



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 7VVZ / pdb_00007vvz
EMDB ID : EMD-32150
Title : NuA4 bound to the nucleosome
Authors : Qu, K.; Chen, Z.
Deposited on : 2021-11-09
Resolution : 8.80 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:

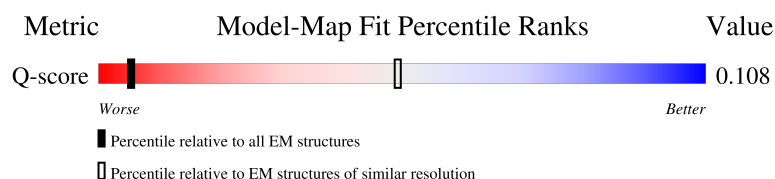
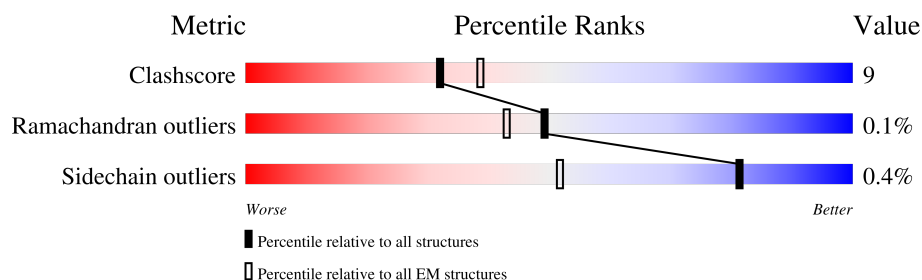
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.80 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.



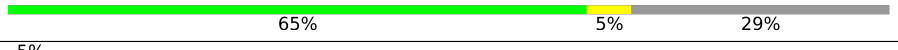
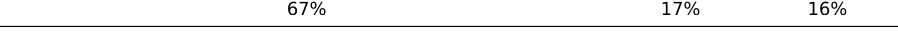
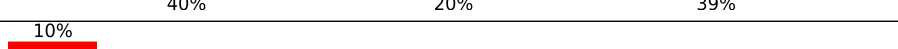
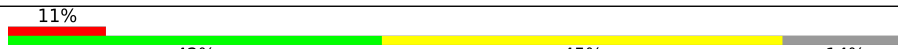
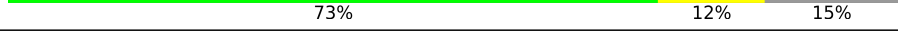
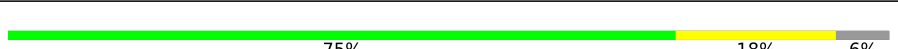
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	265 (8.30 - 9.30)

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	Y	113	10% 31% 10% 59%
2	V	282	5% 30% 10% 60%
3	H	832	26% 6% 68%
3	T	832	7% 23% 10% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	A	136	
4	O	136	
5	B	103	
5	Q	103	
6	N	130	
6	S	130	
7	D	126	
7	U	126	
8	P	445	
9	W	207	
10	I	207	
11	X	9	
12	E	1168	
13	F	489	
14	G	375	
15	K	476	
16	L	3744	

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 61920 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 Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	46	Total	C	N	O	S	0	0
			396	245	64	86	1		

- Molecule 2 is a protein called Chromatin modification-related protein YNG2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	113	Total	C	N	O	S	0	0
			923	583	158	179	3		

- Molecule 3 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	274	Total	C	N	O	S	0	0
			2294	1441	403	441	9		
3	H	269	Total	C	N	O	S	0	0
			2250	1427	380	438	5		

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	96	Total	C	N	O	S	0	0
			791	500	151	137	3		
4	A	94	Total	C	N	O	S	0	0
			774	489	147	135	3		

- Molecule 5 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	80	Total	C	N	O	S	0	0
			641	405	125	110	1		
5	B	87	Total	C	N	O	S	0	0
			703	442	142	118	1		

- Molecule 6 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	S	106	Total	C	N	O	0	0
			814	513	159	142		
6	N	106	Total	C	N	O	0	0
			814	513	159	142		

- Molecule 7 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	92	Total	C	N	O	S	0	0
			719	453	129	135	2		
7	D	93	Total	C	N	O	S	0	0
			725	456	130	137	2		

- Molecule 8 is a protein called Histone acetyltransferase ESA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	270	Total	C	N	O	S	0	0
			2286	1481	380	415	10		

- Molecule 9 is a DNA chain called DNA (207-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	180	Total	C	N	O	P	0	0
			3666	1739	667	1080	180		

- Molecule 10 is a DNA chain called DNA (207-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	179	Total	C	N	O	P	0	0
			3695	1746	696	1074	179		

- Molecule 11 is a protein called Epl1 arginine anchor.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	9	Total	C	N	O	0	0
			82	53	19	10		

- Molecule 12 is a protein called Chromatin modification-related protein EAF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	415	Total	C	N	O	S	0	0
			3448	2193	619	622	14		

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	983	ARG	-	expression tag	UNP Q06337
E	984	THR	-	expression tag	UNP Q06337
E	985	LEU	-	expression tag	UNP Q06337
E	986	GLN	-	expression tag	UNP Q06337
E	987	VAL	-	expression tag	UNP Q06337
E	988	ASP	-	expression tag	UNP Q06337
E	989	TRP	-	expression tag	UNP Q06337
E	990	SER	-	expression tag	UNP Q06337
E	991	HIS	-	expression tag	UNP Q06337
E	992	PRO	-	expression tag	UNP Q06337
E	993	GLN	-	expression tag	UNP Q06337
E	994	PHE	-	expression tag	UNP Q06337
E	995	GLU	-	expression tag	UNP Q06337
E	996	LYS	-	expression tag	UNP Q06337
E	997	HIS	-	expression tag	UNP Q06337
E	998	HIS	-	expression tag	UNP Q06337
E	999	HIS	-	expression tag	UNP Q06337
E	1000	HIS	-	expression tag	UNP Q06337
E	1001	HIS	-	expression tag	UNP Q06337
E	1002	HIS	-	expression tag	UNP Q06337
E	1003	HIS	-	expression tag	UNP Q06337
E	1004	HIS	-	expression tag	UNP Q06337
E	1005	HIS	-	expression tag	UNP Q06337
E	1006	HIS	-	expression tag	UNP Q06337
E	1007	HIS	-	expression tag	UNP Q06337
E	1008	HIS	-	expression tag	UNP Q06337
E	1009	ASP	-	expression tag	UNP Q06337
E	1010	TYR	-	expression tag	UNP Q06337
E	1011	ASP	-	expression tag	UNP Q06337
E	1012	ILE	-	expression tag	UNP Q06337
E	1013	PRO	-	expression tag	UNP Q06337
E	1014	THR	-	expression tag	UNP Q06337
E	1015	THR	-	expression tag	UNP Q06337
E	1016	ALA	-	expression tag	UNP Q06337
E	1017	SER	-	expression tag	UNP Q06337
E	1018	VAL	-	expression tag	UNP Q06337
E	1019	ASP	-	expression tag	UNP Q06337

