



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:19 AM UTC

PDB ID : 8BH3 / pdb_00008bh3
EMDB ID : EMD-16044
Title : DNA-PK Ku80 mediated dimer bound to PAXX
Authors : Hardwick, S.W.; Chaplin, A.K.
Deposited on : 2022-10-28
Resolution : 4.55 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

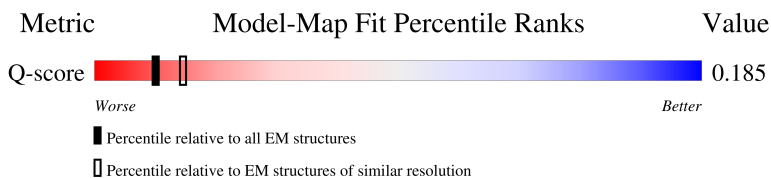
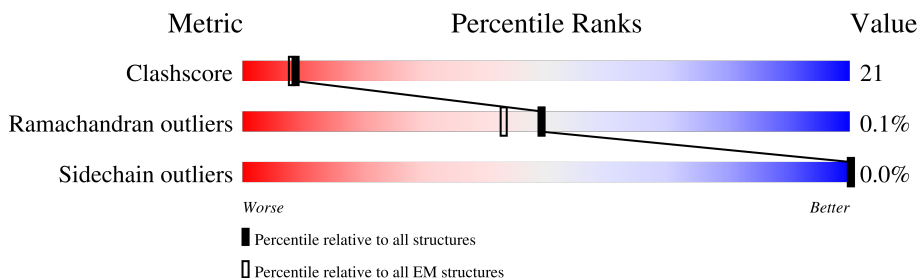
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.55 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.



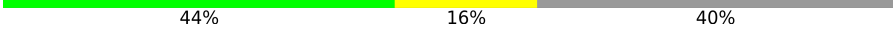
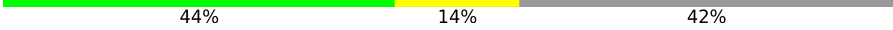
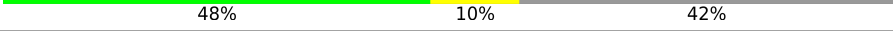
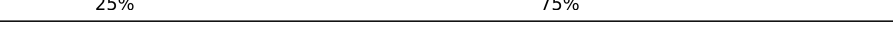
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2458 (4.05 - 5.04)

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

Mol	Chain	Length	Quality of chain
1	A	4128	
1	S	4128	
2	B	609	
2	T	609	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	732	 53%38%9%
3	L	732	 52%37%11%
4	D	204	 46%58%14%28%
4	M	204	 48%66%14%20%
5	G	336	 18%44%16%40%
5	H	336	 26%44%14%42%
5	P	336	 25%51%8%40%
5	Q	336	 26%48%10%42%
6	I	911	 17%10%73%
6	R	911	 17%10%73%
7	j	25	 12%88%
8	i	27	 33%67%
9	d	26	 19%81%
10	e	28	 25%75%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 89245 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3550	Total	C	N	O	S	0	0
			27927	17939	4728	5074	186		
1	S	3540	Total	C	N	O	S	0	0
			27999	18001	4725	5087	186		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	507	Total	C	N	O	S	0	0
			4038	2587	686	747	18		
2	T	502	Total	C	N	O	S	0	0
			4014	2569	680	747	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	668	Total	C	N	O	S	0	0
			5292	3382	884	1000	26		
3	L	652	Total	C	N	O	S	0	0
			5174	3304	871	973	26		

- Molecule 4 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	147	Total	C	N	O	S	0	0
			1075	689	183	197	6		
4	M	164	Total	C	N	O	S	0	0
			1195	754	207	228	6		

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

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

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	246	Total	C	N	O	S	0	0
			1977	1256	336	372	13		
6	R	246	Total	C	N	O	S	0	0
			1958	1240	332	373	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	27	Total	C	N	O	P	0	0
			552	265	102	158	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	26	Total	C	N	O	P	0	0
			528	253	89	160	26		

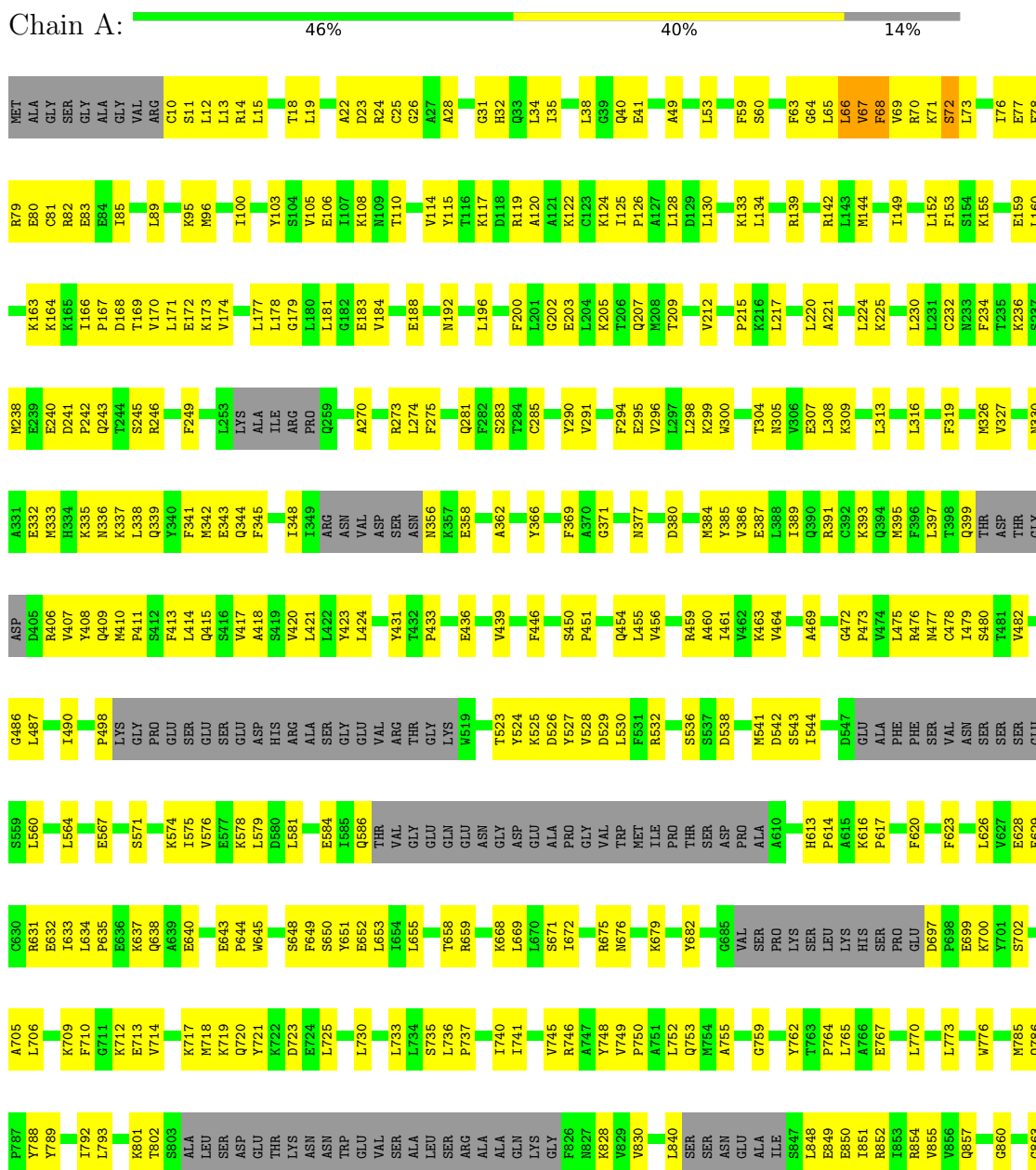
- Molecule 10 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	28	Total	C	N	O	P	0	0
			573	275	107	163	28		

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



HIS	H1830	H1687	A1595	G1513	C1432	E1354	E1265	C1183	L1111	V1021	H941	Q864
GLY	C1831	L1688	A1598	L1514	L1436	G1355	F1270	R1184	H1115	D1022	Q844	Q865
CYS	D1834	K1689	G1599	L1515	Y1437	W1356	F1271	H1185	A1116	T1024	F944	L870
ILE	A1835	G1690	M1600	E1516	G1438	K1357	L1271	K1186	D1117	T1024	Q947	L871
THR	V1693	V1693	M1601	A1517	L1439	L1358	R1274	S1187	E1118	R1025	Q953	THR
GLU	T1694	T1694	D1602	A1518	F1439	L1359	R1275	I1188	K1119	R1026	Q954	VAL
GLY	L1695	L1695	G1603	C1525	D1444	K1360	V1276	E1189	S1120	R1034	Q955	THR
ASP	F1696	F1696	S1604	L1528	R1445	H1367	G1277	K1193	L1121	E1035	P956	SER
SER	F1697	F1697	R1605	L1529	S1446	K1368	L1278	P1196	G1122	W1039	P957	ASP
THR	R1698	R1698	E1607	L1532	R1447	M1369	L1279	L1197	T1123	Q1043	H958	GLU
SER	F1699	F1699	R1608	L1533	L1448	K1370	L1282	L1201	C1127	Q1043	Y959	M879
LEU	THR	THR	Q1611	V1537	V1452	V1371	L1282	M1201	C1128	Q1043	Q960	M880
GLY	SER	SER	K1612	L1538	V1453	L1372	L1290	R1202	Q1049	Q1049	R961	K881
GLY	GLY	GLY	H1613	THR	A1454	V1373	V1294	S1203	S1052	S1052	Y962	D857
SER	GLY	GLY	Q1614	ALA	A1455	Q1374	F1295	M1205	M1065	M1065	K963	R888
SER	GLY	GLY	L1618	SER	K1456	P1379	F1296	L1206	L1071	L1071	L972	E889
LEU	GLY	GLY	L1621	LEU	Q1457	P1380	F1297	W1207	S1058	S1058	C974	K890
LEU	GLY	GLY	T1621	SER	L1458	G1382	L1298	L1208	K1061	K1061	Q978	L892
GLN	SER	SER	H1625	SER	H1459	F1384	E1299	E1215	I1138	I1138	Y979	F894
ASN	GLY	GLY	H1628	GLY	R1460	N1385	S1300	E1215	E1139	E1139	Y980	A895
GLU	SER	SER	K1628	SER	N1465	I1386	I1307	S1218	L1145	L1145	R981	F898
SER	VAL	VAL	W1632	VAL	N1466	G1387	K1311	G1226	M1146	M1146	Q982	R899
GLY	ILE	ILE	H1632	ILE	I1467	D1388	C1312	G1227	A1147	A1147	L983	E900
GLY	ILE	ILE	W1632	ILE	L1468	V1389	F1313	G1228	A1148	A1148	Y984	M901
GLY	ILE	ILE	S1637	H1552	P1469	Q1390	GLY	C1229	K1149	K1149	E985	K902
GLY	ILE	ILE	L1638	S1554	H1477	V1391	THR	Q1230	K1150	K1150	L987	P903
GLY	ILE	ILE	L1639	S1554	S1478	M1392	GLY	G1231	R1151	R1151	Y988	V904
GLY	ILE	ILE	E1640	Y1558	V1479	N1392	GLY	P1232	R1152	R1152	L987	I905
GLY	ILE	ILE	E1640	F1559	L1480	A1393	ALA	I1235	L1153	L1153	Q990	F910
GLY	ILE	ILE	K1642	Y1560	T1481	P1396	ASN	I1235	P1154	P1154	Q990	F910
GLY	ILE	ILE	V1645	L1562	E1482	N1401	ARG	Q1238	G1155	G1155	H993	R913
GLY	ILE	ILE	V1645	L1562	L1483	L1402	T1322	P1239	S1160	S1160	W994	V914
GLY	ILE	ILE	V1645	L1562	L1483	M1403	ARG	T1240	A1161	A1161	F995	T915
GLY	ILE	ILE	V1645	L1562	L1483	K1404	E1326	LEU	S1162	S1162	T996	E916
GLY	ILE	ILE	V1645	L1562	L1483	A1405	E1326	LEU	L1163	L1163	N997	L917
GLY	ILE	ILE	V1645	L1562	L1483	L1406	R1329	TRP	C1164	C1164	N998	A918
GLY	ILE	ILE	V1645	L1562	L1483	K1407	Y1330	LEU	L1165	L1165	K999	L919
GLY	ILE	ILE	V1645	L1562	L1483	M1408	M1331	ARG	D1167	D1167	K1000	
GLY	ILE	ILE	V1645	L1562	L1483		Y1332	GLY	E1086	E1086	Q1004	D923
GLY	ILE	ILE	V1645	L1562	L1483	Y1411	V1332	PRO	F1089	F1089	A1008	R924
GLY	ILE	ILE	V1645	L1562	L1483	K1412	S1333	PHE	E1092	E1092	L1009	Q925
GLY	ILE	ILE	V1645	L1562	L1483	D1413	K1334	GLY	L1010	L1010	K927	T926
GLY	ILE	ILE	V1645	L1562	L1483	I1414	C1335	S1249	L1011	L1011	V928	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	T1336	GLY	L1012	L1012	A1008	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1013	L1013	L1009	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1014	L1014	E1011	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1015	L1015	A1012	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1016	L1016	I1013	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1017	L1017	F1099	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1018	L1018	V1100	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1019	L1019	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1020	L1020	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1021	L1021	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1022	L1022	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1023	L1023	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1024	L1024	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1025	L1025	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1026	L1026	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1027	L1027	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1028	L1028	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1029	L1029	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1030	L1030	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1031	L1031	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1032	L1032	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1033	L1033	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1034	L1034	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1035	L1035	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1036	L1036	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1037	L1037	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1038	L1038	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1039	L1039	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1040	L1040	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1041	L1041	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1042	L1042	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1043	L1043	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1044	L1044	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1045	L1045	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1046	L1046	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1047	L1047	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1048	L1048	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1049	L1049	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1050	L1050	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1051	L1051	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1052	L1052	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1053	L1053	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1054	L1054	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1055	L1055	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1056	L1056	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1057	L1057	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1058	L1058	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1059	L1059	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1060	L1060	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1061	L1061	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1062	L1062	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1063	L1063	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1064	L1064	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1065	L1065	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1066	L1066	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1067	L1067	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1068	L1068	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1069	L1069	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1070	L1070	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1071	L1071	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1072	L1072	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1073	L1073	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1074	L1074	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1075	L1075	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1076	L1076	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1077	L1077	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1078	L1078	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1079	L1079	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1080	L1080	F1101	
GLY	ILE	ILE	V1645	L1562	L1483	L1415	V1337	GLY	L1081	L1081	F1101	
GLY	ILE	ILE	V1645	L1562								

