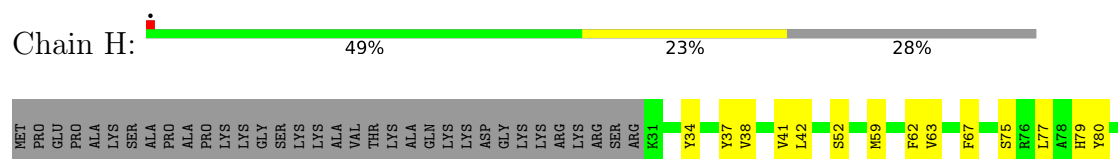
- Molecule 3: Histone H2AX

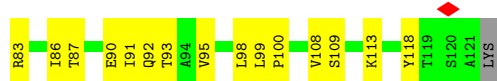


- Molecule 4: Histone H2B type 1-J

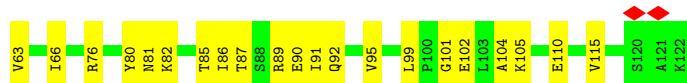
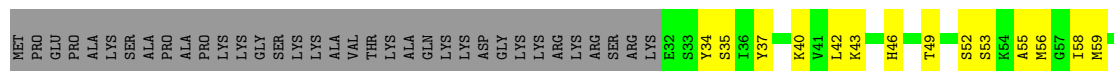