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1020	GLY	-	expression tag	UNP Q06337
E	1021	SER	-	expression tag	UNP Q06337
E	1022	GLU	-	expression tag	UNP Q06337
E	1023	ASN	-	expression tag	UNP Q06337
E	1024	LEU	-	expression tag	UNP Q06337
E	1025	TYR	-	expression tag	UNP Q06337
E	1026	PHE	-	expression tag	UNP Q06337
E	1027	GLN	-	expression tag	UNP Q06337
E	1028	GLY	-	expression tag	UNP Q06337
E	1029	SER	-	expression tag	UNP Q06337
E	1030	PRO	-	expression tag	UNP Q06337
E	1031	GLN	-	expression tag	UNP Q06337
E	1032	GLN	-	expression tag	UNP Q06337
E	1033	ASN	-	expression tag	UNP Q06337
E	1034	LYS	-	expression tag	UNP Q06337
E	1035	THR	-	expression tag	UNP Q06337
E	1036	ALA	-	expression tag	UNP Q06337
E	1037	ALA	-	expression tag	UNP Q06337
E	1038	LEU	-	expression tag	UNP Q06337
E	1039	ALA	-	expression tag	UNP Q06337
E	1040	GLN	-	expression tag	UNP Q06337
E	1041	HIS	-	expression tag	UNP Q06337
E	1042	ASP	-	expression tag	UNP Q06337
E	1043	GLU	-	expression tag	UNP Q06337
E	1044	ALA	-	expression tag	UNP Q06337
E	1045	VAL	-	expression tag	UNP Q06337
E	1046	ASP	-	expression tag	UNP Q06337
E	1047	ASN	-	expression tag	UNP Q06337
E	1048	LYS	-	expression tag	UNP Q06337
E	1049	PHE	-	expression tag	UNP Q06337
E	1050	ASN	-	expression tag	UNP Q06337
E	1051	LYS	-	expression tag	UNP Q06337
E	1052	GLU	-	expression tag	UNP Q06337
E	1053	GLN	-	expression tag	UNP Q06337
E	1054	GLN	-	expression tag	UNP Q06337
E	1055	ASN	-	expression tag	UNP Q06337
E	1056	ALA	-	expression tag	UNP Q06337
E	1057	PHE	-	expression tag	UNP Q06337
E	1058	TYR	-	expression tag	UNP Q06337
E	1059	GLU	-	expression tag	UNP Q06337
E	1060	ILE	-	expression tag	UNP Q06337
E	1061	LEU	-	expression tag	UNP Q06337

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1062	HIS	-	expression tag	UNP Q06337
E	1063	LEU	-	expression tag	UNP Q06337
E	1064	PRO	-	expression tag	UNP Q06337
E	1065	ASN	-	expression tag	UNP Q06337
E	1066	LEU	-	expression tag	UNP Q06337
E	1067	ASN	-	expression tag	UNP Q06337
E	1068	GLU	-	expression tag	UNP Q06337
E	1069	GLU	-	expression tag	UNP Q06337
E	1070	GLN	-	expression tag	UNP Q06337
E	1071	ARG	-	expression tag	UNP Q06337
E	1072	ASN	-	expression tag	UNP Q06337
E	1073	ALA	-	expression tag	UNP Q06337
E	1074	PHE	-	expression tag	UNP Q06337
E	1075	ILE	-	expression tag	UNP Q06337
E	1076	GLN	-	expression tag	UNP Q06337
E	1077	SER	-	expression tag	UNP Q06337
E	1078	LEU	-	expression tag	UNP Q06337
E	1079	LYS	-	expression tag	UNP Q06337
E	1080	ASP	-	expression tag	UNP Q06337
E	1081	ASP	-	expression tag	UNP Q06337
E	1082	PRO	-	expression tag	UNP Q06337
E	1083	SER	-	expression tag	UNP Q06337
E	1084	GLN	-	expression tag	UNP Q06337
E	1085	SER	-	expression tag	UNP Q06337
E	1086	ALA	-	expression tag	UNP Q06337
E	1087	ASN	-	expression tag	UNP Q06337
E	1088	LEU	-	expression tag	UNP Q06337
E	1089	LEU	-	expression tag	UNP Q06337
E	1090	ALA	-	expression tag	UNP Q06337
E	1091	GLU	-	expression tag	UNP Q06337
E	1092	ALA	-	expression tag	UNP Q06337
E	1093	LYS	-	expression tag	UNP Q06337
E	1094	LYS	-	expression tag	UNP Q06337
E	1095	LEU	-	expression tag	UNP Q06337
E	1096	ASN	-	expression tag	UNP Q06337
E	1097	ASP	-	expression tag	UNP Q06337
E	1098	ALA	-	expression tag	UNP Q06337
E	1099	GLN	-	expression tag	UNP Q06337
E	1100	ALA	-	expression tag	UNP Q06337
E	1101	PRO	-	expression tag	UNP Q06337
E	1102	LYS	-	expression tag	UNP Q06337
E	1103	VAL	-	expression tag	UNP Q06337