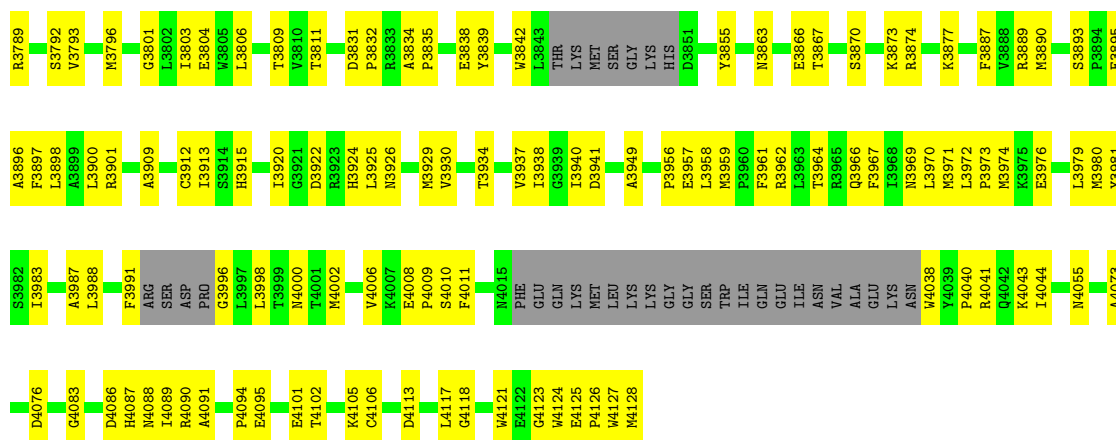
S3047	E2946	Q2864	D2779	LEU	THR	P2573	F2389	Q2324	R2254	I2182	GLU	GLN	PHE
K3048	T2947	H2865	L2760	GLY	LEU	N2574	H2390	L2325	L2255	H2183	GLU	SER	GLU
L3049		A2866	D2781	LEU	THR	P2575	G2391	L2326	I2256	A2184	GLU	TYR	ASN
K3050	K2850	A2867	D2782	PRO	GLN	M2576	V2392	L2327	F2257	M2185	SER	LEU	LEU
L3051	Q2951	L2868	Q2783	GLY	THR	F2577	L2393	R2328	E2258	V2187	VAL	TYR	ILE
K3052	I2952	L2869	L2784	ASP	ALA	E2578	K2394		K2259	V2187	PRO	SER	ASP
L3053				GLU	ASP		T2395	M2331	F2260	E2188	R2120	SER	LEU
Q3054	S2955	V2876	L2785	VAL	GLY	L2581	L2396	E2332	S2261	I2189	D2121	GLN	LYS
			K2786	ASP	ARG	S2582		E2333		V2190	L2122	ASN	ARG
D3059	L2958	S2883	L2787	ASN	SER		E2399	K2334	D2264	A2191	P2123	PRO	ARG
Q3059		S2788	L2788	LYS	SER	Q2587	L2402	N2335		S2124	S2124	ARG	TYR
	D2964	S2789	L2790	VAL	PHE	D2491	L2403	I2336	D2269	I2193	N2125	PRO	ASN
F3064	Y2965	Q2885	L2791	LYS	ASP	L2591	C2403	L2337	D2270	L2194	N2126	ALA	PHE
	S2866	R2891	L2791	GLY	TRP		R2404	E2338	S2271	S2195	K2127	PRO	PRO
K3067	E2967	L2892	L2794	ALA	LEU	W2595	V2405	E2339	G2272	W2196		VAL	VAL
H3070	A2968	Q2795	G2721	ALA	THR	R2596	Q2496	S2340	G2273	T2197		GLU	GLU
G3071	A2969	E2894	R2722	ALA	GLY	F2597	M2408	L2341	I2274	PHE	N2132	ARG	VAL
E3072	Q2971	A2896	T2793	SER	SER	T2603	Q2414	F2343	Q2275	L2199	N2135	ARG	VAL
			D2724	THR	ASP	PRO	S2417	L2344	G2278		P2139	ARG	PRO
K3075	K2978	R2899	D2724	ASP	ASP	MET	K2418		M2281	L2211	L2140	GLU	MET
	Q2979	L2900	L2728	PRO	PRO	PHE	K2503	K2347	A2282	A2212	N2141	GLN	GLU
E3079	W2981	L2901	R2731	VAL	LEU	VAL		Q2348	A2282	N2213	T2142	ARG	ARG
		ALA		VAL	VAL	GLU	Q2422	L2349	N2283	R2214	R2143	LYS	LYS
Y3082	G2984	GLU	D2735	ASP	HIS	THR	R2425	H2352	L2285	L2216	F2145	LYS	LYS
	E2985	LEU	Q2736	THR	THR	ALA	H2426	Q2353	F2286	R2217	L2146	VAL	TYR
E3085	F2986	PRO	E2737	SER	SER	GLN	L2517	N2354	P2287	F2218	A2147	HIS	ILE
L3088	T2987	ALA	K2738	PRO	PRO	GLN	D2428	T2355	Y2288	L2219	K2148	ASP	GLU
L3088	E2988	LYS	L2739	SER	SER	LYS	D2429	M2356		M2220	L2149	ASP	ILE
L3089	A2989	ARG	S2740	SER	SER	THR	E2430	E2357	Q2291		V2150	VAL	ARG
Y3090	E2990	VAL	L2741	ASP	ASP	LEU	R2431	D2358	C2292		T2151	LEU	LYS
	K2991	ARG	M2742	SER	SER	GLN	W2525	K2359	G2292	H2225		GLU	LYS
D3094	C3001	GLY	R2745	LEU	LEU	THR	S2526	F2360	C2293	F2226	E2154	LEU	ALA
D3095		LYS	K2746	LEU	LEU	ARG	H2527	I2361	Q2294	K2227	E2155	GLU	ARG
	E3007	ALA	G2747	PHE	PHE	THR	Y2440	V2362	Q2295	A2229	V2156	MET	GLU
K3100	W3008	ARG	V2748	ALA	ALA	GLN	K2441	C2363	E2298	V2230	F2157	ASP	ALA
Y3101		L2916	A2749	HIS	HIS	GLU	M2442	L2364	Y2299	F2231	R2158	GLU	ALA
Y3102		Q2834	Q2749	LYS	LYS	GLY	M2443	N2365		R2232		ASN	ALA
I3103	L3011	V2920	Q2750	ARG	ARG	SER	P2444	K2366	A2302	H2233	Y2160	LEU	ASN
Q3104		L2836	Q2751	SER	SER	LEU	K2445	V2367		R2234	A2161	ASP	GLY
	C3014	L2837	K2752	GLU	GLU	SER	L2446		W2164	L2235		SER	ASP
F3110		F2840	R2753	ARG	ARG	ALA		S2370	N2305	E2236		ASP	ASP
M3111	E3022	E2995	E2754	LEU	LEU	ARG	R2452	F2371	L2165	I2237	L2165	GLY	GLY
Q3112	ASN	N2841	K2755	GLN	GLN	TRP	L2845	P2372	S2166	L2238	S2166	PRO	PRO
N3113	PRO	A2927	E2756	ARG	ARG	PRO	L2455	F2373	M2307	K2239	P2167	M2094	SER
Y3114	PRO	K2928		ALA	ALA	VAL	S2547	L2374	S2308	T2240	L2168	A2095	TYR
S3115	ASP	L2929	K2762	PRO	PRO	ALA	V2458	A2375	F2309	L2241	L2169	L2097	MET
	LEU	Y2930		LEU	LEU	GLY	R2549	D2376	R2311	W2242	Q2170	SER	SER
ASN	ASN	R2931	Q2765	LYS	LYS	GLN	H2464	R2377	Y2312	E2243	L2171	L2100	SER
L3120		F2848	D2766	SER	SER	ILE	F2465	F2378	K2313	C2244	K2172		LEU
L3121	Y3029	S2849	V2769	VAL	VAL	ARG	S2466	M2379	Y2316	W2245	A2173	M2104	SER
H3122		F2936	V2770	GLY	GLY	ALA	F2564	N2380	A2317	K2246	S2174	H2105	TYR
Q3123	Y3036	D2937	L2771	PRO	PRO	THR	L2563	A2381	A2318	E2247	E2175	L2108	LEU
L3126	T3039	V2938	Y2772	ASP	ASP	GLN	C2469	R2470	A2319	G2248	ASN	L2108	ALA
T3127		S2856	Y2773	PHE	PHE	GLN	T2566	F2382		L2249	GLY	PRO	GLY
K3128	Y3043	R2940	R2773	GLY	GLY	GLN		F2383	K2330	S2250	GLY	PRO	D2033
L3129	R3044	T2944	H2777	LYS	LYS	HIS	P2570	L2386	V2321	I2251	G2179	PRO	ALA
Q3130	R3046	S2945	G2778	ASP	ASP	LYS	D2571	P2387	V2322	F2252	GLY	PRO	D2036
				PHE	ARG		Y2572	K2388	L2323	Y2253		GLY	W2049

V3132	GLU	D3226	I3227	ASP	V3132
L3135	ASN	S3228	S3229	ASN	L3135
T3136	SER	R3167	I3230	SER	T3136
E3137	MET	I3231	I3231	MET	E3137
I3138	ASN	R3232	S3233	ASN	I3138
O3139	VAL	S3237	S3237	VAL	O3139
E3140	ASP	P3174	D3174	ASP	E3140
GLN	GLN	P3175	P3175	GLN	GLN
F3141	ASP	K3176	K3176	ASP	F3141
I3142	GLY	N3177	N3177	GLY	I3142
A3143	ASP	I3178	I3178	ASP	A3143
S3144	ASP	M3179	M3179	S3144	S3144
S3145	PRO	I3243	I3243	S3145	S3145
S3146	SER	D3244	D3244	S3146	S3146
K3147	ASP	S3245	S3245	K3147	K3147
Q3148	ARG	K3248	K3248	Q3148	Q3148
G3149	GLU	M3256	M3256	G3149	G3149
L3150	GLU	L3259	L3259	L3150	L3150
L3151	VAL	L3262	L3262	L3151	L3151
Q3154	GLN	H3263	H3263	Q3154	Q3154
K3158	GLN	K3264	K3264	K3158	K3158
R3159	GLY	S3265	S3265	R3159	R3159
L3160	GLU	K3267	K3267	L3160	L3160
D3226	GLU	I3268	I3268	D3226	D3226
I3227	ASP	L3197	L3197	I3227	I3227
S3228	ASN	THR	THR	S3228	S3228
R3167	SER	PRO	PRO	R3167	R3167
I3230	MET	LEU	LEU	I3230	I3230
I3231	GLU	GLN	GLN	I3231	I3231
R3232	VAL	E3368	E3368	R3232	R3232
S3237	GLN	E3369	E3369	S3237	S3237
P3174	GLU	E3371	E3371	P3174	P3174
P3175	GLN	E3372	E3372	P3175	P3175
K3176	GLY	E3373	E3373	K3176	K3176
N3177	GLY	E3374	E3374	N3177	N3177
I3178	GLY	E3375	E3375	I3178	I3178
M3179	GLY	E3376	E3376	M3179	M3179
I3243	GLY	E3377	E3377	I3243	I3243
D3244	GLY	E3378	E3378	D3244	D3244
S3245	GLY	E3379	E3379	S3245	S3245
K3248	GLY	E3380	E3380	K3248	K3248
M3256	GLY	E3381	E3381	M3256	M3256
L3259	GLY	E3382	E3382	L3259	L3259
L3262	GLY	E3383	E3383	L3262	L3262
H3263	GLY	E3384	E3384	H3263	H3263
K3264	GLY	E3385	E3385	K3264	K3264
S3265	GLY	E3386	E3386	S3265	S3265
K3267	GLY	E3387	E3387	K3267	K3267
I3268	GLY	E3388	E3388	I3268	I3268
L3197	GLY	E3389	E3389	L3197	L3197
THR	GLY	E3390	E3390	THR	THR
PRO	GLY	E3391	E3391	PRO	PRO
LEU	GLY	E3392	E3392	LEU	LEU
GLN	GLY	E3393	E3393	GLN	GLN
A3441	GLY	E3394	E3394	A3441	A3441
Y3442	GLY	E3395	E3395	Y3442	Y3442
P3443	GLY	E3396	E3396	P3443	P3443
K3372	GLY	E3397	E3397	K3372	K3372
V3373	GLY	E3398	E3398	V3373	V3373
R3380	GLY	E3399	E3399	R3380	R3380
H3384	GLY	E3400	E3400	H3384	H3384
A3888	GLY	E3401	E3401	A3888	A3888
V3389	GLY	E3402	E3402	V3389	V3389
Q3390	GLY	E3403	E3403	Q3390	Q3390
A3391	GLY	E3404	E3404	A3391	A3391
S3286	GLY	E3405	E3405	S3286	S3286
R3287	GLY	E3406	E3406	R3287	R3287
S3288	GLY	E3407	E3407	S3288	S3288
R3289	GLY	E3408	E3408	R3289	R3289
Q3291	GLY	E3409	E3409	Q3291	Q3291
G3292	GLY	E3410	E3410	G3292	G3292
Q3293	GLY	E3411	E3411	Q3293	Q3293
Q3296	GLY	E3412	E3412	Q3296	Q3296
T3303	GLY	E3413	E3413	T3303	T3303
V3304	GLY	E3414	E3414	V3304	V3304
S3305	GLY	E3415	E3415	S3305	S3305
L3306	GLY	E3416	E3416	L3306	L3306
L3307	GLY	E3417	E3417	L3307	L3307
D3308	GLY	E3418	E3418	D3308	D3308
E3309	GLY	E3419	E3419	E3309	E3309
N3319	GLY	E3420	E3420	N3319	N3319
I3320	GLY	E3421	E3421	I3320	I3320
L3321	GLY	E3422	E3422	L3321	L3321
A3322	GLY	E3423	E3423	A3322	A3322
F3323	GLY	E3424	E3424	F3323	F3323
R3324	GLY	E3425	E3425	R3324	R3324
D3325	GLY	E3426	E3426	D3325	D3325
K3326	GLY	E3427	E3427	K3326	K3326
M3240	GLY	E3428	E3428	M3240	M3240
L3328	GLY	E3429	E3429	L3328	L3328
L3329	GLY	E3430	E3430	L3329	L3329
L3330	GLY	E3431	E3431	L3330	L3330
T3333	GLY	E3432	E3432	T3333	T3333
T3337	GLY	E3433	E3433	T3337	T3337
A3340	GLY	E3434	E3434	A3340	A3340
D3354	GLY	E3435	E3435	D3354	D3354
L3360	GLY	E3436	E3436	L3360	L3360
S3364	GLY	E3437	E3437	S3364	S3364
SER	GLY	E3438	E3438	SER	SER
GLU	GLY	E3439	E3439	GLU	GLU
ALA	GLY	E3440	E3440	ALA	ALA
GLY	GLY	E3441	E3441	GLY	GLY
PRO	GLY	E3442	E3442	PRO	PRO
ALA	GLY	E3443	E3443	ALA	ALA
G3408	GLY	E3444	E3444	G3408	G3408
I3410	GLY	E3445	E3445	I3410	I3410
Y3413	GLY	E3446	E3446	Y3413	Y3413
M3414	GLY	E3447	E3447	M3414	M3414
L3415	GLY	E3448	E3448	L3415	L3415
F3416	GLY	E3449	E3449	F3416	F3416
F3419	GLY	E3450	E3450	F3419	F3419
C3420	GLY	E3451	E3451	C3420	C3420
D3421	GLY	E3452	E3452	D3421	D3421
Q3422	GLY	E3453	E3453	Q3422	Q3422
Q3423	GLY	E3454	E3454	Q3423	Q3423
L3424	GLY	E3455	E3455	L3424	L3424
R3425	GLY	E3456	E3456	R3425	R3425
E3428	GLY	E3457	E3457	E3428	E3428
E3429	GLY	E3458	E3458	E3429	E3429
ASN	GLY	E3459	E3459	ASN	ASN
ALA	GLY	E3460	E3460	ALA	ALA
ALA	GLY	E3461	E3461	ALA	ALA
VAL	GLY	E3462	E3462	VAL	VAL
ILE	GLY	E3463	E3463	ILE	ILE
ASP	GLY	E3464	E3464	ASP	ASP
ALA	GLY	E3465	E3465	ALA	ALA
GLU	GLY	E3466	E3466	GLU	GLU
LEU	GLY	E3467	E3467	LEU	LEU
GLN	GLY	E3468	E3468	GLN	GLN
A3441	GLY	E3469	E3469	A3441	A3441
Y3442	GLY	E3470	E3470	Y3442	Y3442
P3443	GLY	E3471	E3471	P3443	P3443
K3444	GLY	E3472	E3472	K3444	K3444
L3445	GLY	E3473	E3473	L3445	L3445
V3446	GLY	E3474	E3474	V3446	V3446
I33535	GLY	E3475	E3475	I33535	I33535
S3536	GLY	E3476	E3476	S3536	S3536
S3539	GLY	E3477	E3477	S3539	S3539
T3545	GLY	E3478	E3478	T3545	T3545
K3550	GLY	E3479	E3479	K3550	K3550
N3551	GLY	E3480	E3480	N3551	N3551
K3552	GLY	E3481	E3481	K3552	K3552
E3553	GLY	E3482	E3482	E3553	E3553
F3554	GLY	E3483	E3483	F3554	F3554
I3558	GLY	E3484	E3484	I3558	I3558
Q3564	GLY	E3485	E3485	Q3564	Q3564
I3568	GLY	E3486	E3486	I3568	I3568
F3571	GLY	E3487	E3487	F3571	F3571
A3574	GLY	E3488	E3488	A3574	A3574
L3575	GLY	E3489	E3489	L3575	L3575
P3581	GLY	E3490	E3490	P3581	P3581
F3585	GLY	E3491	E3491	F3585	F3585
W3588	GLY	E3492	E3492	W3588	W3588
S3589	GLY	E3493	E3493	S3589	S3589
N3590	GLY	E3494	E3494	N3590	N3590
D3591	GLY	E3495	E3495	D3591	D3591
V3592	GLY	E3496	E3496	V3592	V3592
R3593	GLY	E3497	E3497	R3593	R3593
A3597	GLY	E3498	E3498	A3597	A3597
LYS	GLY	E3499	E3499	LYS	LYS
THR	GLY	E3500	E3500	THR	THR
A3511	GLY	E3501	E3501	A3511	A3511
V3512	GLY	E3502	E3502	V3512	V3512
A3513	GLY	E3503	E3503	A3513	A3513
V3514	GLY	E3504	E3504	V3514	V3514
Q3515	GLY	E3505	E3505	Q3515	Q3515
H3516	GLY	E3506	E3506	H3516	H3516
S3517	GLY	E3507	E3507	S3517	S3517
V3519	GLY	E3508	E3508	V3519	V3519
E3520	GLY	E3509	E3509	E3520	E3520
I3521	GLY	E3510	E3510	I3521	I3521
T3522	GLY	E3511	E3511	T3522	T3522
H3716	GLY	E3512	E3512	H3716	H3716
Y3717	GLY	E3513	E3513	Y3717	Y3717
M3613	GLY	E3514	E3514	M3613	M3613
R3718	GLY	E3515	E3515	R3718	R3718
G3618	GLY	E3516	E3516	G3618	G3618
P3620	GLY	E3517	E3517	P3620	P3620
L3625	GLY	E3518	E3518	L3625	L3625
G3626	GLY	E3519	E3519	G3626	G3626
A3627	GLY	E3520	E3520	A3627	A3627
F3628	GLY	E3521	E3521	F3628	F3628
R3629	GLY	E3522	E3522	R3629	R3629
R3630	GLY	E3523	E3523	R3630	R3630
T3633	GLY	E3524	E3524	T3633	T3633
Q3634	GLY	E3525	E3525	Q3634	Q3634
K3638	GLY	E3526	E3526	K3638	K3638
E3639	GLY	E3527	E3527	E3639	E3639
F3640	GLY	E3528	E3528	F3640	F3640
G3647	GLY	E3529	E3529	G3647	G3647
GLY	GLY	E3530	E3530	GLY	GLY
SER	GLY	E3531	E3531	SER	SER
LYS	GLY	E3532	E3532	LYS	LYS
LEU	GLY	E3533	E3533	LEU	LEU
ARG	GLY	E3534	E3534	ARG	ARG
MET	GLY	E3535	E3535	MET	MET
L3751	GLY	E3536	E3536	L3751	L3751
L3752	GLY	E3537	E3537	L3752	L3752
S3657	GLY	E3538	E3538	S3657	S3657
D3658	GLY	E3539	E3539	D3658	D3658
F3659	GLY	E3540	E3540	F3659	F3659
N3660	GLY	E3541	E3541	N3660	N3660
D3661	GLY	E3542	E3542	D3661	D3661
N3664	GLY	E3543	E3543	N3664	N3664
M3665	GLY	E3544	E3544	M3665	M3665
K3675	GLY	E3545	E3545	K3675	K3675
P3676	GLY	E3546	E3546	P3676	P3676
F3677	GLY	E3547	E3547	F3677	F3677
G3678	GLY	E3548	E3548	G3678	G3678
N3679	GLY	E3549	E3549	N3679	N3679
D3761	GLY	E3550	E3550	D3761	D3761
Q3762	GLY	E3551	E3551	Q3762	Q3762
R3763	GLY	E3552	E3552	R3763	R3763
N3772	GLY	E3553	E3553	N3772	N3772
L3788	GLY	E3554	E3554	L3788	L3788
R3789					