- Molecule 4: Histone H2B type 1-J

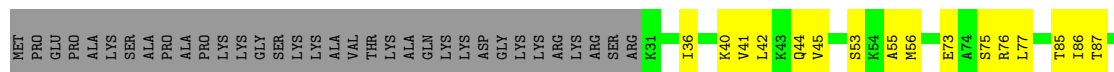




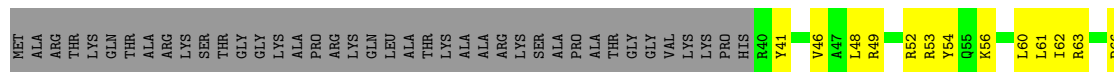
• Molecule 4: Histone H2B type 1-J



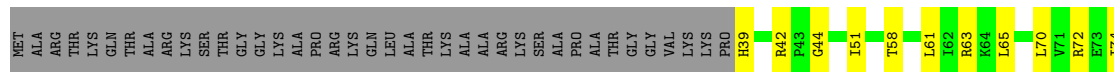
• Molecule 4: Histone H2B type 1-J



• Molecule 5: Histone H3.1

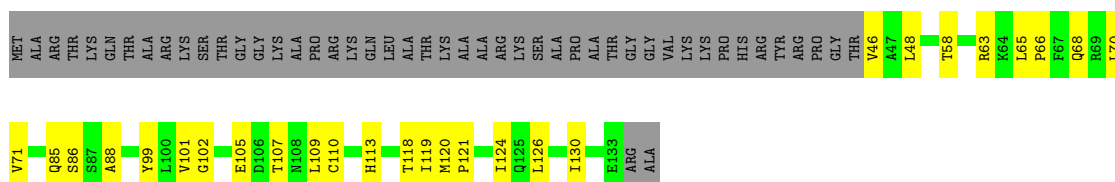


• Molecule 5: Histone H3.1

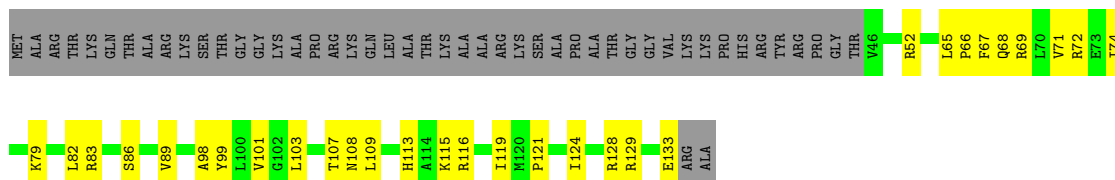


• Molecule 5: Histone H3.1

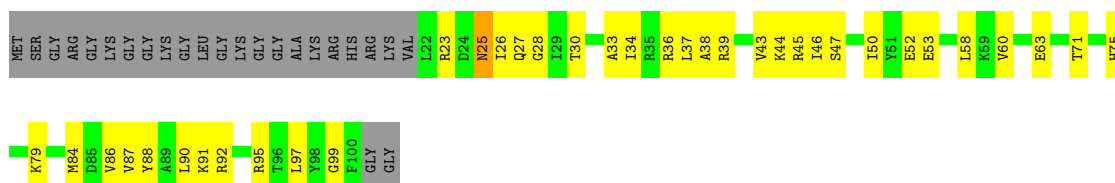




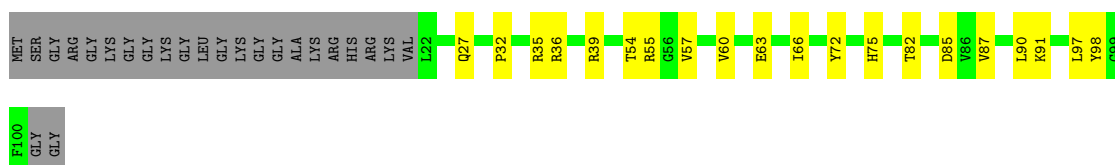
• Molecule 5: Histone H3.1



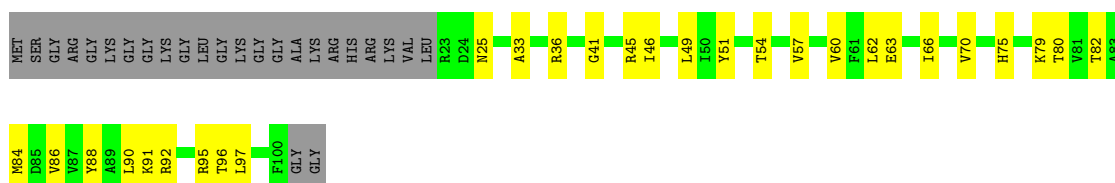
• Molecule 6: Histone H4



• Molecule 6: Histone H4

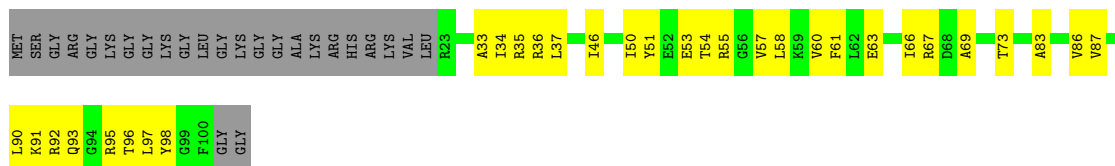


• Molecule 6: Histone H4



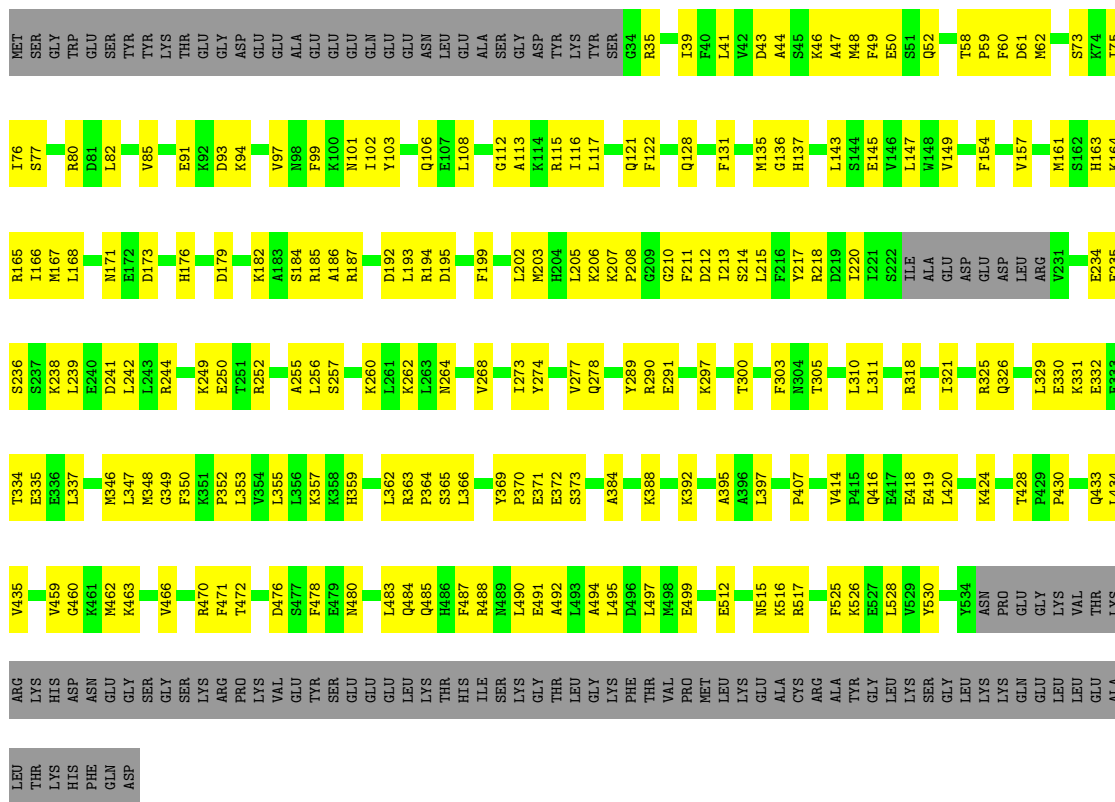
• Molecule 6: Histone H4





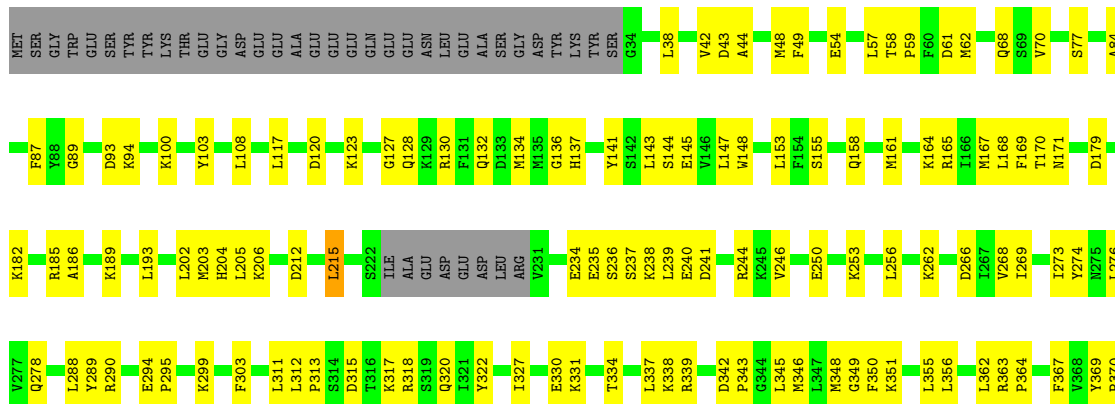
- Molecule 7: X-ray repair cross-complementing protein 6

Chain K: 

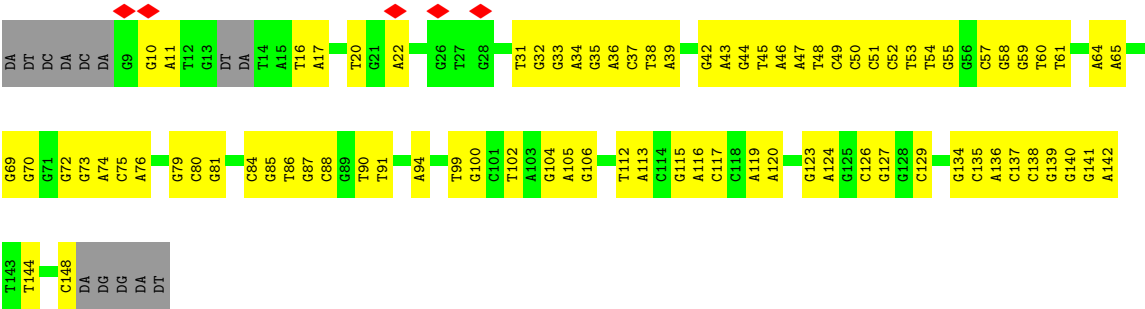


- Molecule 7: X-ray repair cross-complementing protein 6

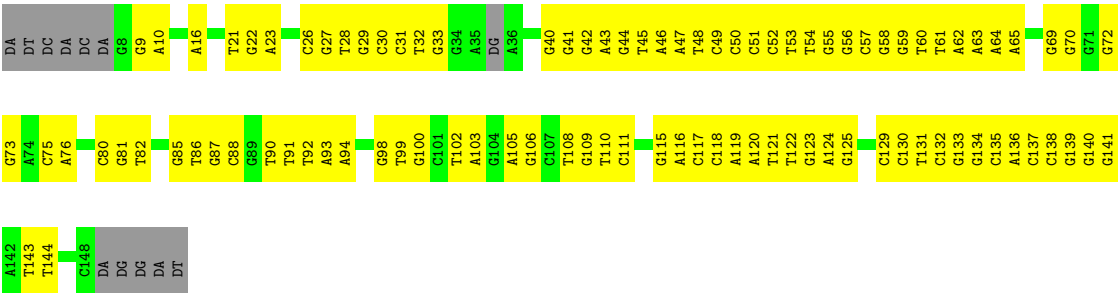
Chain M:  51% 29% 19%







• Molecule 9: DNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	77373	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.87	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.994	Depositor
Minimum map value	-0.606	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.21	Depositor
Map size (Å)	1038.24, 1038.24, 1038.24	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.472, 2.472, 2.472	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	O	0.15	0/28610	0.36	0/38654
1	o	0.17	0/28521	0.39	0/38527
2	L	0.11	0/5337	0.31	0/7193
2	N	0.14	0/5210	0.33	0/7024
2	l	0.10	0/4200	0.30	0/5673
2	n	0.10	0/4187	0.30	0/5654
3	C	0.13	0/777	0.37	0/1050
3	G	0.11	0/755	0.26	0/1021
3	c	0.12	0/789	0.35	0/1064
3	g	0.10	0/761	0.29	0/1029
4	D	0.15	0/716	0.46	0/963
4	H	0.12	0/714	0.30	0/961
4	d	0.12	0/719	0.33	0/967
4	h	0.12	0/729	0.30	0/979
5	A	0.12	0/788	0.31	0/1057
5	E	0.12	0/805	0.36	0/1079
5	a	0.11	0/725	0.29	0/972
5	e	0.11	0/729	0.35	0/977
6	B	0.13	0/638	0.30	0/856
6	F	0.10	0/638	0.30	0/856
6	b	0.11	0/627	0.28	0/841
6	f	0.10	0/616	0.30	0/827
7	K	0.16	0/4018	0.33	0/5418
7	M	0.11	0/4048	0.32	0/5454
7	k	0.11	0/4036	0.28	0/5439
7	m	0.10	0/4001	0.28	0/5395
8	I	0.32	0/3169	0.50	0/4882
8	i	0.34	0/3216	0.52	0/4956
9	J	0.30	0/3240	0.48	0/5003
9	j	0.31	0/3261	0.48	0/5035
All	All	0.17	0/116580	0.37	0/159806

There are no bond length outliers.