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1104	ASP	-	expression tag	UNP Q06337
E	1105	ASN	-	expression tag	UNP Q06337
E	1106	LYS	-	expression tag	UNP Q06337
E	1107	PHE	-	expression tag	UNP Q06337
E	1108	ASN	-	expression tag	UNP Q06337
E	1109	LYS	-	expression tag	UNP Q06337
E	1110	GLU	-	expression tag	UNP Q06337
E	1111	GLN	-	expression tag	UNP Q06337
E	1112	GLN	-	expression tag	UNP Q06337
E	1113	ASN	-	expression tag	UNP Q06337
E	1114	ALA	-	expression tag	UNP Q06337
E	1115	PHE	-	expression tag	UNP Q06337
E	1116	TYR	-	expression tag	UNP Q06337
E	1117	GLU	-	expression tag	UNP Q06337
E	1118	ILE	-	expression tag	UNP Q06337
E	1119	LEU	-	expression tag	UNP Q06337
E	1120	HIS	-	expression tag	UNP Q06337
E	1121	LEU	-	expression tag	UNP Q06337
E	1122	PRO	-	expression tag	UNP Q06337
E	1123	ASN	-	expression tag	UNP Q06337
E	1124	LEU	-	expression tag	UNP Q06337
E	1125	ASN	-	expression tag	UNP Q06337
E	1126	GLU	-	expression tag	UNP Q06337
E	1127	GLU	-	expression tag	UNP Q06337
E	1128	GLN	-	expression tag	UNP Q06337
E	1129	ARG	-	expression tag	UNP Q06337
E	1130	ASN	-	expression tag	UNP Q06337
E	1131	ALA	-	expression tag	UNP Q06337
E	1132	PHE	-	expression tag	UNP Q06337
E	1133	ILE	-	expression tag	UNP Q06337
E	1134	GLN	-	expression tag	UNP Q06337
E	1135	SER	-	expression tag	UNP Q06337
E	1136	LEU	-	expression tag	UNP Q06337
E	1137	LYS	-	expression tag	UNP Q06337
E	1138	ASP	-	expression tag	UNP Q06337
E	1139	ASP	-	expression tag	UNP Q06337
E	1140	PRO	-	expression tag	UNP Q06337
E	1141	SER	-	expression tag	UNP Q06337
E	1142	GLN	-	expression tag	UNP Q06337
E	1143	SER	-	expression tag	UNP Q06337
E	1144	ALA	-	expression tag	UNP Q06337
E	1145	ASN	-	expression tag	UNP Q06337

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1146	LEU	-	expression tag	UNP Q06337
E	1147	LEU	-	expression tag	UNP Q06337
E	1148	ALA	-	expression tag	UNP Q06337
E	1149	GLU	-	expression tag	UNP Q06337
E	1150	ALA	-	expression tag	UNP Q06337
E	1151	LYS	-	expression tag	UNP Q06337
E	1152	LYS	-	expression tag	UNP Q06337
E	1153	LEU	-	expression tag	UNP Q06337
E	1154	ASN	-	expression tag	UNP Q06337
E	1155	ASP	-	expression tag	UNP Q06337
E	1156	ALA	-	expression tag	UNP Q06337
E	1157	GLN	-	expression tag	UNP Q06337
E	1158	ALA	-	expression tag	UNP Q06337
E	1159	PRO	-	expression tag	UNP Q06337
E	1160	LYS	-	expression tag	UNP Q06337
E	1161	VAL	-	expression tag	UNP Q06337
E	1162	ASP	-	expression tag	UNP Q06337
E	1163	ALA	-	expression tag	UNP Q06337
E	1164	ASN	-	expression tag	UNP Q06337
E	1165	SER	-	expression tag	UNP Q06337
E	1166	ALA	-	expression tag	UNP Q06337
E	1167	ALA	-	expression tag	UNP Q06337
E	1168	LEU	-	expression tag	UNP Q06337

- Molecule 13 is a protein called Actin-related protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	414	Total	C	N	O	S	0	0
			3278	2088	541	638	11		

- Molecule 14 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	357	Total	C	N	O	S	0	0
			2788	1772	468	531	17		

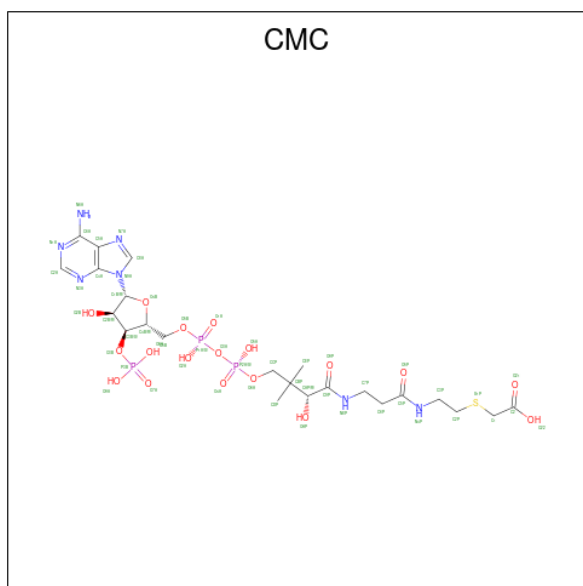
- Molecule 15 is a protein called SWR1-complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	237	Total	C	N	O	S	0	0
			1989	1275	337	370	7		

- Molecule 16 is a protein called Transcription-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	3513	Total	C	N	O	S	0	0
			28729	18596	4776	5237	120		

- Molecule 17 is CARBOXYMETHYL COENZYME *A (CCD ID: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).

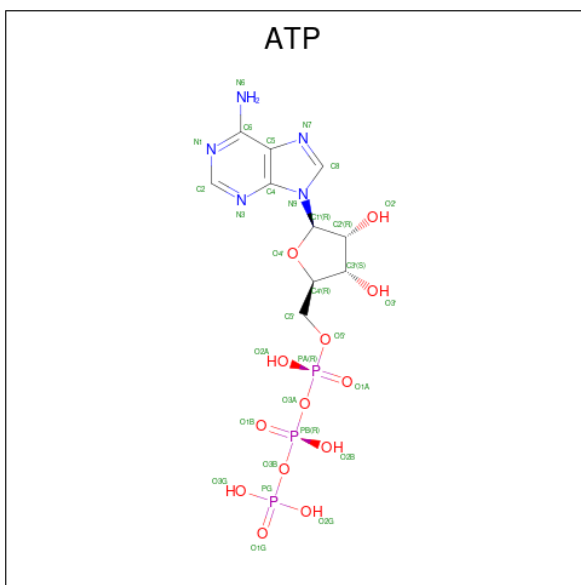


Mol	Chain	Residues	Atoms						AltConf
17	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