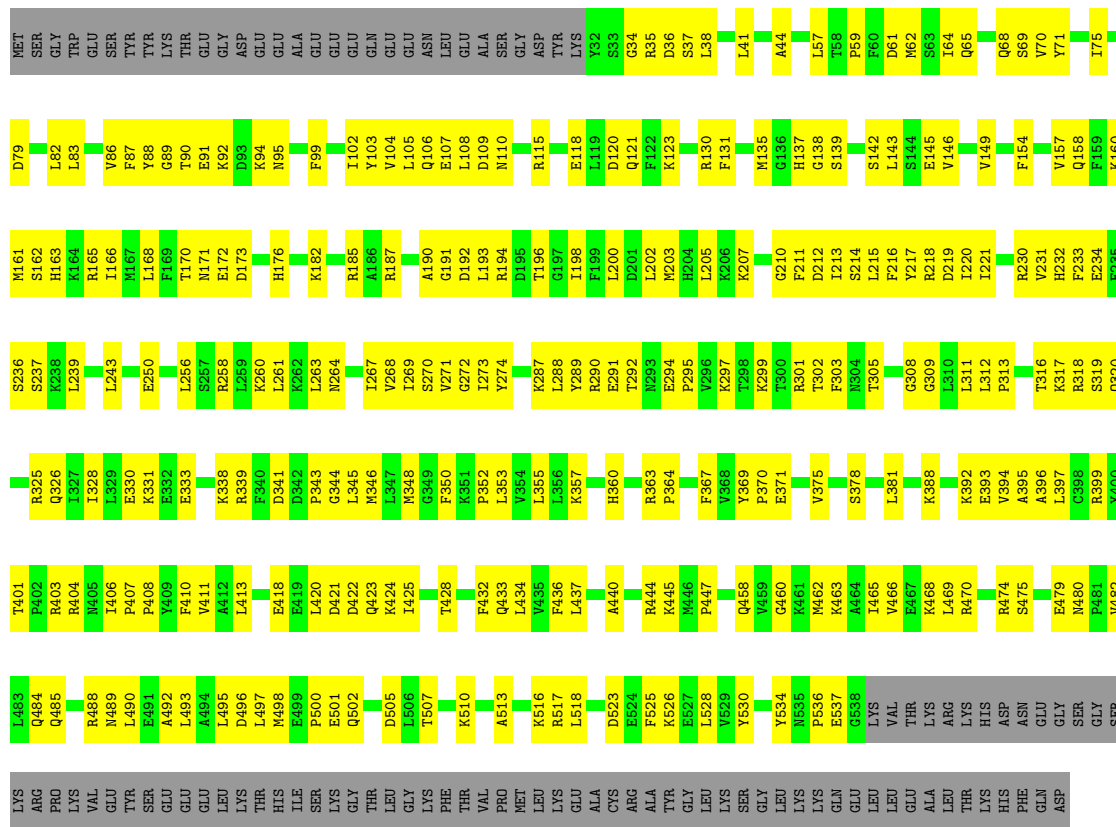
T169	ARG	ASP	T432	ARG	GLU	G665	L736	SER	K381	Y1107	Y1192	T1275
V170	PRO	SER	P433	THR	GLN	F666	F737	ALA	S882	M1108	K1193	A1278
L171	Q259	ASN	V494	GLY	GLU	Y667	H738	LEU	Y883	E1109	F1194	Q1278
E172	Q261	LYS	L435	W519	ASN	K668	N739	SER	D887	H1115	V1195	L1279
K173	D261	LYS	L438	P522	ASP	L669	T740	ARG	K888	A1116	P1197	Q1280
V174	Y265	LYS	L438	T523	GLY	L670	I741	ALA	K889	D1117	L1198	V1281
Y175	Y265	LYS	L438	T524	ASP	S671	E742	GLN	K890	E1118	P1199	L1282
E176	Y265	LYS	L438	T525	ASP	L672	Q753	LYS	K891	G1121	N1201	T1284
L177	P268	LYS	F446	K526	ALA	R675	M754	GLY	K892	T1123	M1205	K1292
V184	P268	LYS	P447	K526	PRO	K678	Q753	LYS	K893	T1124	K1209	A1293
H185	A270	LYS	Q448	K526	VAL	L680	W758	GLY	K894	Q1125	F1209	F1297
P186	A270	LYS	Y449	K526	VAL	L681	G759	GLY	K895	Q1126	D1210	L1298
M189	L274	LYS	S450	Y527	TRP	Y682	L759	LYS	K896	C1127	V1211	E1299
F186	F275	LYS	P451	Y528	MET	Y683	L759	LYS	K897	C1128	K1213	S1300
M189	F275	LYS	K452	D529	ILE	L680	L759	LYS	K898	I1131	F1219	I1301
N195	H278	LYS	M453	L530	THR	Y682	L759	LYS	K899	D1132	F1219	H1304
L196	Q281	LYS	L455	F531	THR	Y682	L759	LYS	K899	H1133	L1220	D1305
F197	L286	LYS	L455	Q454	THR	Y682	L759	LYS	K899	C1134	I1221	I1307
R198	L286	LYS	L455	Q454	THR	Y682	L759	LYS	K899	C1135	E1225	C1312
A199	F294	LYS	V462	M540	THR	Y682	L759	LYS	K899	C1136	G1226	F1313
F200	E295	LYS	V462	M541	THR	Y682	L759	LYS	K899	C1137	G1227	GLY
L201	V296	LYS	V464	D542	THR	Y682	L759	LYS	K899	C1138	G1227	GLY
M208	L297	LYS	A469	S543	THR	Y682	L759	LYS	K899	C1139	G1227	GLY
E214	L298	LYS	A469	S543	THR	Y682	L759	LYS	K899	C1140	G1227	GLY
L217	K299	LYS	L475	I544	THR	Y682	L759	LYS	K899	C1141	G1227	GLY
L220	W300	LYS	L475	I544	THR	Y682	L759	LYS	K899	C1142	G1227	GLY
A221	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1143	G1227	GLY
C223	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1144	G1227	GLY
L224	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1145	G1227	GLY
K225	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1146	G1227	GLY
G226	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1147	G1227	GLY
L227	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1148	G1227	GLY
S228	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1149	G1227	GLY
S229	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1150	G1227	GLY
L230	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1151	G1227	GLY
S237	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1152	G1227	GLY
E240	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1153	G1227	GLY
Q243	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1154	G1227	GLY
T244	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1155	G1227	GLY
S245	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1156	G1227	GLY
R246	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1157	G1227	GLY
E247	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1158	G1227	GLY
L248	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1159	G1227	GLY
F249	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1160	G1227	GLY
N250	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1161	G1227	GLY
F251	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1162	G1227	GLY
V252	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1163	G1227	GLY
L253	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1164	G1227	GLY
LYS	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1165	G1227	GLY
ILE	C301	LYS	N477	D547	THR	Y682	L759	LYS	K899	C1166	G1227	GLY