There are no bond angle outliers.

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	O	28053	0	28316	1046	0
1	o	27969	0	28250	1129	0
2	L	5240	0	5249	200	0
2	N	5114	0	5119	215	0
2	l	4117	0	4135	118	0
2	n	4106	0	4133	101	0
3	C	767	0	812	41	0
3	G	745	0	779	31	0
3	c	779	0	823	30	0
3	g	751	0	784	28	0
4	D	706	0	719	38	0
4	H	703	0	714	32	0
4	d	708	0	724	24	0
4	h	718	0	740	26	0
5	A	778	0	813	33	0
5	E	794	0	831	26	0
5	a	717	0	753	30	0
5	e	721	0	759	28	0
6	B	631	0	670	38	0
6	F	631	0	670	14	0
6	b	620	0	651	23	0
6	f	610	0	641	27	0
7	K	3940	0	3982	168	0
7	M	3970	0	4037	143	0
7	k	3958	0	4022	87	0
7	m	3923	0	3971	86	0
8	I	2829	0	1562	66	0
8	i	2871	0	1583	129	0
9	J	2886	0	1571	75	0
9	j	2905	0	1583	97	0
All	All	113260	0	109396	3808	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 17.

The worst 5 of 3808 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:328:GLU:O	2:l:332:LYS:HB2	1.54	1.05
9:j:55:DG:N2	9:j:56:DG:H22	1.62	0.97
9:j:55:DG:N2	9:j:56:DG:N2	2.12	0.96
1:o:3686:TRP:HA	1:o:3690:PHE:HB3	1.46	0.93
9:j:55:DG:C2	9:j:56:DG:N2	2.40	0.89

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	O	3438/4128 (83%)	3136 (91%)	300 (9%)	2 (0%)	48	83
1	o	3427/4128 (83%)	3081 (90%)	341 (10%)	5 (0%)	48	83
2	L	648/732 (88%)	583 (90%)	65 (10%)	0	100	100
2	N	632/732 (86%)	577 (91%)	54 (8%)	1 (0%)	43	77
2	l	513/732 (70%)	473 (92%)	40 (8%)	0	100	100
2	n	513/732 (70%)	478 (93%)	35 (7%)	0	100	100
3	C	98/143 (68%)	83 (85%)	14 (14%)	1 (1%)	12	47
3	G	96/143 (67%)	96 (100%)	0	0	100	100
3	c	100/143 (70%)	92 (92%)	8 (8%)	0	100	100
3	g	97/143 (68%)	93 (96%)	3 (3%)	1 (1%)	12	47
4	D	90/126 (71%)	80 (89%)	10 (11%)	0	100	100
4	H	89/126 (71%)	86 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	89/126 (71%)	86 (97%)	2 (2%)	1 (1%)	11	45
4	h	90/126 (71%)	86 (96%)	4 (4%)	0	100	100
5	A	93/136 (68%)	89 (96%)	4 (4%)	0	100	100
5	E	94/136 (69%)	89 (95%)	5 (5%)	0	100	100
5	a	86/136 (63%)	80 (93%)	6 (7%)	0	100	100
5	e	86/136 (63%)	78 (91%)	8 (9%)	0	100	100
6	B	77/103 (75%)	75 (97%)	2 (3%)	0	100	100
6	F	77/103 (75%)	74 (96%)	3 (4%)	0	100	100
6	b	76/103 (74%)	76 (100%)	0	0	100	100
6	f	76/103 (74%)	75 (99%)	1 (1%)	0	100	100
7	K	489/609 (80%)	455 (93%)	34 (7%)	0	100	100
7	M	489/609 (80%)	454 (93%)	33 (7%)	2 (0%)	30	67
7	k	489/609 (80%)	468 (96%)	21 (4%)	0	100	100
7	m	485/609 (80%)	457 (94%)	27 (6%)	1 (0%)	43	77
All	All	12537/15652 (80%)	11500 (92%)	1023 (8%)	14 (0%)	49	83

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	76	ILE
3	C	19	SER
1	o	1557	GLU
2	N	299	ASP
7	M	215	LEU

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	O	3106/3671 (85%)	3103 (100%)	3 (0%)	88	88
1	o	3090/3671 (84%)	3089 (100%)	1 (0%)	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	585/649 (90%)	585 (100%)	0	100	100
2	N	570/649 (88%)	570 (100%)	0	100	100
2	l	461/649 (71%)	461 (100%)	0	100	100
2	n	460/649 (71%)	460 (100%)	0	100	100
3	C	77/106 (73%)	77 (100%)	0	100	100
3	G	74/106 (70%)	74 (100%)	0	100	100
3	c	77/106 (73%)	77 (100%)	0	100	100
3	g	75/106 (71%)	75 (100%)	0	100	100
4	D	75/105 (71%)	75 (100%)	0	100	100
4	H	74/105 (70%)	74 (100%)	0	100	100
4	d	76/105 (72%)	76 (100%)	0	100	100
4	h	78/105 (74%)	78 (100%)	0	100	100
5	A	82/111 (74%)	82 (100%)	0	100	100
5	E	84/111 (76%)	84 (100%)	0	100	100
5	a	76/111 (68%)	76 (100%)	0	100	100
5	e	77/111 (69%)	77 (100%)	0	100	100
6	B	65/79 (82%)	64 (98%)	1 (2%)	57	71
6	F	65/79 (82%)	65 (100%)	0	100	100
6	b	62/79 (78%)	62 (100%)	0	100	100
6	f	62/79 (78%)	62 (100%)	0	100	100
7	K	439/548 (80%)	439 (100%)	0	100	100
7	M	445/548 (81%)	445 (100%)	0	100	100
7	k	443/548 (81%)	443 (100%)	0	100	100
7	m	438/548 (80%)	438 (100%)	0	100	100
All	All	11216/13734 (82%)	11211 (100%)	5 (0%)	100	100

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	415	GLN
1	O	2137	ILE
1	O	2295	GLN
6	B	25	ASN
1	o	3383	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	673	HIS
6	f	93	GLN
5	e	85	GLN
7	K	485	GLN
6	B	25	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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.

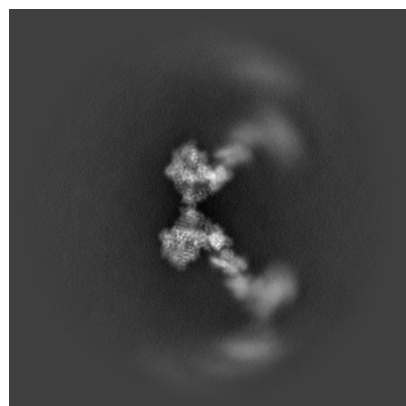
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53237. These allow visual inspection of the internal detail of the map and identification of artifacts.