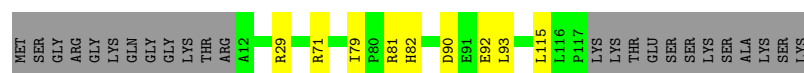
Mol	Chain	Residues	Atoms		AltConf
18	F	1	Total	Mg	0
			1	1	
18	G	1	Total	Mg	0
			1	1	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



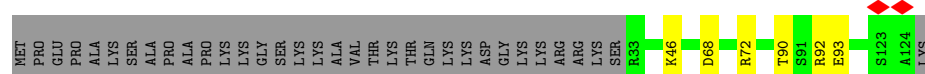
Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total 31	C 10	N 5	O 13	P 3	0
19	G	1	Total 31	C 10	N 5	O 13	P 3	0

Chain N: 



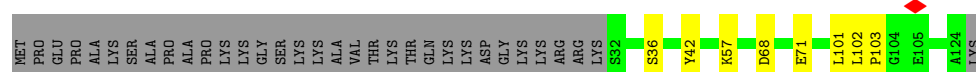
• Molecule 7: Histone H2B 1.1

Chain U: 

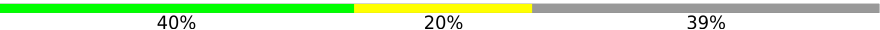


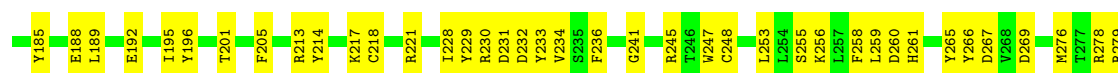
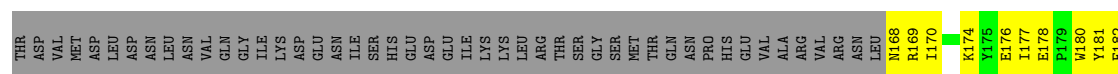
• Molecule 7: Histone H2B 1.1

Chain D: 



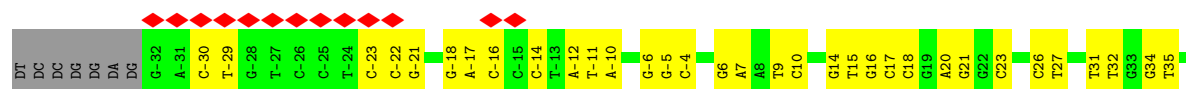
• Molecule 8: Histone acetyltransferase ESA1

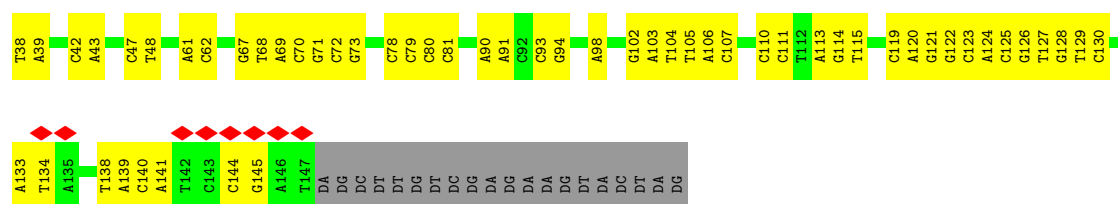
Chain P: 



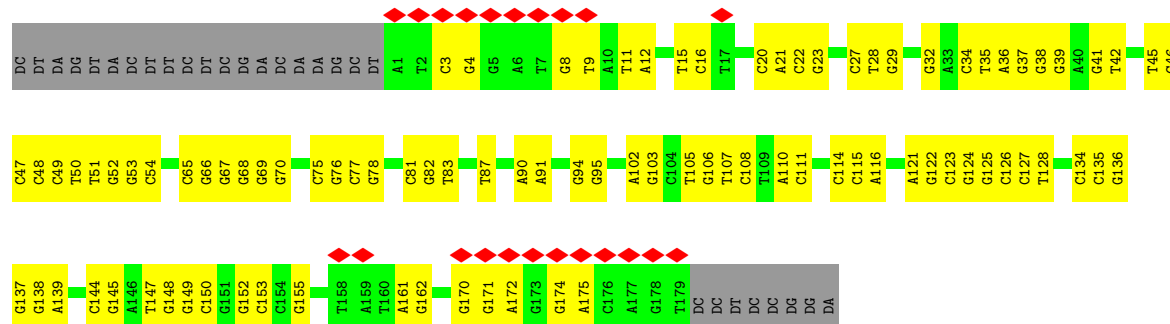
• Molecule 9: DNA (207-mer)

Chain W: 

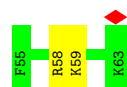
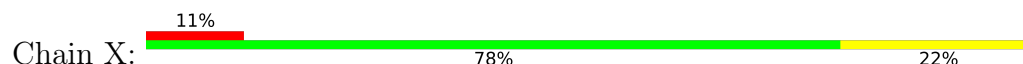




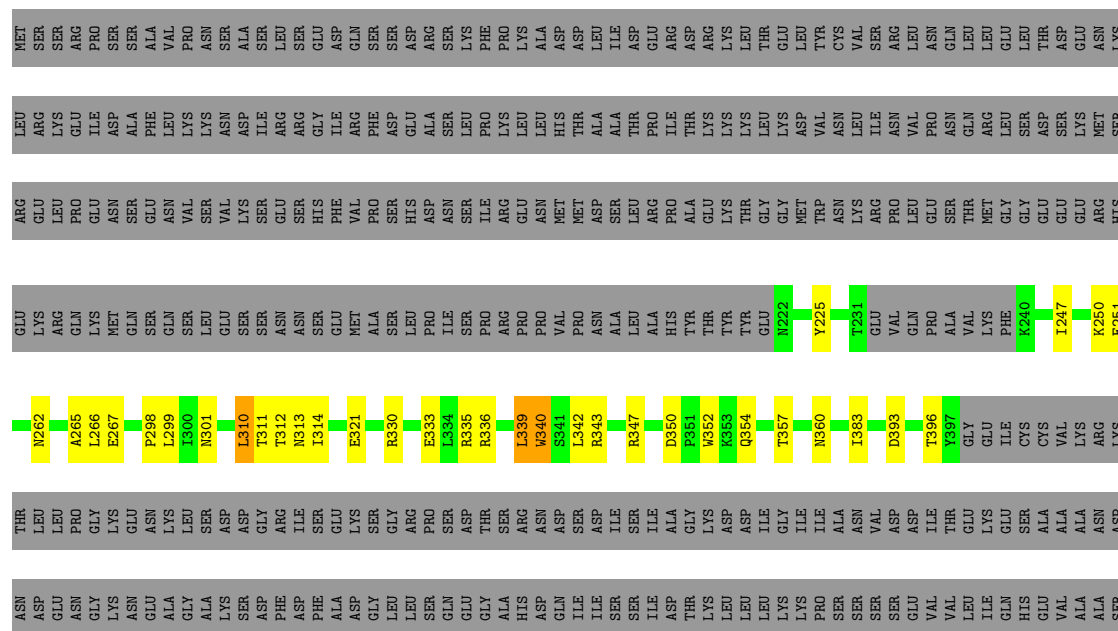
• Molecule 10: DNA (207-mer)