E2410	L2344	S2261	A2191	S2124	ARG	VAL	A1922	LEU	Q1779	GLY	Q1614	SER	Q1426	W1356
L2411	V2345		T2192	W2125	PRO	GLU	A1922	ASN	S1780	GLY	K1617	LEU	K1357	K1357
Y2412	A2346	N2270	L2193	M2126	ALA	VAL	N1926	GLU	F1781	SER	K1617	GLY	D1444	L1358
F2413	K2347	S2271	L2194	K2127	THR	GLU	M1926	SER	F1782	NET	L1707	SER	R1445	L1359
Q2414	Q2348	V2272	S2195	L2196	GLY	VAL	ALA	T1862	R1783	E1708	T1620	SER	S1446	K1360
L2415	L2349	G2273	W2196		ARG	PRO	GLY	F1863	R1784	E1709	L1623	GLN	R1447	K1361
K2416	K2350	I2274	W2196		PHE	MET	GLU	D1864	I1785	L1710	L1623	GLY	L1448	
S2417	Q2351	Q2275	L2199	G2194	ARG	GLU	ASN			R1711	Q1624	SER	V1452	T1366
K2418	H2352	L2276	A2200	N2195	ARG	ARG	GLN	I1867	R1788	R1712	H1625	SER	H1367	H1367
	Q2353	L2277	T2201	W2196	ARG	GLU	LEU	T1868	T1793	V1713	W1626	ILE	L1368	M1369
V2421	N2354	P2202	Q2353	L2197	GLU	LYS	L1934			L1714	K1627	HIS	L1458	
	T2355	L2279	T2203	G2194	GLN	TYR	E1935	M1871	L1797	Q1716	D1630	F1553	H1459	R1370
N2424	K2356	V2280		N2195	ARG	TYR	E1935	G1872		E1715	D1630	F1553	R1460	V1371
R2425	E2357	M2281	P2206	R2143	ASP	ILE	R1937	Y1873		Q1716	S1631	H1555	L1372	L1372
H2426	D2358	A2282	K2207	L2144	PRO	GLU	R1938		V1801	I1718	S1631	H1555	L1373	Q1373
R2427	K2359	F2145	D2208	F2145	THR	ILE	L1939	I1877	M1804	V1719	W1632	Y1558	I1467	Q1374
	F2360	D2284	E2209	L2146	VAL	ARG	Y1940	D1878	R1806	H1721	L1468	Y1558	L1375	T1375
		L2285	V2210		HIS	LYS		V1879	R1806	F1722	P1469	L1562	L1376	T1376
E2430	N2365	P2286	L2211	L2149	ASP	GLU	C1947	M1880	LYS	P1731	V1645	E1565	C1377	C1377
R2431	K2366	P2287		V2150	ASP	ALA	A1948	V1881	ASP	M1724	L1646	E1565	E1378	E1378
Q2432	K2367		R2214	I2151	VAL	ARG	C1954		PRO	P1731	L1649	E1567	V1479	V1479
K2433	T2368	Q2291	L2215	T2153	LEU	GLU	L1959	ASP	ASP	N1738	K1651	N1568	L1483	G1383
C2435	K2369	C2292	L2216	T2153	GLU	ALA	F1961	HIS	R1816	V1740	K1651	E1570	G1384	E1570
L2436	S2370	G2293	H2217	E2154	LEU	ALA	Y1961	ALA		H1741	L1663	L1571	N1385	N1385
D2437	F2371	I2284	F2218	E2155	GLU	ALA	Y1962	LYS	V1820	C1742	S1664	L1577	K1489	K1489
I2438	P2372	Q2295	L2219	V2156	MET	GLY	Q1963	GLU	R1822	M1743	H1665	A1578	G1490	G1490
	F2373		M2220	F2157	ASP			GLY	S1823	K1744	T1663	L1577	I1491	I1491
Y2440	L2374	Y2299		R2158	ASP	ASP		GLY	S1823	K1744	T1663	L1577	V1389	V1389
K2441	A2375	N2305	V2223	P2159	LEU	ASP	L1959	VAL	R1816	V1740	T1663	L1577	A1390	A1390
M2442	D2376	K2306	F2224	Q2161	ASN	GLY	F1961	ALA		H1741	T1663	L1577	PRO	PRO
N2443	R2377	N2307	H2225	A2161	ASN	GLY	Y1962	LYS	V1820	C1742	S1664	L1577	GLY	GLY
P2444	F2378	S2308	K2226	K2162	H2091	SER	Q1963	GLU	R1822	M1743	H1665	A1578	ASP	ASP
K2445	M2379	F2309	K2227	H2163	E2092	MET		GLY	S1823	K1744	T1663	L1577	GLU	GLU
L2446	V2382	Y2312	F2231	L2165	M2094	THR		GLY	S1823	K1744	T1663	L1577	GLN	GLN
E2450	F2383	K2312	R2232	S2166	L2097	LEU		GLY	S1823	K1744	T1663	L1577	CYS	CYS
L2451	F2384	K2313	H2233	P2167		LEU		GLY	S1823	K1744	T1663	L1577	LEU	LEU
R2462	L2385	E2314	N2234	L2168		SER		GLY	S1823	K1744	T1663	L1577	PRO	PRO
	L2386	V2315	L2235	L2169	L2100	SER		GLY	S1823	K1744	T1663	L1577	LEU	LEU
L2465	P2387	Y2316	E2236	Q2170	V2101	THR		GLY	S1823	K1744	T1663	L1577	LEU	LEU
N2466	K2388	T2237	L2237	L2171	K2102	ALA		GLY	S1823	K1744	T1663	L1577	PRO	PRO
P2467	F2389	E2321	I2238	A2172		ASP		GLY	S1823	K1744	T1663	L1577	PRO	PRO
		V2322	L2241	A2173	R2106	S2034		CYS	R1837	S1755	L1684	M1592	G1513	G1513
E2460	V2392			S2174	L2107			ILE	R1837	S1755	L1684	M1592	L1514	L1514
H2464	T2395	L2327	C2244	E2175	L2108	Q2042		THR	F1840	P1756	D1685	V1593	L1515	L1515
P2465	L2396	W2245	W2245	N2176	GLY	F2043		GLU	S1841	L1758	D1685	V1593	E1516	E1516
S2466	C2397	Y2329	K2246	GLY	PRO	D2044		GLY	S1841	L1758	D1685	V1593	L1517	L1517
	L2398	V2330	D2247	G2179	PRO			GLY	S1841	L1758	D1685	V1593	L1517	L1517
C2469	R2399	M2331	C2248	E2180	GLN	G2048		ASN	V1844	E1760	L1688	M1600	R1527	R1527
R2470	V2400	E2332	L2249	G2181	GLY	V2049		LEU	V1845	L1761	K1689	M1600	W1529	W1529
E2471	L2401	R2333	L2249	G2181	GLU	Q2050		ILE	I1848	E1764	V1693	M1600	S1530	S1530
Q2472	L2402	K2334	P2252	H2183	ASP	SER	ASP	ASP	D1849	E1769	L1696	M1604	L1531	L1531
M2473	C2403	Y2253	Y2253	H2183	SER	TYR	LEU	LYS	V1850	E1769	L1696	M1604	L1532	L1532
	R2404	L2254	R2254	M2185	VAL	TYR	GLY	LYS	L1851	E1769	L1696	M1604	L1532	L1532
	V2405	L2255	L2255	M2185	VAL	TYR	GLY	ARG	L1851	E1769	L1696	M1604	L1532	L1532
	E2406	L2256	L2256	V2186	PRO	SER	ARG	ARG	L1851	E1769	L1696	M1604	L1532	L1532
	G2407	E2339	L2257	V2187	R2120	SER	TYR	TYR	L1851	E1769	L1696	M1604	L1532	L1532
H2481	D2482	N2408	F2257	E2188	D2121	GLN	ASN	GLN	L1851	E1769	L1696	M1604	L1532	L1532
N2483			F2260	V2190	L2122	ASP	PHE	THR	L1851	E1769	L1696	M1604	L1532	L1532
					P2123	PRO	PRO	LYS	L1851	E1769	L1696	M1604	L1532	L1532

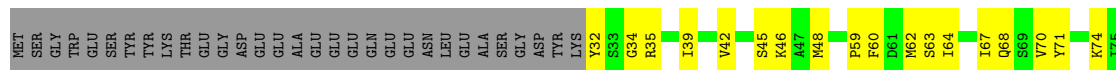


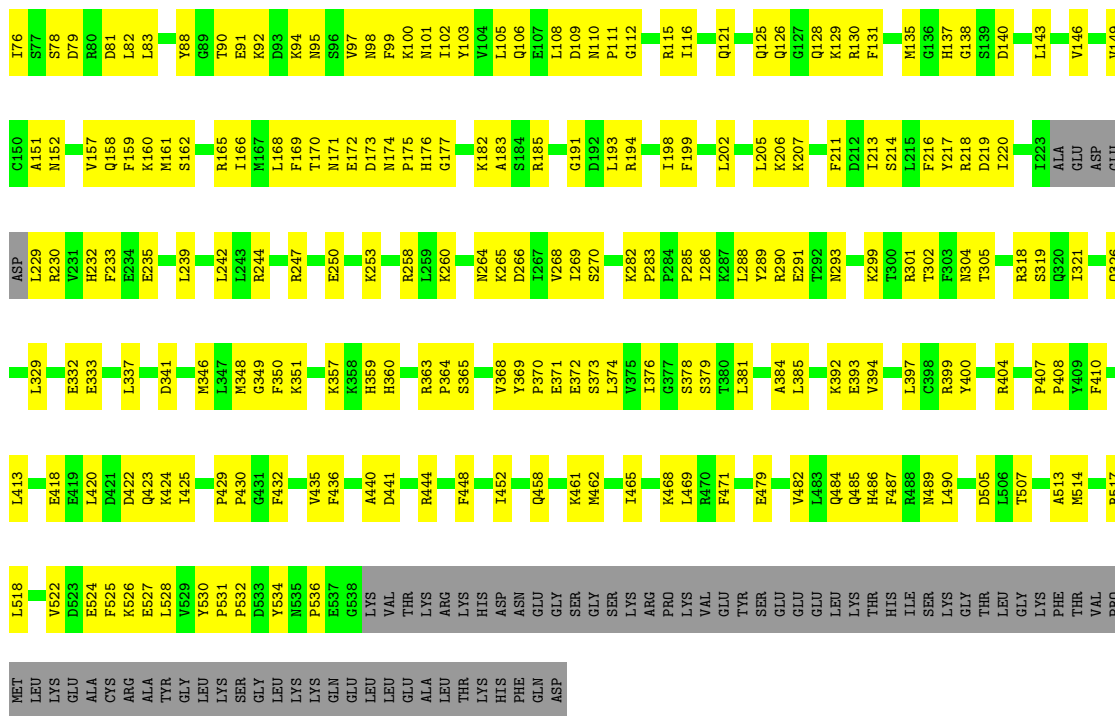


• Molecule 2: X-ray repair cross-complementing protein 6



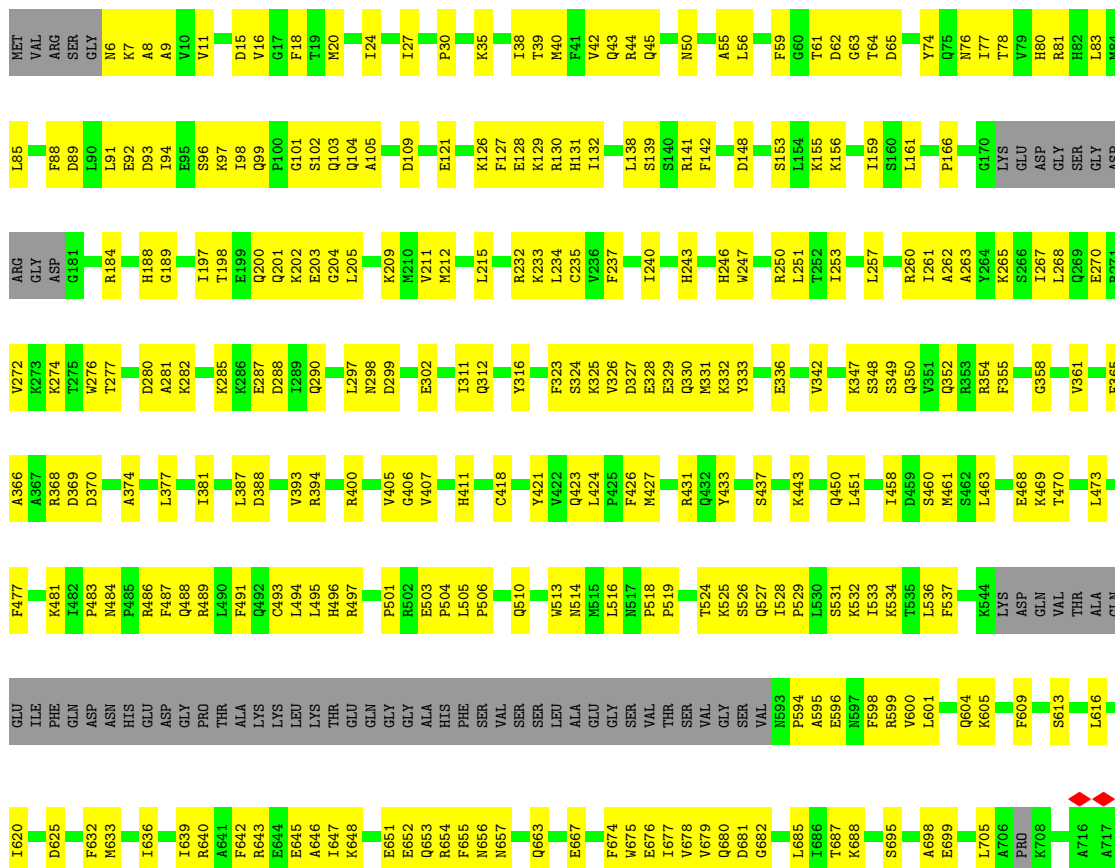
• Molecule 2: X-ray repair cross-complementing protein 6





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

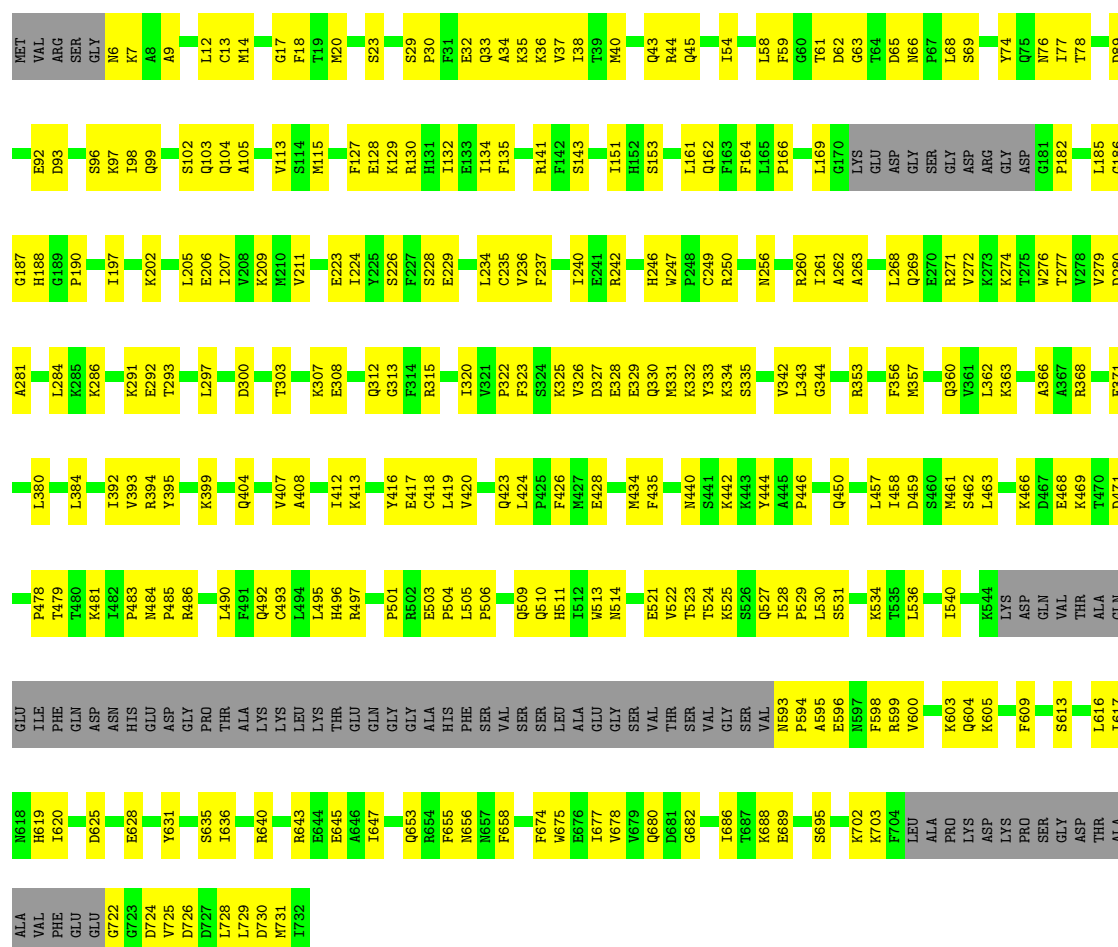
Chain C: 53% 38% 9%

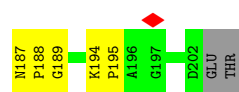




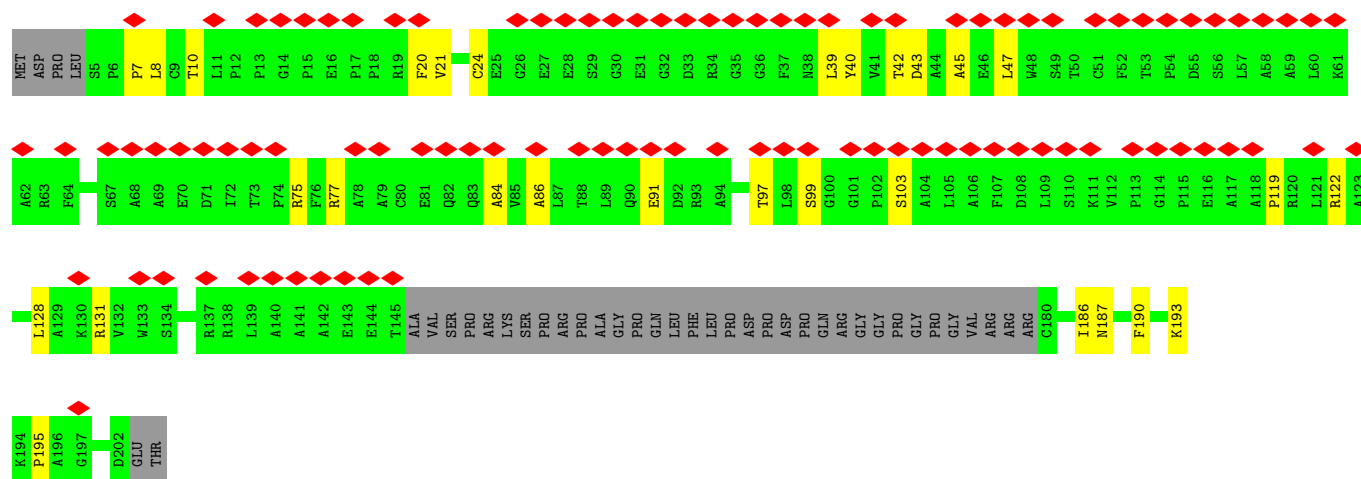
• Molecule 3: X-ray repair cross-complementing protein 5