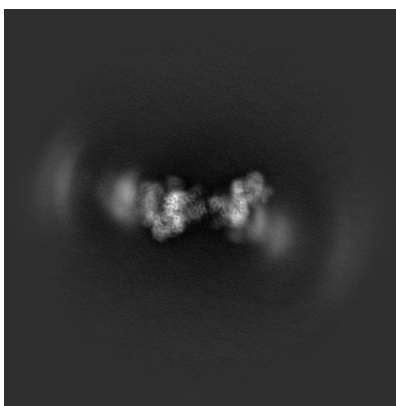
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

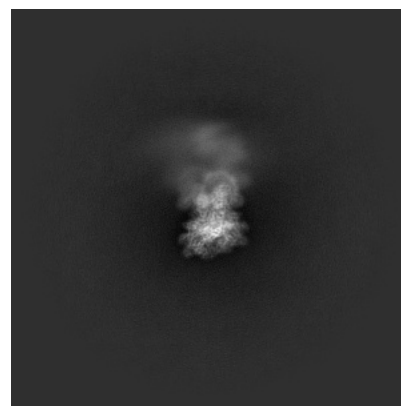
6.1.1 Primary map



X

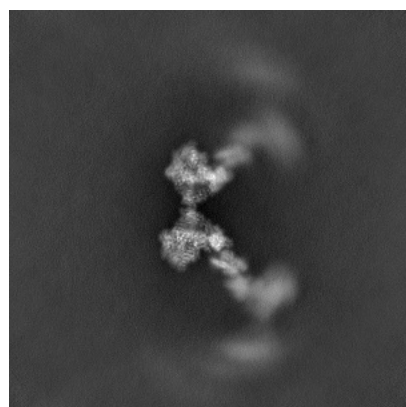


Y

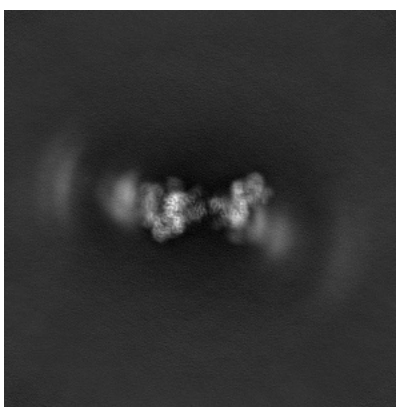


Z

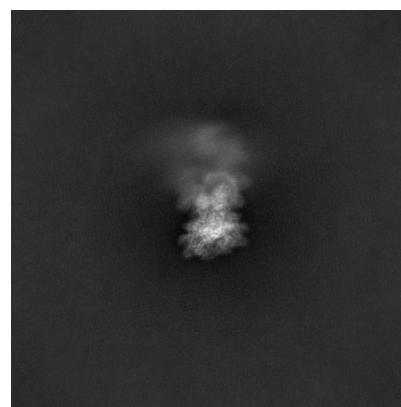
6.1.2 Raw map



X



Y

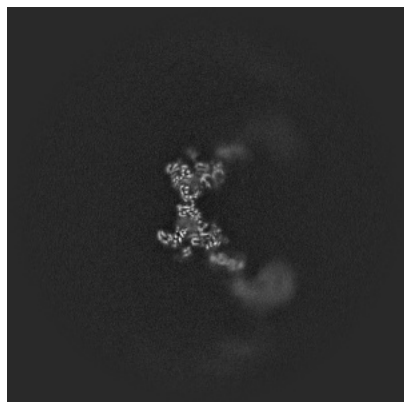


Z

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

6.2 Central slices [i](#)

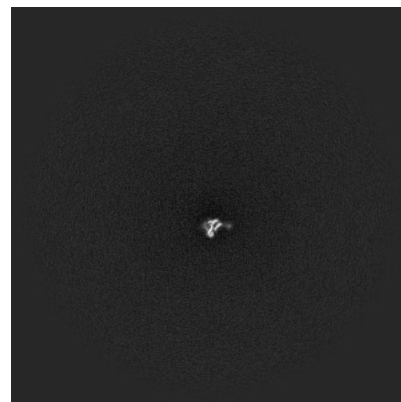
6.2.1 Primary map



X Index: 210

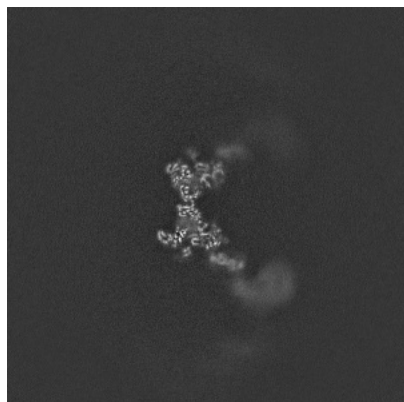


Y Index: 210



Z Index: 210

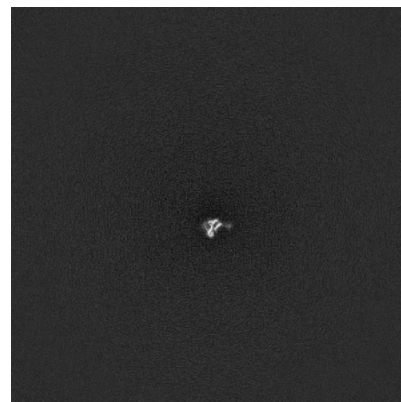
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

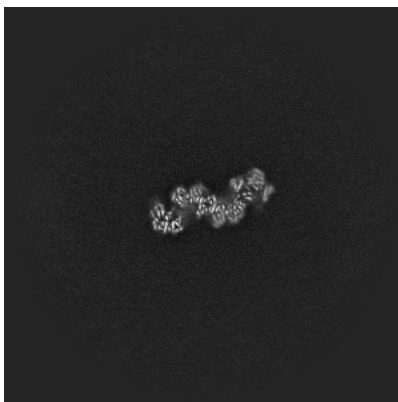
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

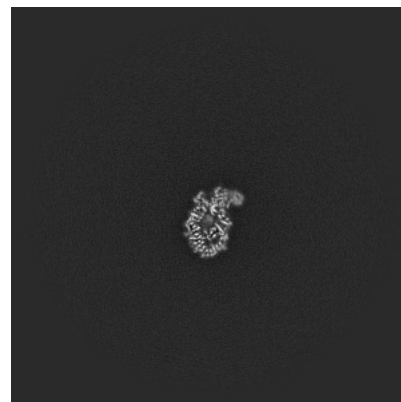
6.3.1 Primary map



X Index: 220



Y Index: 189

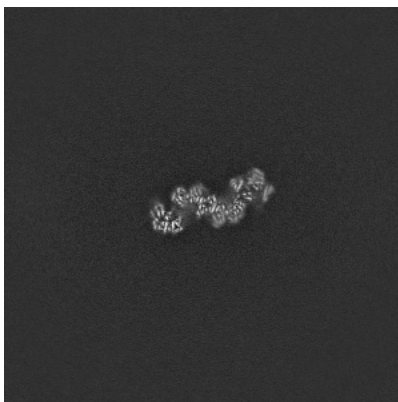


Z Index: 181

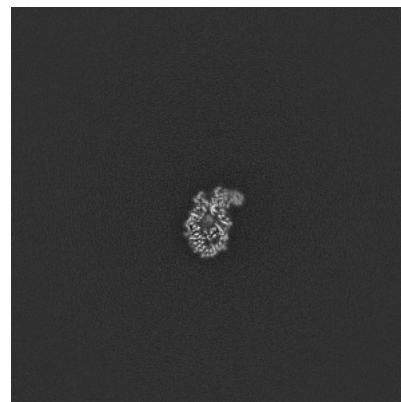
6.3.2 Raw map



X Index: 220



Y Index: 189

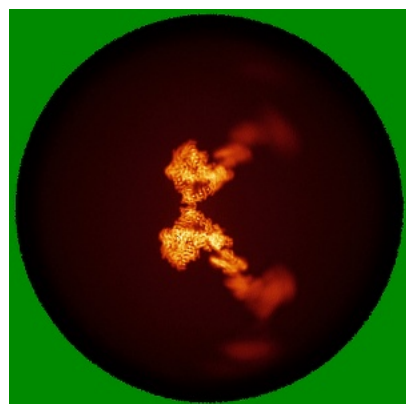


Z Index: 181

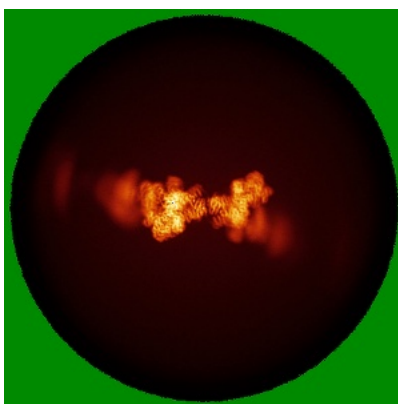
The images above show the largest variance slices of the map in three orthogonal directions.