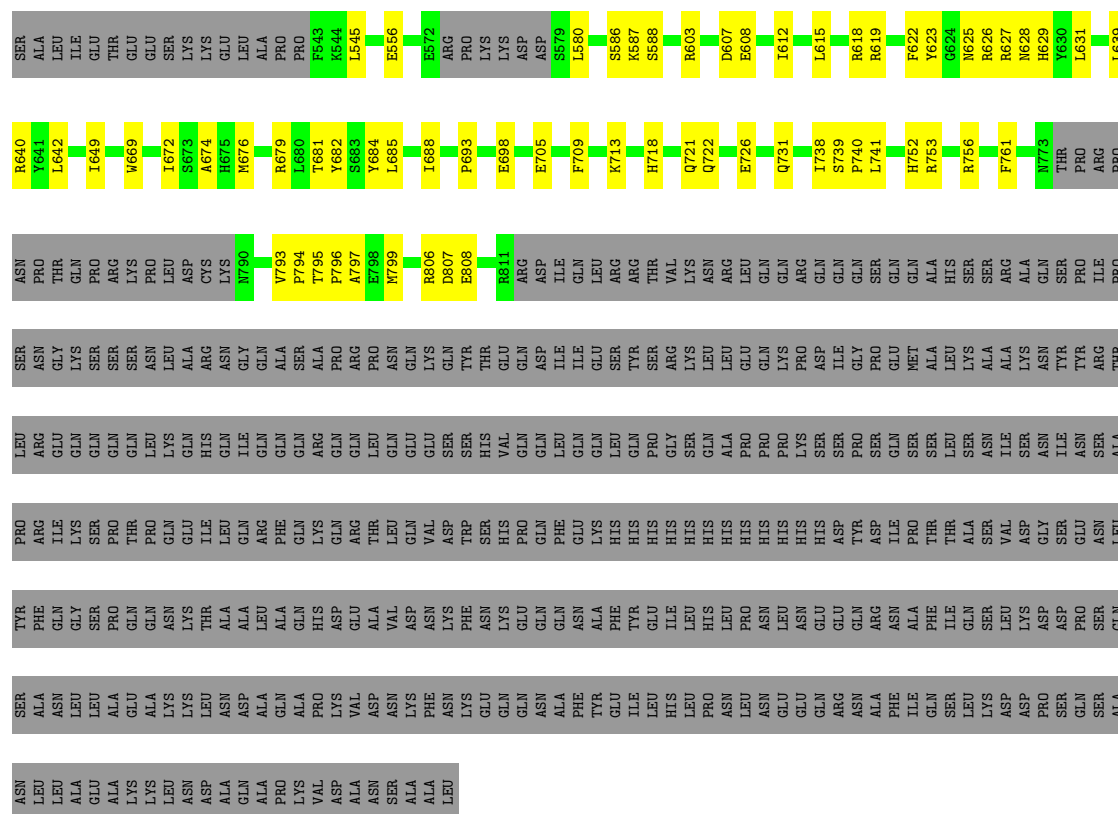


• Molecule 11: Epl1 arginine anchor



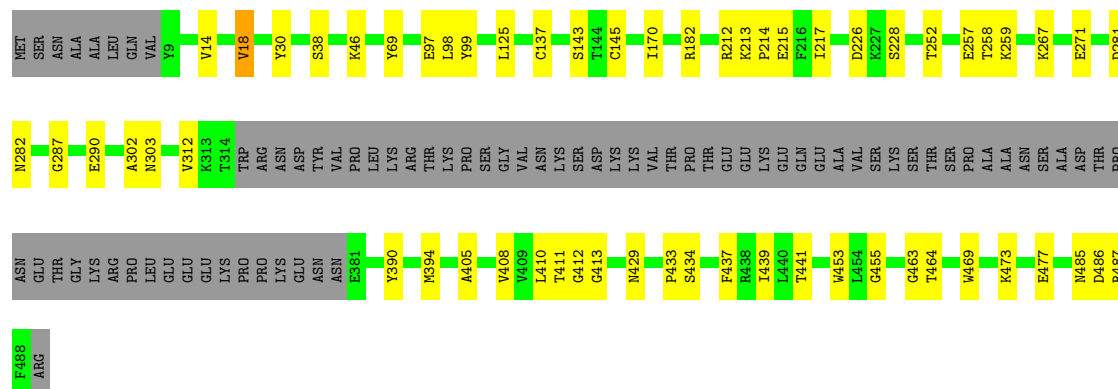
• Molecule 12: Chromatin modification-related protein EAF1