Chain L: 52% 37% 11%

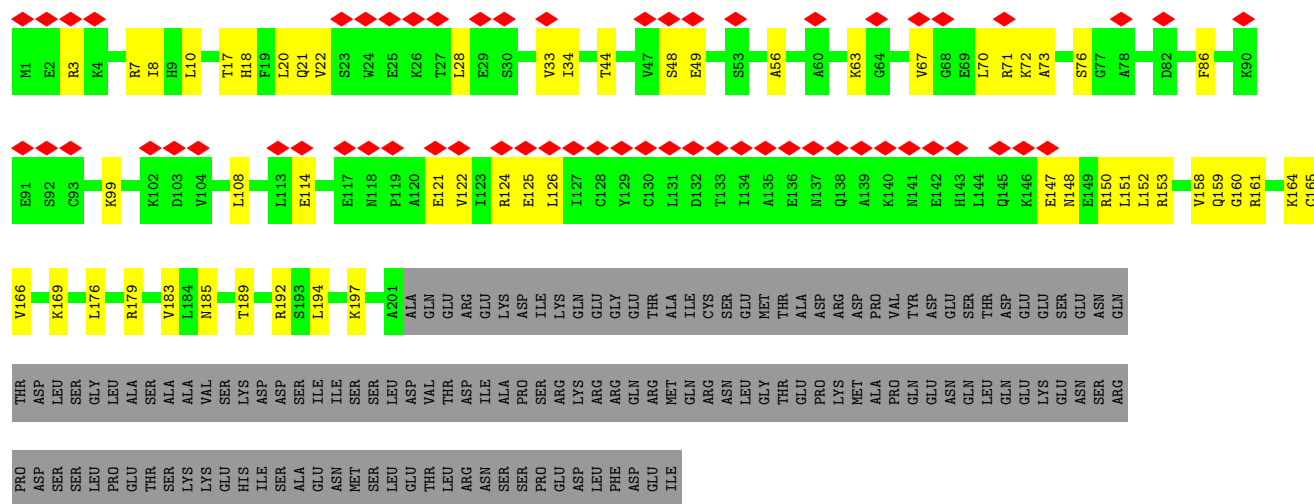
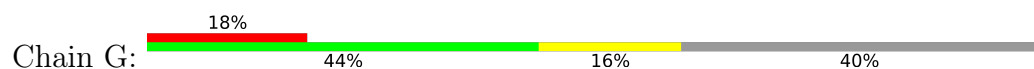




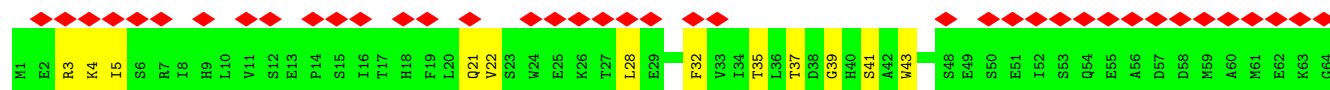
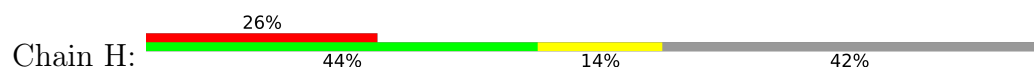
• Molecule 4: Protein PAXX



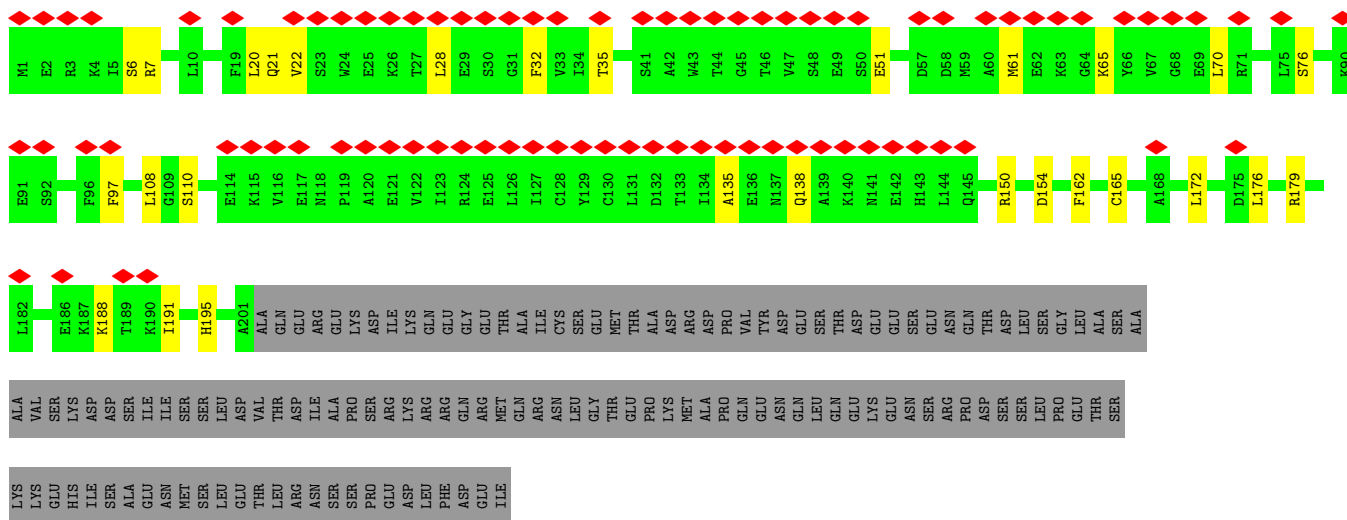
• Molecule 5: DNA repair protein XRCC4



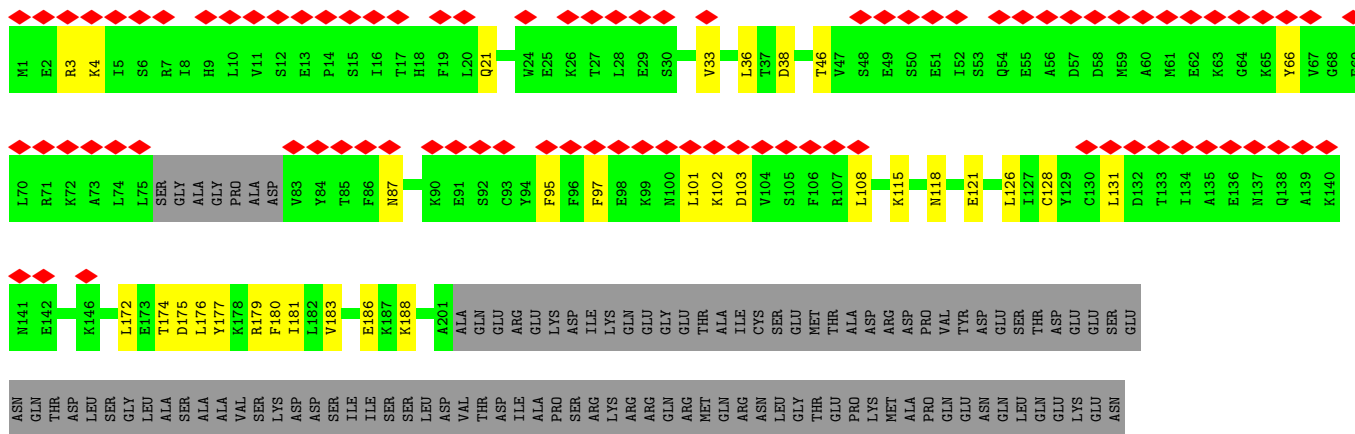
• Molecule 5: DNA repair protein XRCC4



- Molecule 5: DNA repair protein XRCC4



- Molecule 5: DNA repair protein XRCC4



SER ARG
PRO ASP
SER SER
LEU LEU
PRO PRO
GLU GLU
THR THR
SER SER
LYS LYS
GLU GLU
HIS HIS
ILE ILE
SER SER
ALA ALA
GLU GLU
ASN ASN
MET MET
SER SER
LEU LEU
GLU GLU
THR THR
LEU LEU

• Molecule 6: DNA ligase 4

Chain I:  73%

MET ALA
ALA ALA
SER SER
GLN GLN
THR THR
SER SER
LEU LEU
PRO PRO
GLU GLU
THR THR
SER SER
LYS LYS
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

THR ASP
ASP SER
PHE PHE
TYR TYR
PRO PRO
ALA ALA
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

ASP ALA
ALA GLY
SER SER
PHE PHE
TYR TYR
PRO PRO
ALA ALA
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

LEU GLU
GLN GLN
TRP TRP
PHE PHE
ILE ILE
ARG ARG
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

THR LEU
LEU PHE
PHE SER
ALA ALA
PHE PHE
LYS LYS
PRO PRO
GLU GLU
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

GLN PHE
GLY GLY
ALA ALA
SER SER
PHE PHE
TYR TYR
PRO PRO
ALA ALA
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

GLN THR
THR CYS
TYR TYR
VAL VAL
PHE PHE
ASP ASP
VAL VAL
MET MET
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

ALA ILE
ASP ASP
LYS LYS
ARG ARG
GLU GLU
GLY GLY
ILE ILE
MET MET
VAL VAL
SER SER
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

SER HIS
HIS PHE
PHE LEU
LEU LEU
CYS CYS
VAL VAL
ALA ALA
VAL VAL
SER SER
PRO PRO
GLY GLY
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

GLY THR
THR GLU
GLY LYS
LYS LYS
VAL VAL
SER SER
PRO PRO
GLY GLY
ILE ILE
MET MET
VAL VAL
SER SER
PRO PRO
GLY GLY
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

GLN LEU
LEU ARG
GLY GLY
LYS LYS
ALA ALA
SER SER
PRO PRO
GLY GLY
ILE ILE
MET MET
VAL VAL
SER SER
PRO PRO
GLY GLY
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
THR THR
SER SER
LEU LEU
PHE PHE
VAL VAL
HIS HIS
VAL VAL
PRO PRO
GLN GLN
LYS LYS
ASP ASP
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
MET MET
ALA ALA
SER SER
THR THR
LEU LEU
GLU GLU
ILE ILE
ARG ARG
THR THR
LEU LEU

E663 F664
C665 V666
M667 S668
D677 L678
E679 E680
I682 A683
E684 E685
G686 G687
Y688 Y689
P693 T697
V700 I701
A702 G703
N706 I707
I708 I709
K710 I713
L714 S715
N716 K717
H718 D719
W720 W721
K722 W725
E728 C729
F730 S734
F735 W736
Q739 P740
R741

F742 M743
I744 H745
M746 K751
E752 H753
F754 A755
R756 E757
Y758 S764
I767 G768
I768 I781
K782 N783
S784 Q787
I796 A797
D798 L799
E800 C901
Y801 E902
R802 L903
Q904 W805
L810 S811
M812 F813
R814 H815
H816 T817
V818 K841
A842 L843
F847 H848
G849 A850
K851 A857
E858 P740
G859

V860 S861
H862 V863
L864 L865
G866 E867
K876 F877
F878 T881
R884 K885
F886 L889
K890 GLU
SER SER
TRP TRP
VAL VAL
THR THR
ASP ASP
LYS LYS
ILE ILE
D899 K900
C901 E902
L903 Q904
W905 L810
S811 M812
F813 R814
H815 H816
T817 V818
K841 A842
L843 F847
H848 G849
A850 K851
A857 E858
P740 G859

V860 S861
H862 V863
L864 L865
G866 E867
K876 F877
F878 T881
R884 K885
F886 L889
K890 GLU
SER SER
TRP TRP
VAL VAL
THR THR
ASP ASP
LYS LYS
ILE ILE
D899 K900
C901 E902
L903 Q904
W905 L810
S811 M812
F813 R814
H815 H816
T817 V818
K841 A842
L843 F847
H848 G849
A850 K851
A857 E858
P740 G859

V860 S861
H862 V863
L864 L865
G866 E867
K876 F877
F878 T881
R884 K885
F886 L889
K890 GLU
SER SER
TRP TRP
VAL VAL
THR THR
ASP ASP
LYS LYS
ILE ILE
D899 K900
C901 E902
L903 Q904
W905 L810
S811 M812
F813 R814
H815 H816
T817 V818
K841 A842
L843 F847
H848 G849
A850 K851
A857 E858
P740 G859

• Molecule 6: DNA ligase 4

Chain R:  73%

MET ALA
ALA ALA
SER SER
GLN GLN
THR THR
SER SER
LEU LEU
PRO PRO
GLU GLU
PHE PHE
ILE ILE
ASP ASP
ALA ALA
LEU LEU
CYS CYS
SER SER
THR THR
LEU LEU
GLU GLU
ARG ARG
ILE ILE
GLN GLN
LYS LYS
SER SER
ILE ILE
GLY GLY
ARG ARG
ALA ALA
GLU GLU
LYS LYS
ILE ILE
ARG ARG
HIS HIS
PHE PHE
ARG ARG
GLU GLU
PHE PHE
LEU LEU
ASP ASP
SER SER
TRP TRP
ARG ARG
LYS LYS
PHE PHE
HIS HIS
ASP ASP
ALA ALA
LEU LEU
HIS HIS
LYS LYS
ASN ASN
HIS HIS
LYS LYS
ASP ASP
HIS HIS
VAL VAL

Chain d: 19% 81%

T14	A15	A16	T17	A18	A19	T20	A21	G22	T23	T24	T25	T26	T27	A28	G29	T30	T31	T32	A33	T34	T35	G36	G37	G38	C39
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 10: DNA (28-MER)

Chain e: 25% 75%

A17	T20	A21	A22	T23	A24	A25	A26	C27	T28	A29	A33	C34	T35	A36	T37	T38	A39	T40	T41	A42	T43	G44
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35211	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 ($e^-/\text{\AA}^2$)	52.1	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	0.940	Depositor
Minimum map value	-0.499	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.061	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.16	0/28471	0.37	1/38509 (0.0%)
1	S	0.15	0/28549	0.36	1/38591 (0.0%)
2	B	0.14	0/4118	0.33	0/5556
2	T	0.13	0/4092	0.32	0/5516
3	C	0.11	0/5393	0.29	0/7273
3	L	0.10	0/5272	0.28	0/7107
4	D	0.08	0/1101	0.23	0/1500
4	M	0.10	0/1223	0.27	0/1665
5	G	0.10	0/1657	0.27	0/2228
5	H	0.09	0/1616	0.23	0/2170
5	P	0.08	0/1657	0.24	0/2228
5	Q	0.11	0/1616	0.25	0/2170
6	I	0.11	0/2021	0.33	0/2727
6	R	0.11	0/1999	0.31	0/2697
7	j	0.20	0/570	0.37	0/876
8	i	0.24	0/620	0.43	0/953
9	d	0.25	0/591	0.44	0/908
10	e	0.21	0/644	0.39	0/990
All	All	0.14	0/91210	0.34	2/123664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2294	ILE	N-CA-C	-5.99	105.85	111.48
1	S	2294	ILE	N-CA-C	-5.46	105.29	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27927	0	27803	1297	0
1	S	27999	0	28062	1232	0
2	B	4038	0	4071	223	0
2	T	4014	0	4065	192	0
3	C	5292	0	5264	237	0
3	L	5174	0	5164	223	0
4	D	1075	0	1060	21	0
4	M	1195	0	1157	21	0
5	G	1628	0	1620	45	0
5	H	1589	0	1587	37	0
5	P	1628	0	1620	22	0
5	Q	1589	0	1587	24	0
6	I	1977	0	1923	95	0
6	R	1958	0	1905	74	0
7	j	509	0	271	31	0
8	i	552	0	301	30	0
9	d	528	0	282	29	0
10	e	573	0	312	30	0
All	All	89245	0	88054	3664	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 21.