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

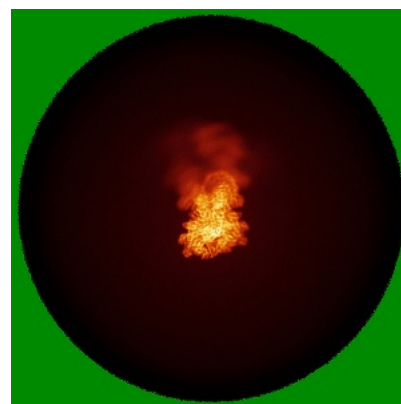
6.4.1 Primary map



X



Y

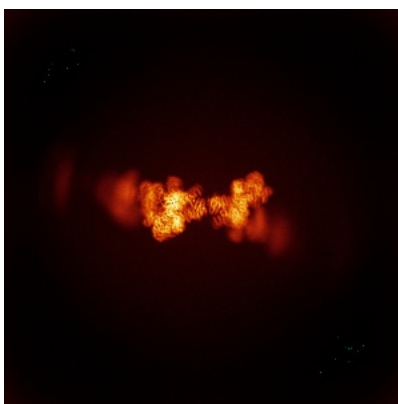


Z

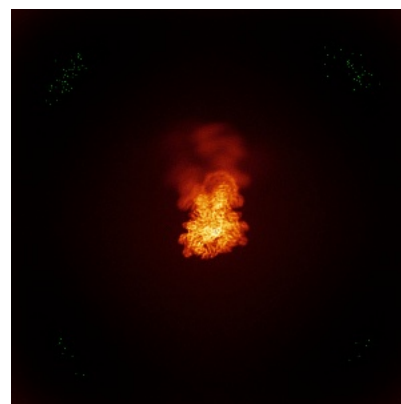
6.4.2 Raw map



X



Y

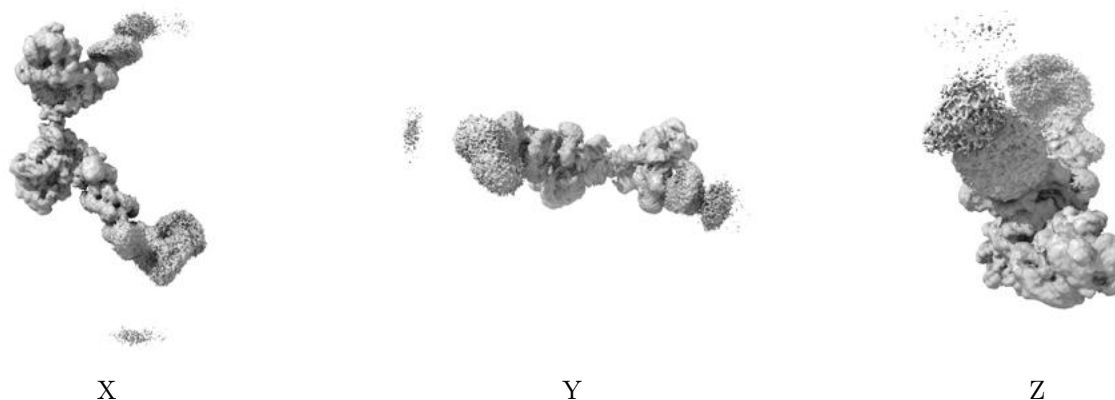


Z

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 0.21. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

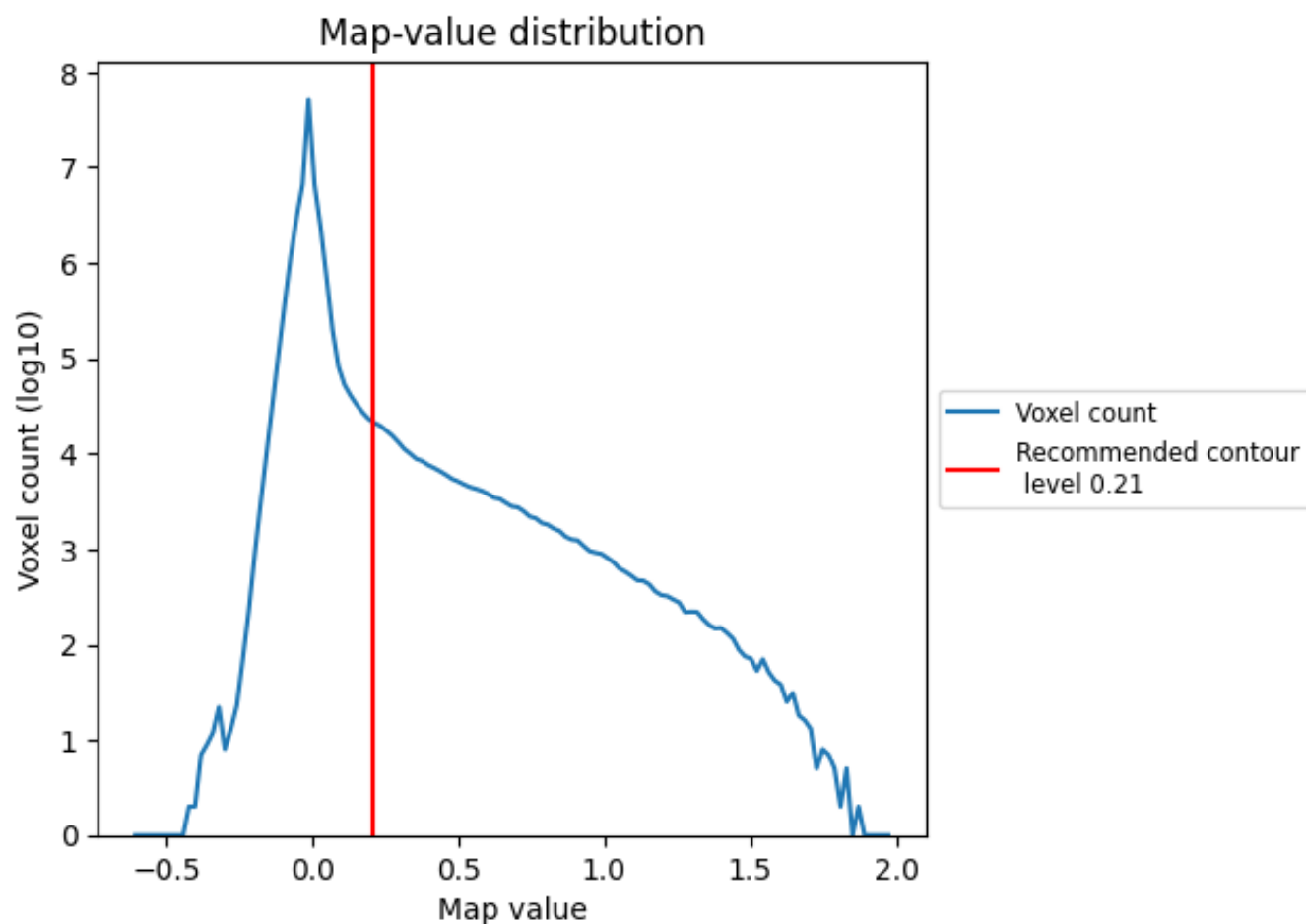
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