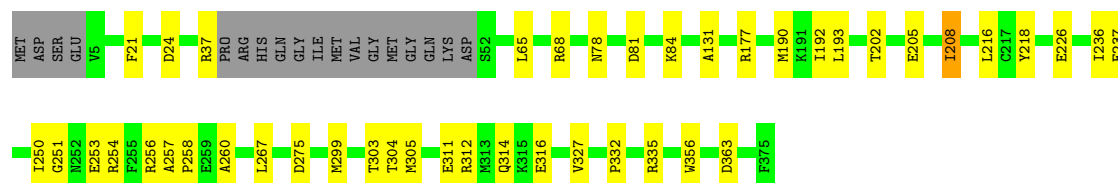
• Molecule 13: Actin-related protein 4

Chain F: 73% 12% 15%

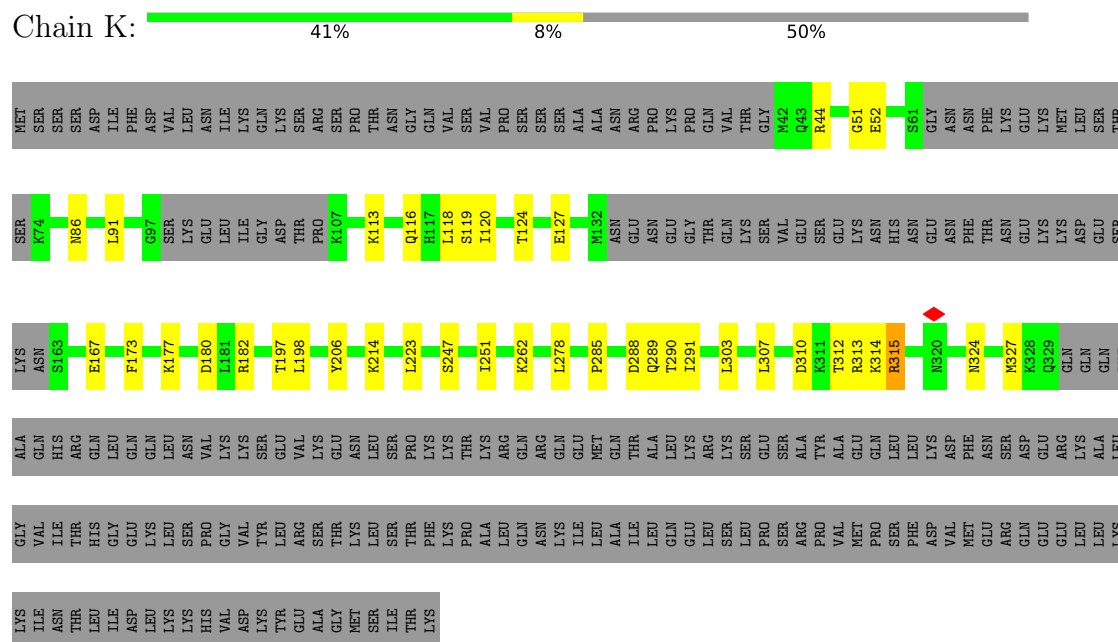


• Molecule 14: Actin

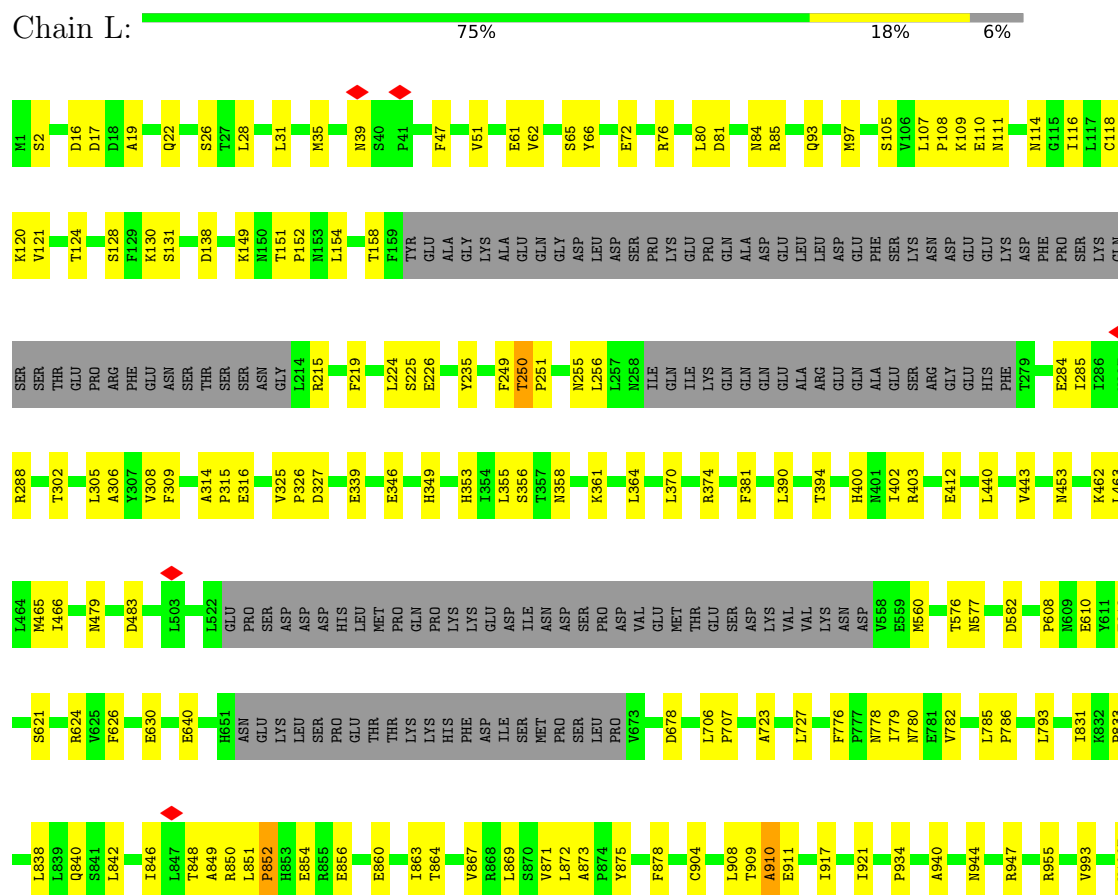
Chain G: 83% 11% 5%



- Molecule 15: SWR1-complex protein 4



- Molecule 16: Transcription-associated protein 1



Q3087	H752	T2437	A2300	S2154	TLE	W1966	S1818	E1683	V1303	H1012
A3088	F2755	E2444	L2301	D2166	ASN	V1975	G1819	W1684	I1320	H1013
L3091	T2756	R2450	L2310	Y2169	PRO	E1976	VAL	K1686	R1014	Y1013
Y3092	D2757	R2456	K2313	Y2172	GLU	Q1981	L1825	K1687	D1327	M1028
S3109	C2762	D2457	Y2316	F2172	ALA	F1988	W1826	K1688	H1328	T1029
T3118	D2768	D2461	L2320	K2177	THR	L1989	D1827	K1704	K1330	K1030
T3118	W2769	E2461	L2320	E2178	THR	L1989	K1829	E1708	Q1331	S1031
F3121	N2770	F2462	S2328	W2179	ALA	H1992	K1830	E1708	S1335	S1032
F3121	S2771	I2463	S2328	I2180	TLE	P1993	P1831	L1716	P1336	A1033
I3128	D2772	P2620	D2341	M2181	TLE	P1993	K1832	L1716	M1547	K1044
W3131	R2773	L2469	D2341	L2184	VAL	M2011	W1833	L1730	P1548	K1044
Y3132	D2774	Q2474	M2344	L2184	ASP	F2016	L1834	E1734	K1340	V1047
F3136	E2777	Q2474	D2344	D2198	ASN	F2016	ASN	E1734	L1345	N1048
F3136	Q3018	E2483	D2345	H2199	ASN	SER	H1838	L1562	M1365	K1051
L3140	K3019	K2484	Q2346	D2200	ASN	ASN	M1839	P1563	T1366	L1052
M3151	A3020	E2485	F2348	H2200	PRO	SER	K1840	P1742	F1367	L1052
V3152	E3021	L2349	R2350	Q2203	ILE	ASN	I1841	Q1565	L1368	I1055
R3153	D2785	R2350	R2350	E2204	ASN	S2022	W1842	R1582	T1369	D1062
R3153	V2786	L2488	V2353	A2205	ASN	S2022	K1843	F1750	F1370	L1063
R3158	R2791	Y2491	V2353	L2206	A2028	A2028	N1844	I1756	R1376	K1093
Q3182	F2794	Y2492	V2369	V2209	I2029	I2029	A1847	K1757	L1377	E1094
ARG	E2805	C2493	A2373	I2236	D2030	D2030	L1849	K1763	L1378	L1098
GLN	S2806	L2494	A2373	I2236	L2031	L2031	A1850	F1767	E1380	D1098
THR	R2807	L2499	R2385	I2243	I2035	I2035	I1851	I1771	D1386	N1105
ALA	K2808	Q2501	F2394	I2243	ARG	Y2037	D1852	A1772	D1389	L1133
THR	E3037	E2502	F2394	Q2248	ALA	W2038	W1853	S1773	P1136	P1136
MET	E3038	Y2503	F2394	E2249	GLU	K2041	H1857	S1773	N1137	N1137
VAL	A3039	L2504	I2397	S2251	THR	T2042	E1863	I1775	Q1397	P1136
MET	N3040	N2521	F2402	S2252	L2116	L2043	D1885	K1776	T1400	D1141
GLY	T3045	K2524	E2405	L2259	L2116	L2043	K1888	Q1779	R1412	L1144
ASP	A3046	K2524	E2405	L2259	L2116	L2043	E1897	K1778	E1426	L1144