The worst 5 of 3664 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)
6:R:814:ARG:H	6:R:850:ALA:H	1.08	0.95
2:T:318:ARG:HB2	2:T:329:LEU:O	1.68	0.94
1:A:174:VAL:O	1:A:177:LEU:HB2	1.69	0.92
2:T:400:TYR:O	2:T:408:PRO:HA	1.68	0.92
1:A:67:VAL:HB	1:A:85:ILE:HD13	1.54	0.89

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	3476/4128 (84%)	3213 (92%)	259 (8%)	4 (0%)	48	83
1	S	3464/4128 (84%)	3210 (93%)	252 (7%)	2 (0%)	48	83
2	B	505/609 (83%)	471 (93%)	34 (7%)	0	100	100
2	T	498/609 (82%)	470 (94%)	28 (6%)	0	100	100
3	C	660/732 (90%)	619 (94%)	41 (6%)	0	100	100
3	L	644/732 (88%)	615 (96%)	29 (4%)	0	100	100
4	D	139/204 (68%)	137 (99%)	2 (1%)	0	100	100
4	M	160/204 (78%)	160 (100%)	0	0	100	100
5	G	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
5	H	190/336 (56%)	188 (99%)	2 (1%)	0	100	100
5	P	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
5	Q	190/336 (56%)	188 (99%)	2 (1%)	0	100	100
6	I	242/911 (27%)	219 (90%)	23 (10%)	0	100	100
6	R	242/911 (27%)	216 (89%)	26 (11%)	0	100	100
All	All	10808/14512 (74%)	10097 (93%)	705 (6%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	S	3304	VAL
1	A	68	PHE
1	A	1231	GLN
1	A	66	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	A	2999/3671 (82%)	2998 (100%)	1 (0%)	100	100
1	S	3045/3671 (83%)	3042 (100%)	3 (0%)	88	88
2	B	443/548 (81%)	443 (100%)	0	100	100
2	T	446/548 (81%)	446 (100%)	0	100	100
3	C	581/649 (90%)	581 (100%)	0	100	100
3	L	570/649 (88%)	570 (100%)	0	100	100
4	D	110/160 (69%)	110 (100%)	0	100	100
4	M	120/160 (75%)	120 (100%)	0	100	100
5	G	180/303 (59%)	180 (100%)	0	100	100
5	H	177/303 (58%)	177 (100%)	0	100	100
5	P	180/303 (59%)	180 (100%)	0	100	100
5	Q	177/303 (58%)	177 (100%)	0	100	100
6	I	218/808 (27%)	218 (100%)	0	100	100
6	R	217/808 (27%)	217 (100%)	0	100	100
All	All	9463/12884 (73%)	9459 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	VAL
1	S	67	VAL
1	S	3301	LEU
1	S	3306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	80	HIS
1	S	1654	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	P	21	GLN
1	S	676	ASN
1	S	2213	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.

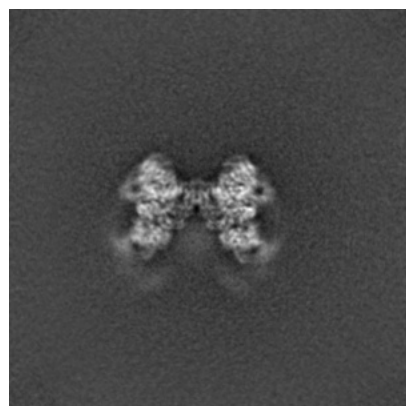
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16044. These allow visual inspection of the internal detail of the map and identification of artifacts.

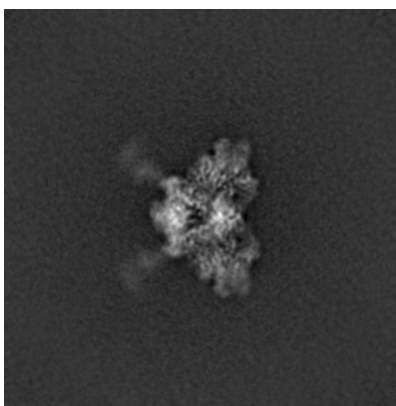
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

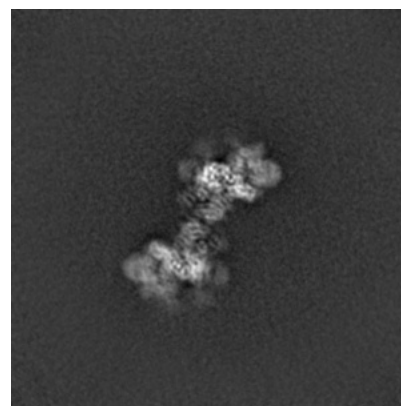
6.1.1 Primary map



X

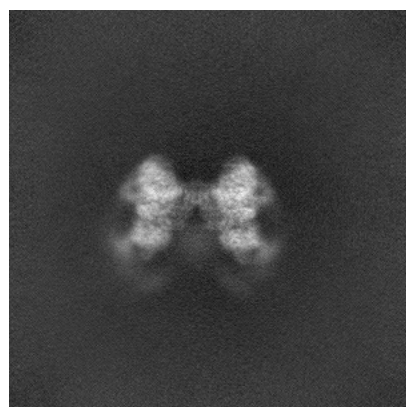


Y

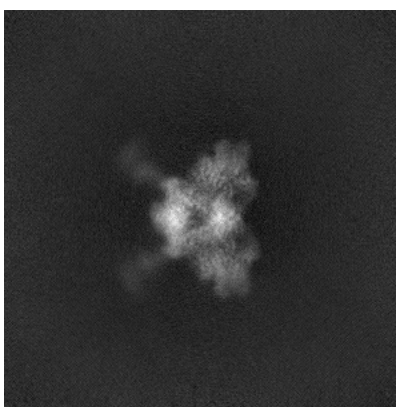


Z

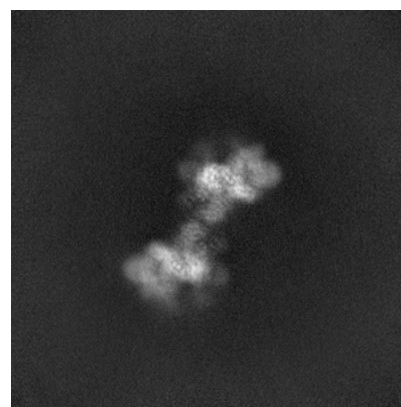
6.1.2 Raw map



X



Y

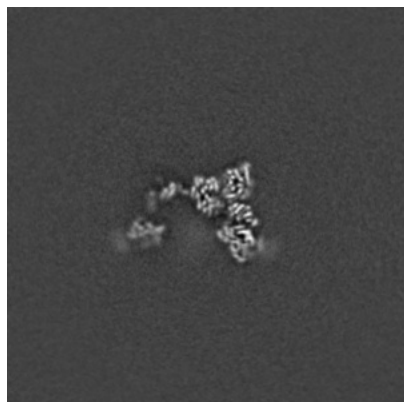


Z

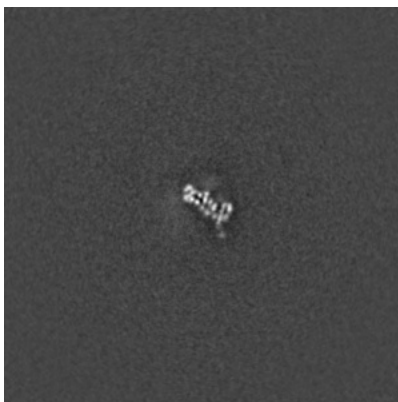
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

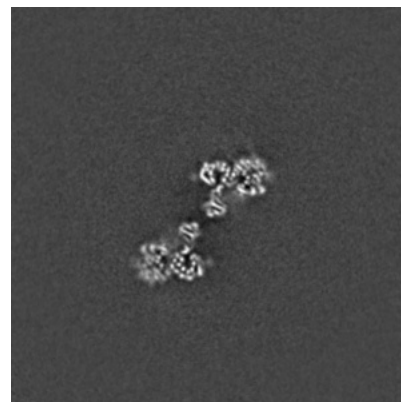
6.2.1 Primary map



X Index: 270



Y Index: 270



Z Index: 270

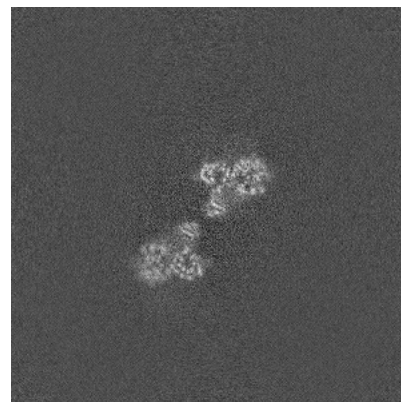
6.2.2 Raw map



X Index: 270



Y Index: 270



Z Index: 270

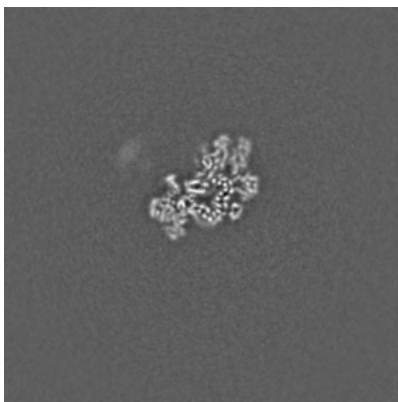
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

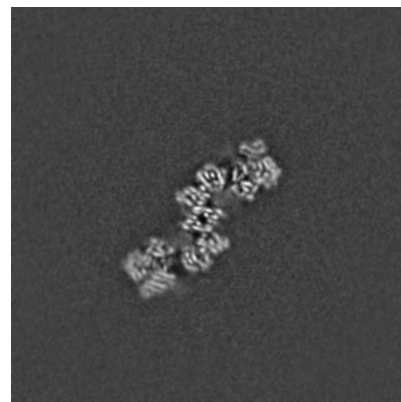
6.3.1 Primary map



X Index: 263

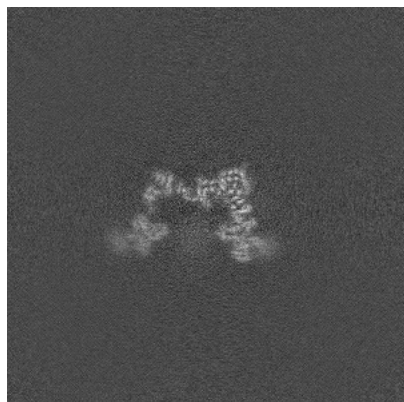


Y Index: 312

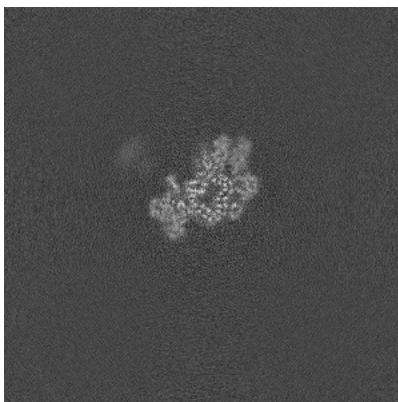


Z Index: 289

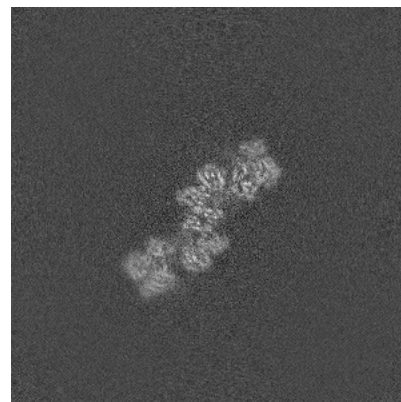
6.3.2 Raw map



X Index: 263



Y Index: 313

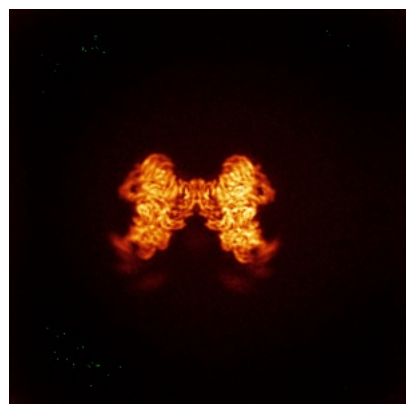


Z Index: 289

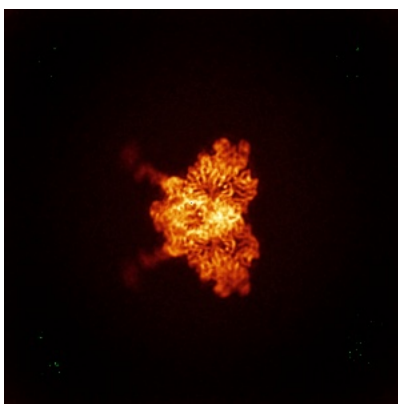
The images above show the largest variance slices of the map in three orthogonal directions.