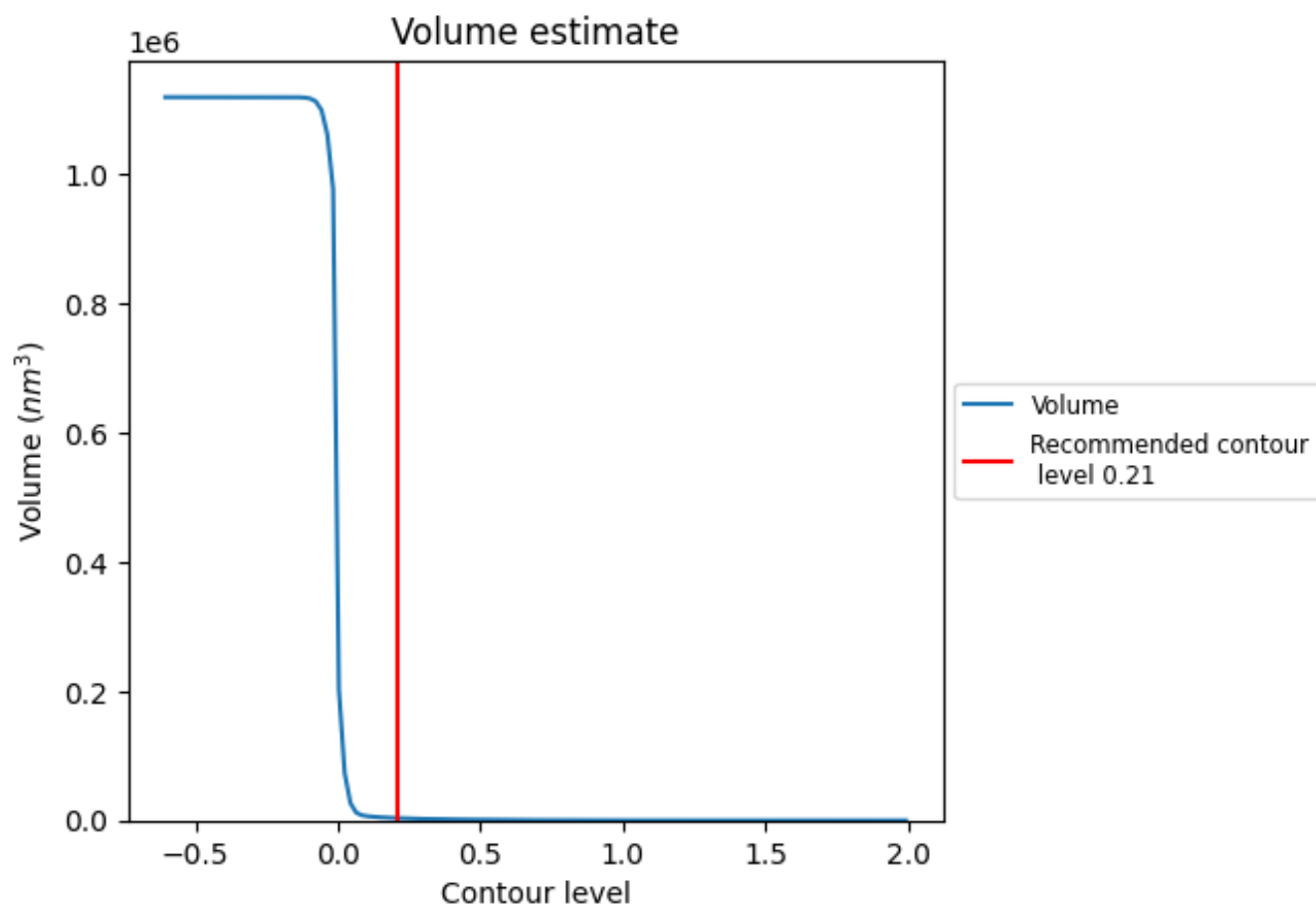
This section contains the results of statistical analysis of the map.

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.

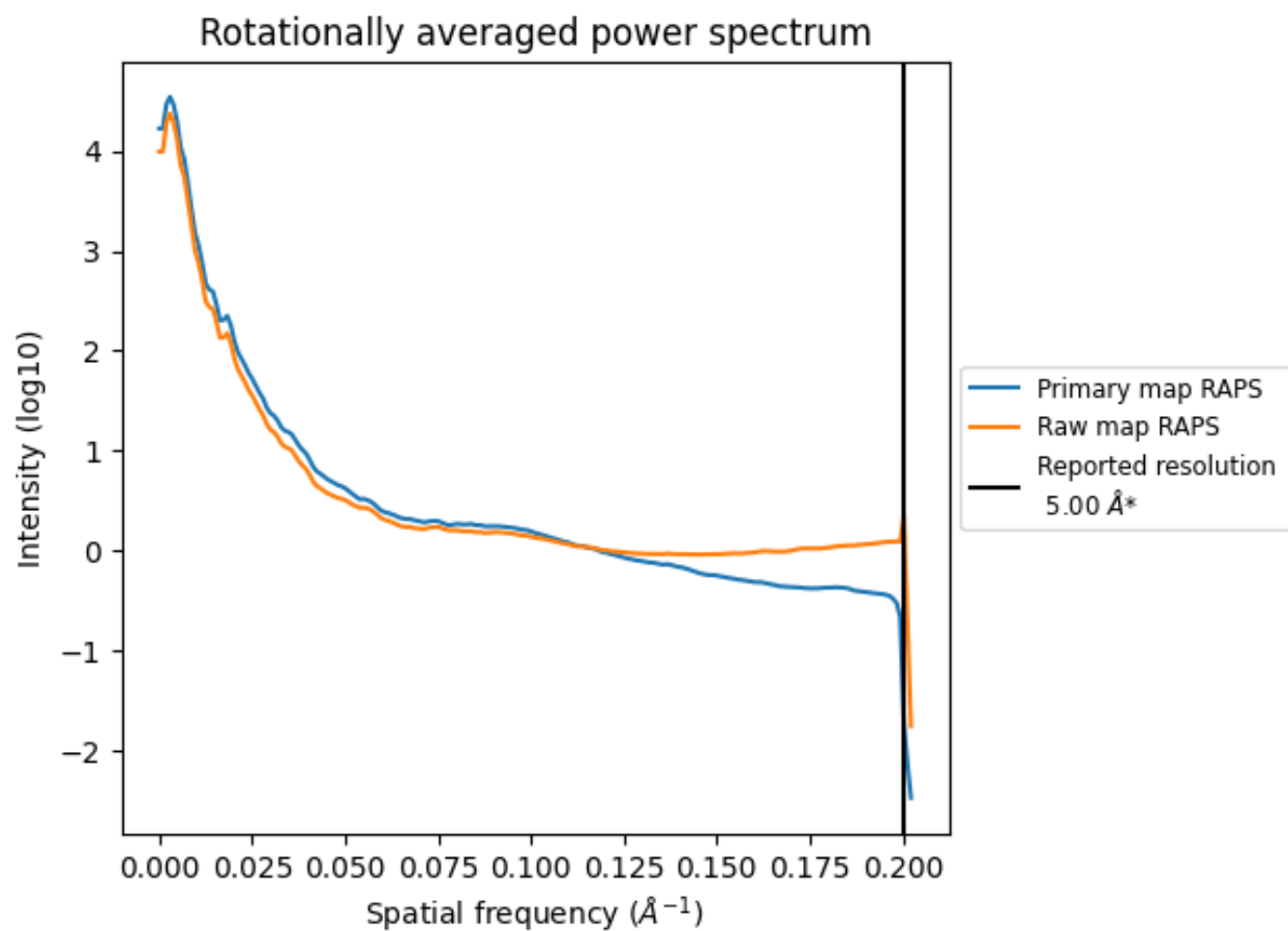
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3518 nm³; this corresponds to an approximate mass of 3178 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 ⓘ