LYS	F3047	S2529	F2407	V2272	L2122	L2043	D1898	E1777	E1427	Y1156
PRO	Q3048	M2530	N2408	P2273	L2123	L2043	ASN	Q1779	P1631	L1144
ASP	D3049	Q2531	N2409	L2274	THR	THR	ASN	Q1779	E1632	Y1156
THR	D3050	Q2531	N2409	L2275	THR	THR	ASN	F1782	E1632	I1171
ASN	Q3059	R2535	T2410	L2275	THR	THR	THR	I1783	E1638	I1171
ASP	Q3059	R2535	T2410	L2275	THR	THR	THR	N1784	E1638	I1171
ARG	F3063	D2540	T2412	P2277	THR	THR	THR	D1785	K1642	L1193
GLY	R3067	F2541	T2413	L2278	THR	THR	THR	A1786	K1642	L1193
ARG	L2917	I2546	R2415	M2279	THR	THR	THR	T1787	E1643	Q1234
P2918	P2918	I2546	R2415	M2279	THR	THR	THR	L1788	L1644	Q1234
Q3203	Q3203	Q2723	N2416	K2284	VAL	ASP	VAL	F1789	F1650	T1271
P3204	Q3204	Q2723	E2417	C2286	ASN	GLY	P1951	V1790	Y1651	T1271
E3210	E3210	Y2726	Q2418	L2285	ASN	ASP	H1954	L1791	L1478	E1277
N3073	N3073	Y2726	F2420	D2288	VAL	VAL	E1955	K1794	E1478	E1277
T3240	T3240	Y2729	L2421	D2288	LEU	VAL	R1956	C1795	S1490	E1278
T3241	T3241	N2574	V2422	D2288	THR	THR	M1957	L1796	D1491	D1278
D3244	D3244	Y2591	T2429	Q2294	PHE	SER	N1958	D1797	H1492	L1280
S3079	S3079	H2592	T2429	K2296	GLN	SER	T1963	L1796	L1503	D1291
R3247	R3247	E2748	R2434	D2297	ASP	SER	P1963	R1799	S1504	D1291
				A2298	ASP	ASP		K1804	L1507	N1298
				M2299	ASP	ASP				

L3248	D3363	P3592
L3249		Y3593
N3250	P3376	E3594
V3251	T3377	R3595
L3252		V3596
	R3389	K3597
Y3260		P3598
N3261	Y3407	L3599
R3262	P3408	L3600
L3263	A3409	K3601
P3264	V3410	
F3265		D3604
P3266	S3413	L3605
R3267		
	N3433	D3610
P3270	V3434	S3611
K3271	E3435	P3612
L3272	T3436	
P3273	R3437	T3625
E3274	R3438	
		Q3629
E3277	I3449	
		F3646
L3280	S3452	
V3281	P3453	E3654
	Q3454	P3655
L3287		D3656
A3289	I3457	N3657
P3290		E3658
Y3291	S3461	L3659
T3292	V3462	
R3293	S3463	L3663
K3295		
	D3481	W3674
	P3482	
	D3483	N3685
D3299		
F3300	Q3486	R3689
K3304	M3489	T3716
P3305		T3717
D3306	K3492	
Y3307	L3493	V3728
R3313	H3497	R3735
L3314	D3498	
	M3506	
V3317	T3507	F3744
R3318		
R3319	T3519	
E3332	S3524	
Q3347	F3544	
E3350	N3566	
L3360	G3579	
N3361		
K3362		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	474949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.268	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	407.02, 407.02, 407.02	wwPDB
Map dimensions	94, 94, 94	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.33, 4.33, 4.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CMC, ATP