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

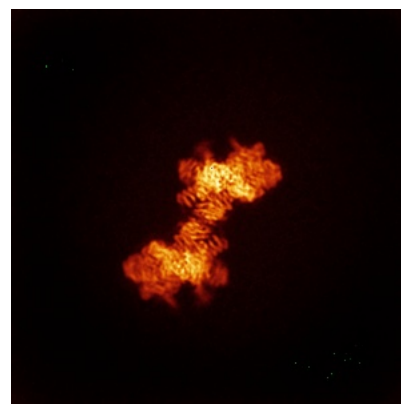
6.4.1 Primary map



X

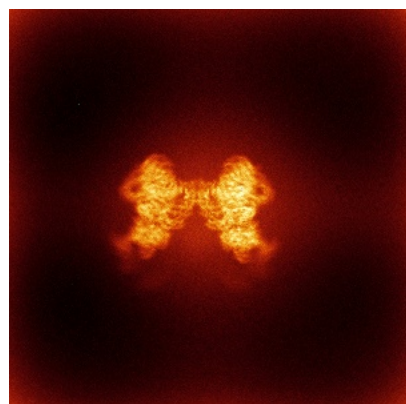


Y

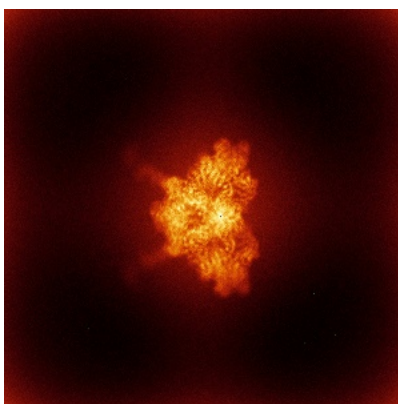


Z

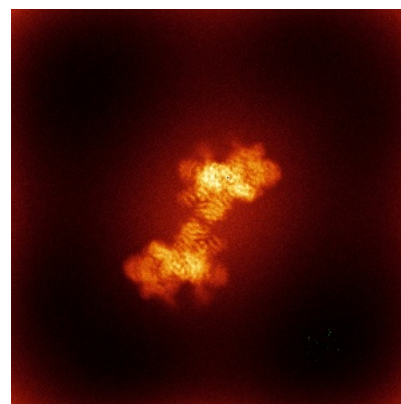
6.4.2 Raw map



X



Y

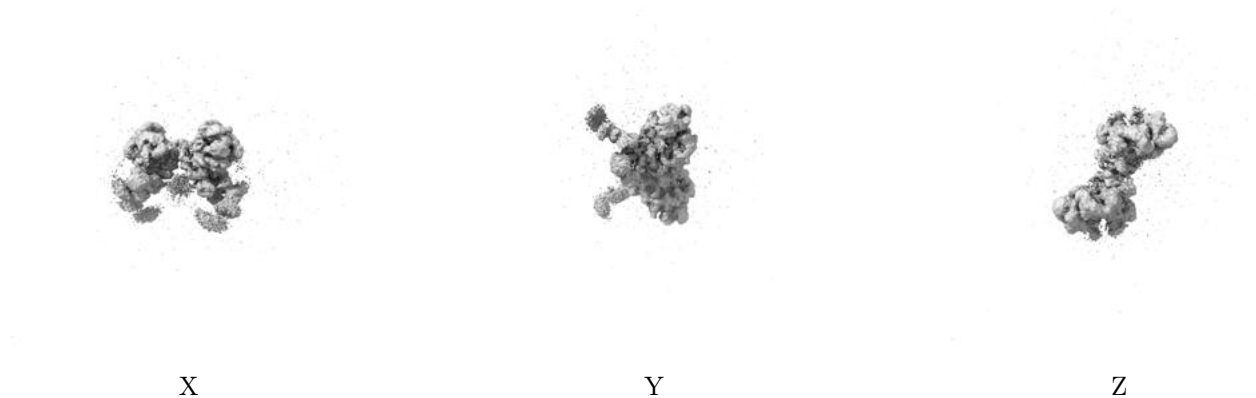


Z

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.

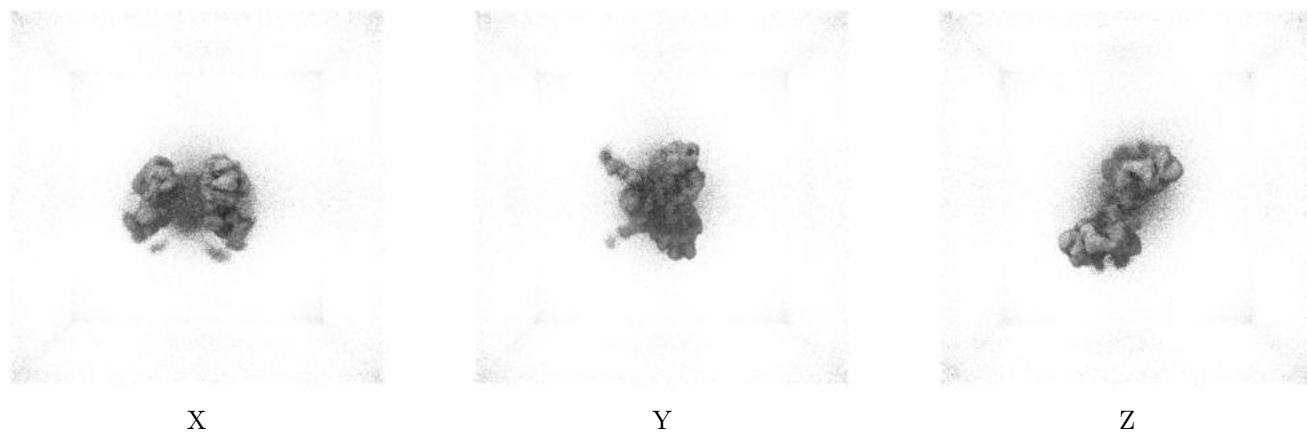
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.061. 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.

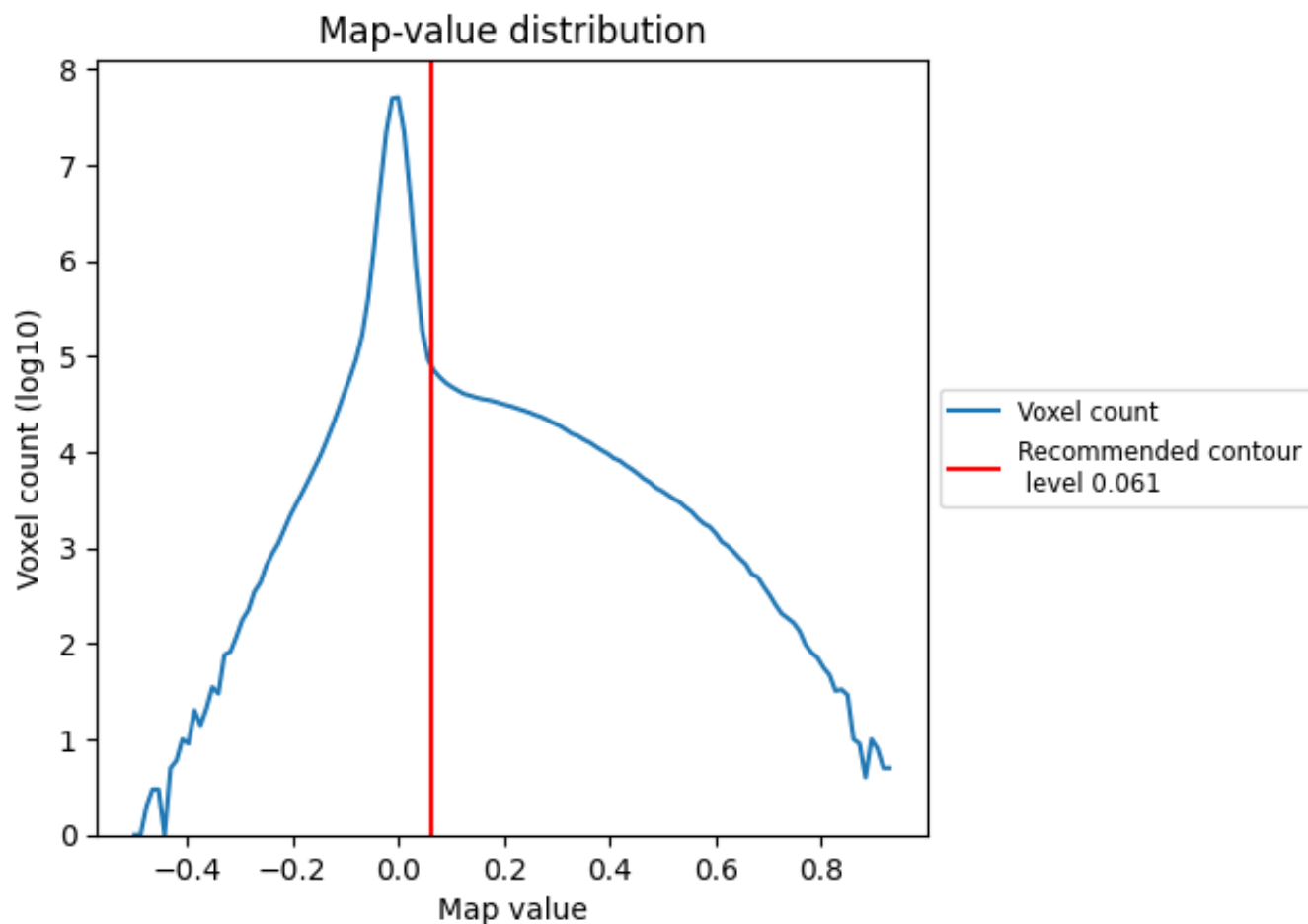
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

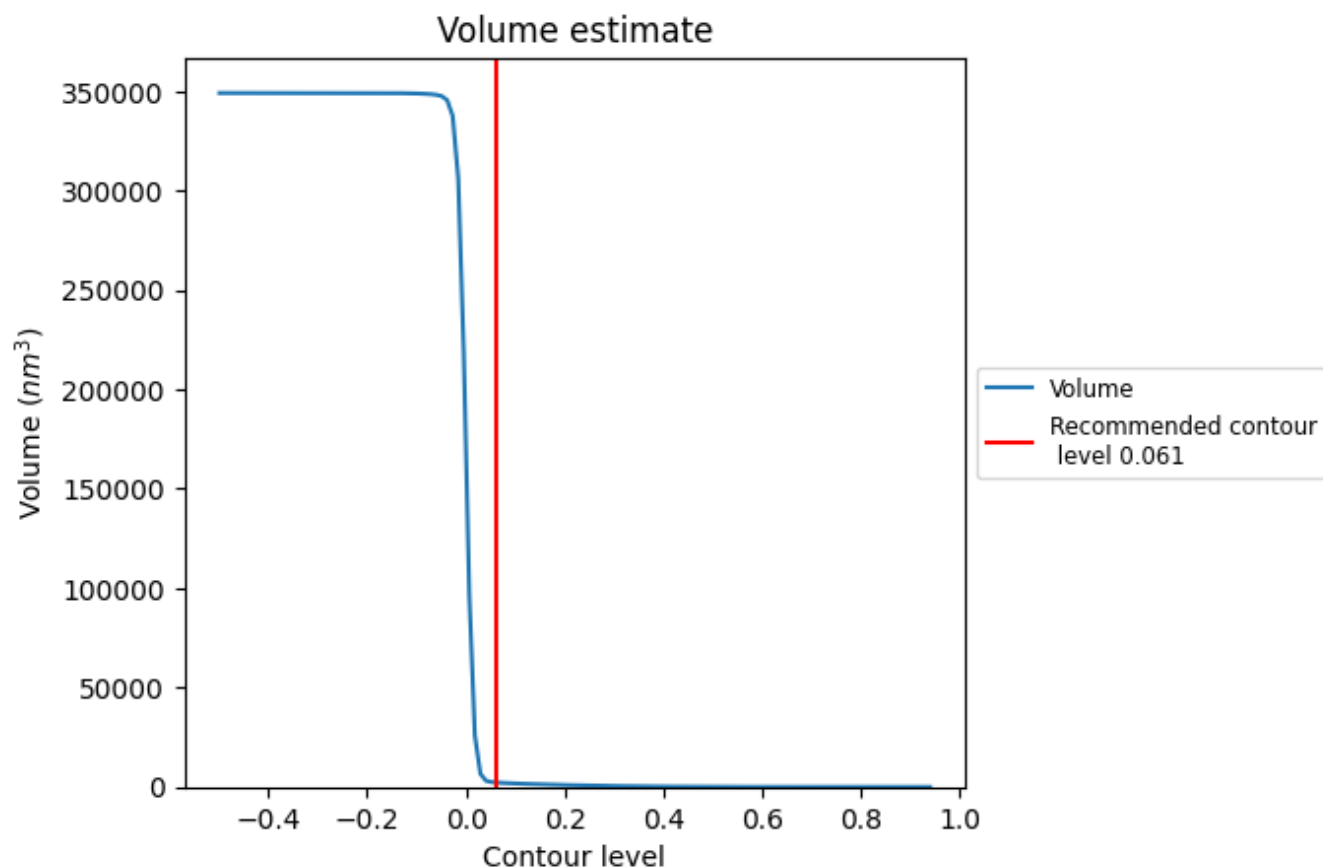
This section contains the results of statistical analysis of the map.

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.

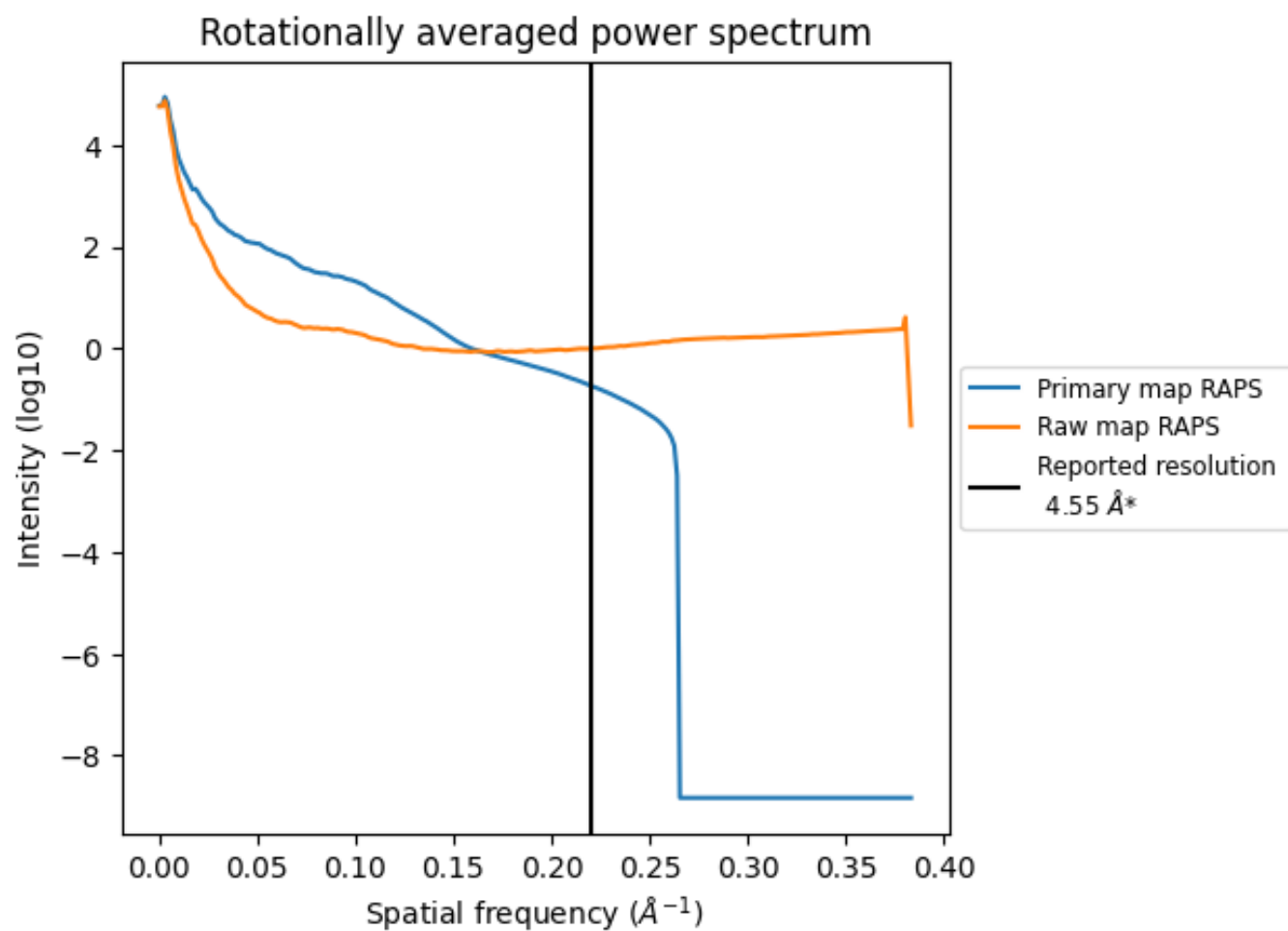
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2251 nm^3 ; this corresponds to an approximate mass of 2033 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 ⓘ