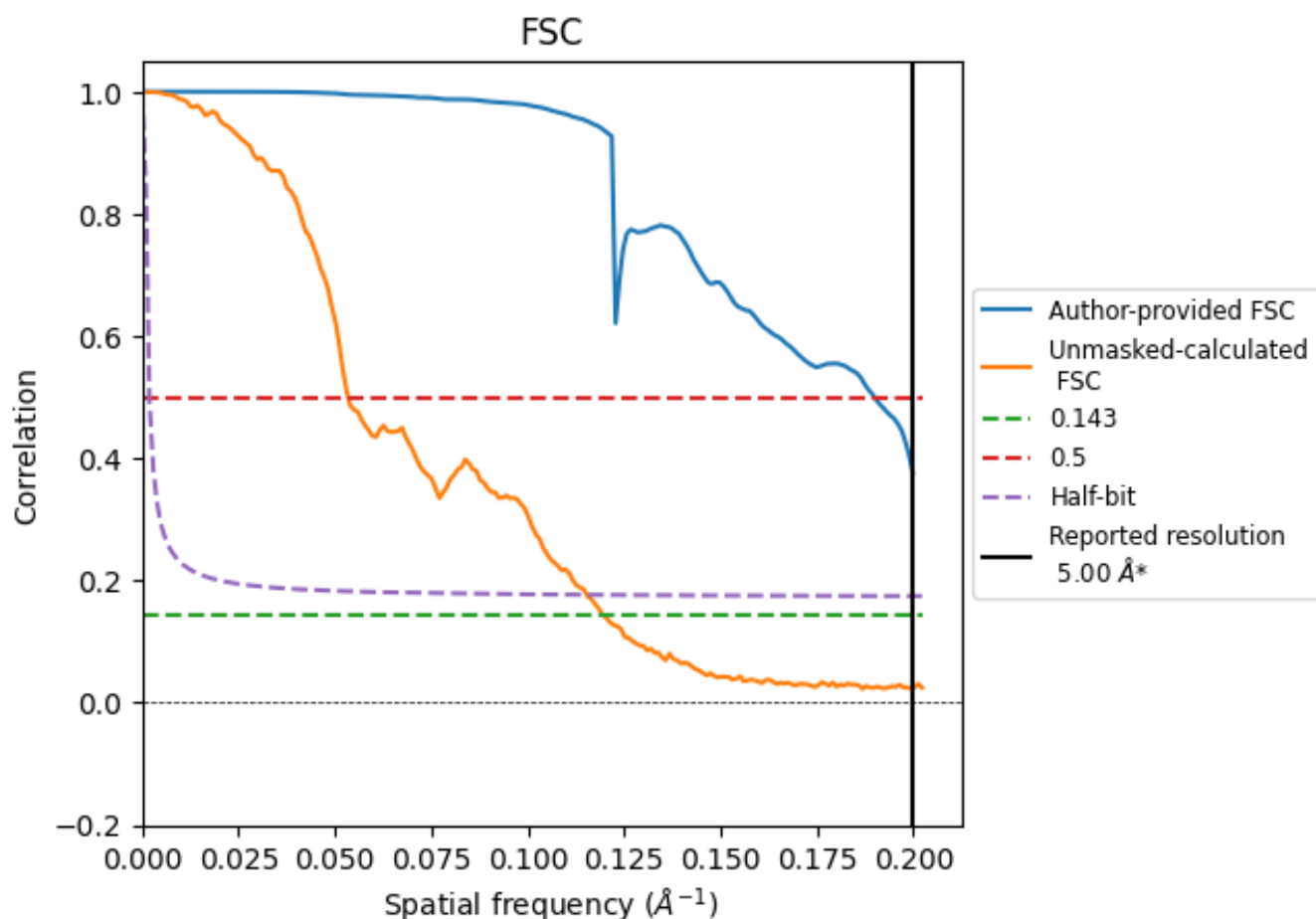


*Reported resolution corresponds to spatial frequency of 0.200 Å⁻¹

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 0.200 Å⁻¹

8.2 Resolution estimates [i](#)

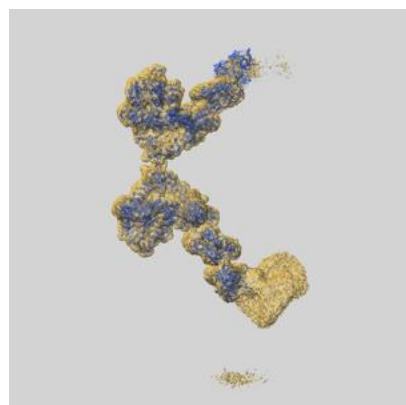
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.00	-	-
Author-provided FSC curve	-	5.27	-
Unmasked-calculated*	8.36	18.73	8.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.36 differs from the reported value 5.0 by more than 10 %

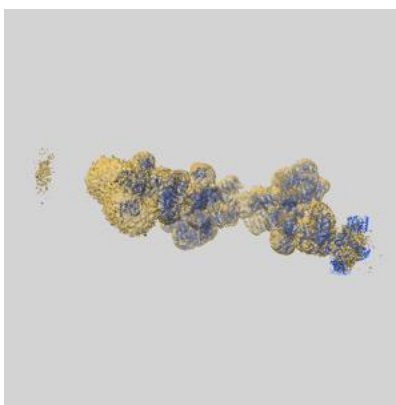
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53237 and PDB model 9QMS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

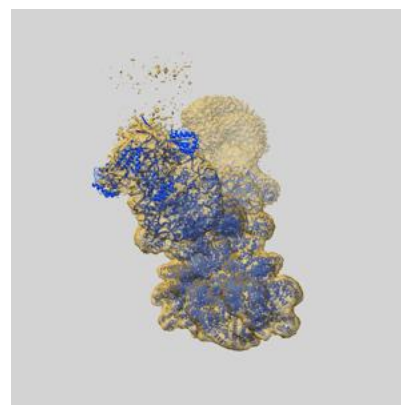
9.1 Map-model overlay [i](#)



X



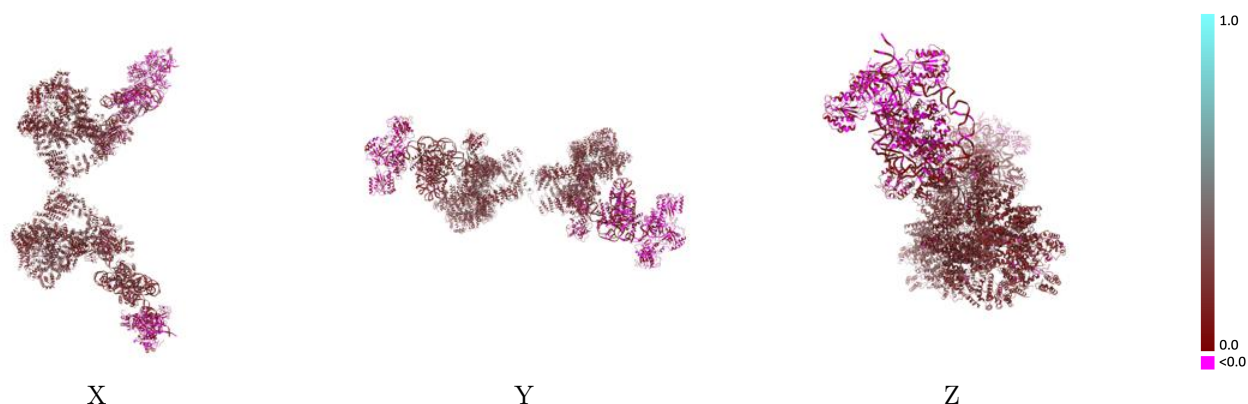
Y



Z

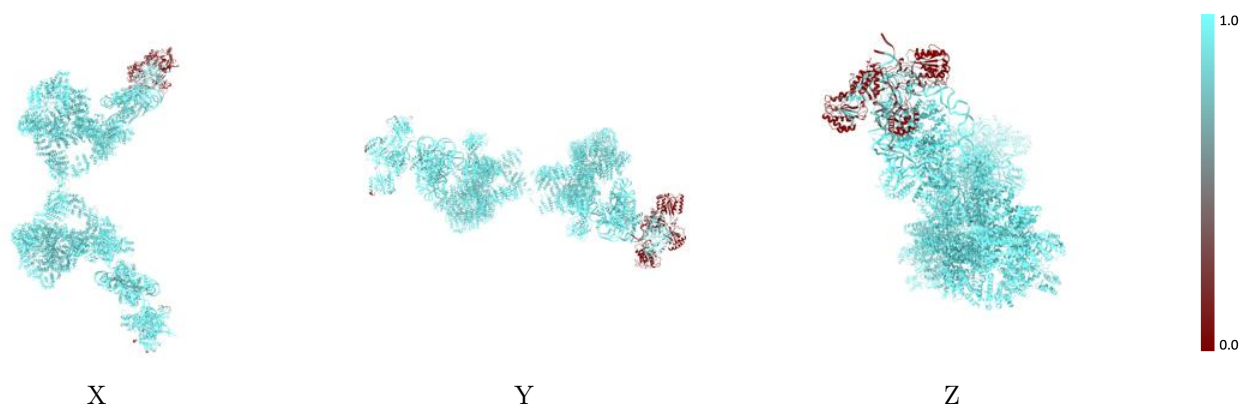
The images above show the 3D surface view of the map at the recommended contour level 0.21 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



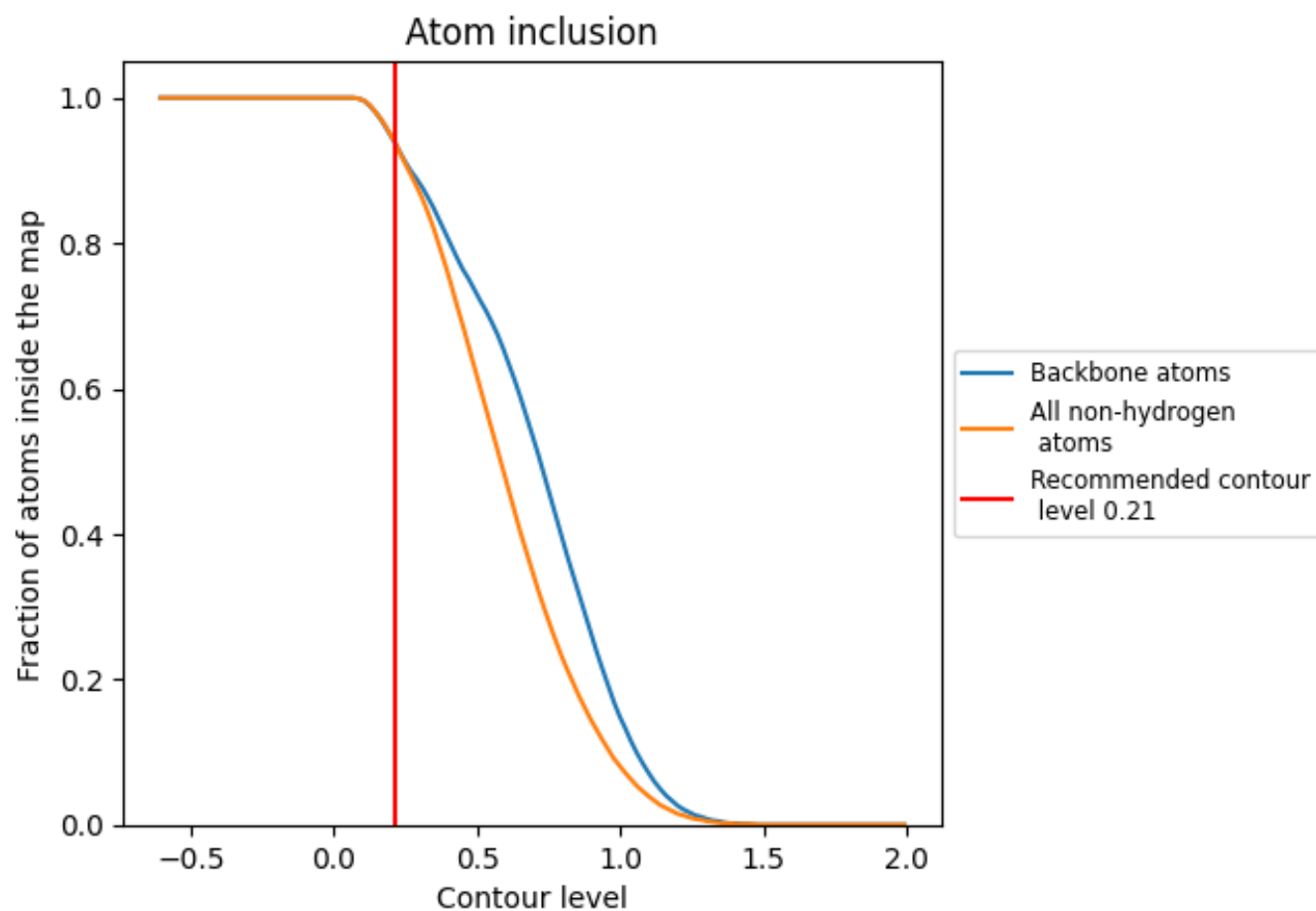
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.21).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.21) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9410	 0.1680
A	 1.0000	 0.1560
B	 1.0000	 0.1600
C	 0.9990	 0.1930
D	 1.0000	 0.2000
E	 1.0000	 0.0780
F	 0.9970	 0.0470
G	 0.9920	 0.0740
H	 0.9940	 0.1010
I	 0.9310	 0.1070
J	 0.9190	 0.1070
K	 0.9990	 0.2320
L	 0.9950	 0.1460
M	 1.0000	 0.1740
N	 0.9990	 0.2040
O	 0.9980	 0.2010
a	 1.0000	 0.0550
b	 1.0000	 0.0610
c	 0.9740	 0.0620
d	 0.9670	 0.0690
e	 1.0000	 0.1690
f	 1.0000	 0.1690
g	 1.0000	 0.1640
h	 1.0000	 0.1770
i	 1.0000	 0.1870
j	 1.0000	 0.2000
k	 0.9320	 0.0600
l	 0.9490	 0.0630
m	 0.2810	 0.0320
n	 0.3350	 0.0270
o	 0.9960	 0.2210