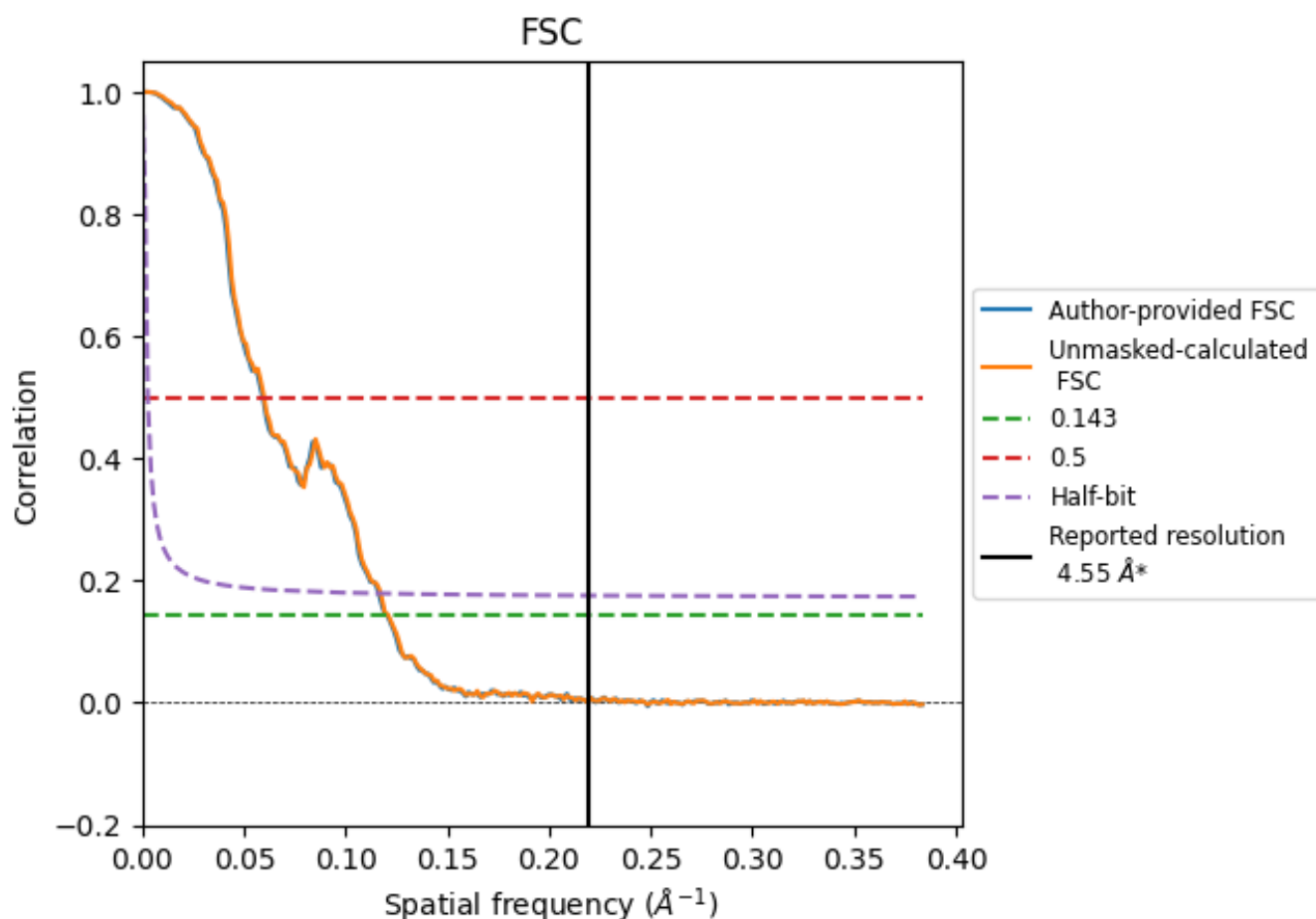


*Reported resolution corresponds to spatial frequency of 0.220 Å⁻¹

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 0.220 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	8.33	16.86	8.61
Unmasked-calculated*	8.27	16.69	8.54

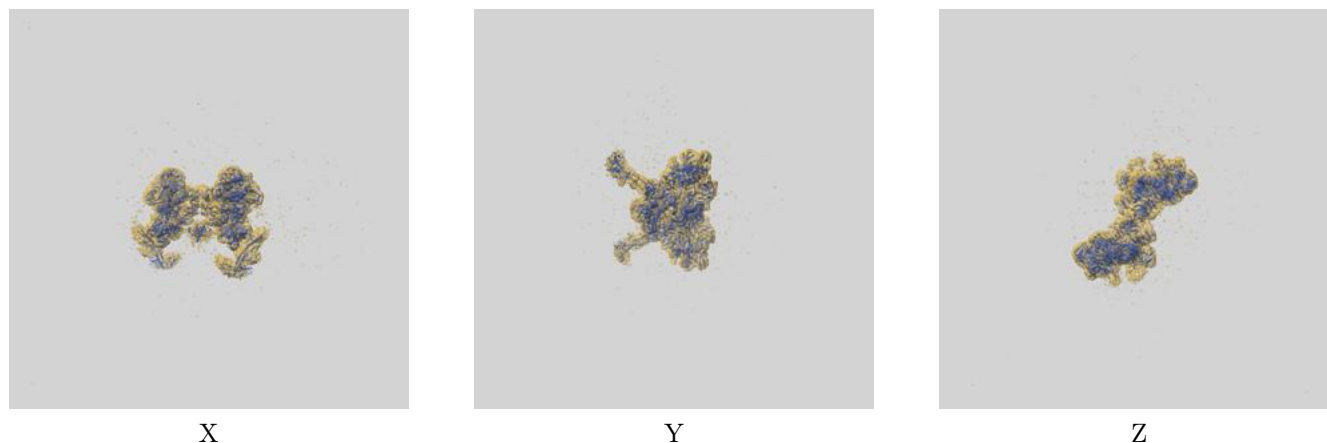
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.33 differs from the reported value 4.55 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.27 differs from the reported value 4.55 by more than 10 %

9 Map-model fit [i](#)

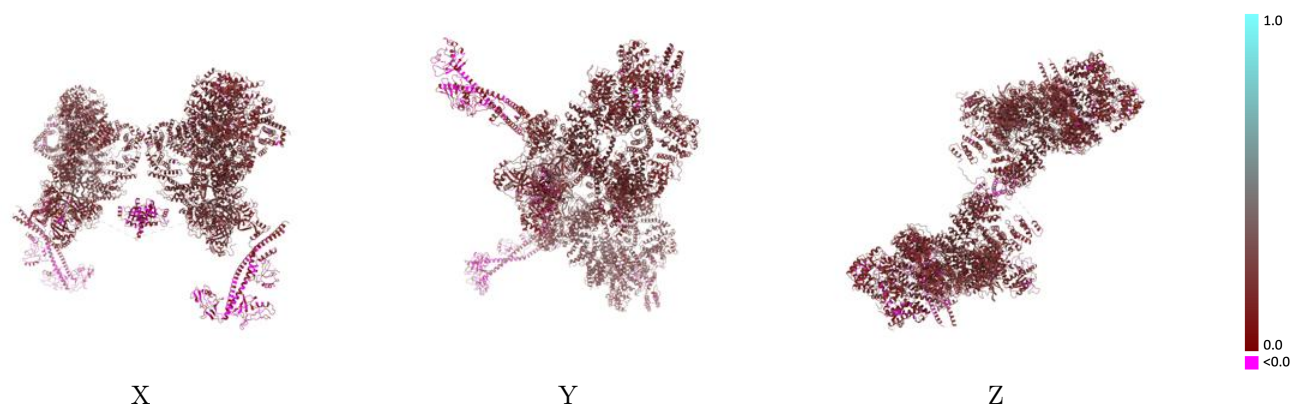
This section contains information regarding the fit between EMDB map EMD-16044 and PDB model 8BH3. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



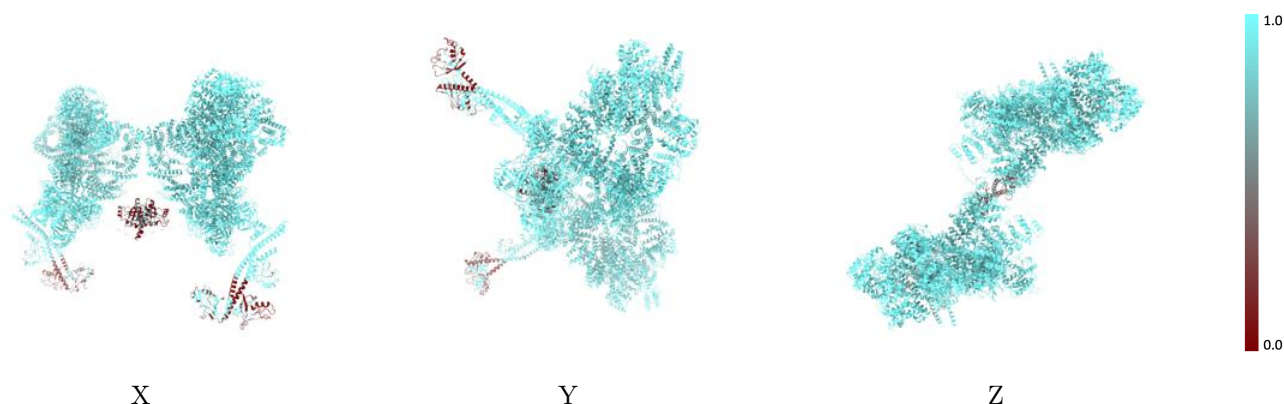
The images above show the 3D surface view of the map at the recommended contour level 0.061 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



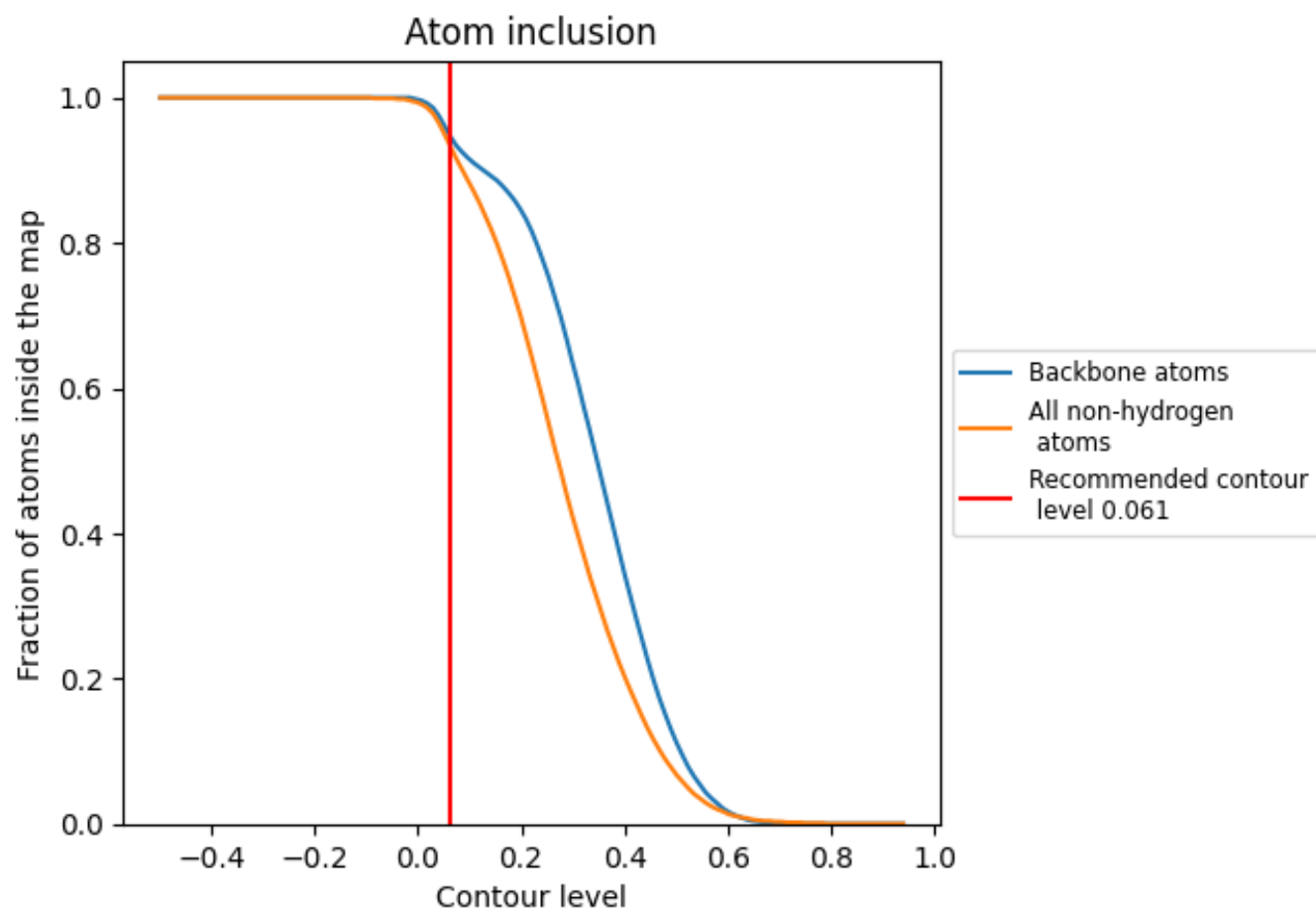
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.061).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.1850
A	 0.9770	 0.2080
B	 0.9830	 0.2240
C	 0.9910	 0.2020
D	 0.3570	 0.0660
G	 0.6710	 0.0690
H	 0.5320	 0.0630
I	 0.9650	 0.1450
L	 0.9950	 0.1760
M	 0.3810	 0.0790
P	 0.5560	 0.0560
Q	 0.5170	 0.0730
R	 0.9550	 0.1280
S	 0.9800	 0.1910
T	 0.9870	 0.1920
d	 0.9920	 0.2600
e	 0.9970	 0.2720
i	 1.0000	 0.2550
j	 0.9900	 0.2460