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	Y	0.14	0/401	0.31	0/535
2	V	0.15	0/934	0.32	0/1251
3	H	0.64	0/2298	0.67	0/3093
3	T	0.14	0/2341	0.37	0/3153
4	A	0.22	0/784	0.35	0/1052
4	O	0.23	0/803	0.35	0/1078
5	B	0.25	0/711	0.44	0/948
5	Q	0.24	0/648	0.40	0/868
6	N	0.21	0/824	0.33	0/1113
6	S	0.21	0/824	0.33	0/1113
7	D	0.24	0/736	0.32	0/991
7	U	0.22	0/730	0.32	0/983
8	P	0.16	0/2347	0.34	0/3171
9	W	0.29	0/4107	0.49	0/6330
10	I	0.29	0/4150	0.48	0/6410
11	X	0.16	0/83	0.51	0/107
12	E	0.65	0/3527	0.62	1/4769 (0.0%)
13	F	0.63	0/3350	0.53	0/4544
14	G	0.51	0/2849	0.47	0/3859
15	K	0.64	0/2036	0.57	0/2739
16	L	0.54	0/29358	0.58	1/39779 (0.0%)
All	All	0.49	0/63841	0.53	2/87886 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
16	L	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	852	PRO	N-CA-C	-5.70	100.73	112.47
12	E	310	LEU	N-CA-C	5.26	119.76	112.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	L	2621	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	396	0	372	10	0
2	V	923	0	955	24	0
3	H	2250	0	2192	56	0
3	T	2294	0	2236	76	0
4	A	774	0	813	6	0
4	O	791	0	828	4	0
5	B	703	0	753	14	0
5	Q	641	0	684	6	0
6	N	814	0	869	8	0
6	S	814	0	869	4	0
7	D	725	0	745	7	0
7	U	719	0	740	5	0
8	P	2286	0	2268	73	0
9	W	3666	0	2018	71	0
10	I	3695	0	2007	67	0
11	X	82	0	92	2	0
12	E	3448	0	3448	102	0
13	F	3278	0	3238	33	0
14	G	2788	0	2760	29	0
15	K	1989	0	1961	41	0
16	L	28729	0	29144	516	0
17	B	51	0	33	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	F	1	0	0	0	0
18	G	1	0	0	0	0
19	F	31	0	12	1	0
19	G	31	0	12	1	0
All	All	61920	0	59049	1034	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 9.

The worst 5 of 1034 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)
12:E:640:ARG:NH2	12:E:726:GLU:OE1	1.98	0.96
16:L:944:ASN:OD1	16:L:947:ARG:NH2	2.01	0.93
12:E:312:THR:OG1	16:L:3728:VAL:O	1.88	0.89
16:L:3244:ASP:OD1	16:L:3247:ARG:NH1	2.13	0.82
15:K:262:LYS:NZ	3:H:545:PRO:O	2.14	0.80

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	Y	44/113 (39%)	44 (100%)	0	0	100	100
2	V	111/282 (39%)	111 (100%)	0	0	100	100
3	H	263/832 (32%)	233 (89%)	29 (11%)	1 (0%)	30	67
3	T	272/832 (33%)	262 (96%)	10 (4%)	0	100	100
4	A	92/136 (68%)	91 (99%)	1 (1%)	0	100	100
4	O	94/136 (69%)	94 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	85/103 (82%)	82 (96%)	3 (4%)	0	100	100
5	Q	78/103 (76%)	77 (99%)	1 (1%)	0	100	100
6	N	104/130 (80%)	104 (100%)	0	0	100	100
6	S	104/130 (80%)	104 (100%)	0	0	100	100
7	D	91/126 (72%)	91 (100%)	0	0	100	100
7	U	90/126 (71%)	90 (100%)	0	0	100	100
8	P	268/445 (60%)	263 (98%)	5 (2%)	0	100	100
11	X	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
12	E	405/1168 (35%)	363 (90%)	41 (10%)	1 (0%)	43	78
13	F	410/489 (84%)	384 (94%)	26 (6%)	0	100	100
14	G	353/375 (94%)	343 (97%)	10 (3%)	0	100	100
15	K	229/476 (48%)	211 (92%)	17 (7%)	1 (0%)	30	67
16	L	3489/3744 (93%)	3203 (92%)	284 (8%)	2 (0%)	48	83
All	All	6589/9755 (68%)	6155 (93%)	429 (6%)	5 (0%)	49	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	K	315	ARG
3	H	500	ILE
16	L	1848	ILE
12	E	340	TRP
16	L	910	ALA

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	Y	44/100 (44%)	44 (100%)	0	100	100
2	V	106/258 (41%)	106 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	256/769 (33%)	253 (99%)	3 (1%)	63	75
3	T	259/769 (34%)	259 (100%)	0	100	100
4	A	82/111 (74%)	82 (100%)	0	100	100
4	O	84/111 (76%)	84 (100%)	0	100	100
5	B	72/79 (91%)	71 (99%)	1 (1%)	59	72
5	Q	66/79 (84%)	66 (100%)	0	100	100
6	N	83/102 (81%)	83 (100%)	0	100	100
6	S	83/102 (81%)	83 (100%)	0	100	100
7	D	79/106 (74%)	78 (99%)	1 (1%)	61	74
7	U	78/106 (74%)	78 (100%)	0	100	100
8	P	253/414 (61%)	252 (100%)	1 (0%)	84	84
11	X	9/9 (100%)	9 (100%)	0	100	100
12	E	379/1054 (36%)	378 (100%)	1 (0%)	86	86
13	F	367/434 (85%)	366 (100%)	1 (0%)	86	86
14	G	305/320 (95%)	303 (99%)	2 (1%)	76	81
15	K	221/441 (50%)	221 (100%)	0	100	100
16	L	3238/3452 (94%)	3222 (100%)	16 (0%)	81	83
All	All	6064/8816 (69%)	6038 (100%)	26 (0%)	81	84

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	L	3252	LEU
16	L	3272	LEU
16	L	3506	MET
16	L	3265	PHE
16	L	3281	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	3041	GLN
16	L	3139	GLN
16	L	3551	GLN
16	L	73	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	L	57	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](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	CMC	B	501	5	51,53,54	0.50	0	72,78,80	0.90	1 (1%)
19	ATP	F	1002	18	32,33,33	0.56	0	48,52,52	0.59	0
19	ATP	G	502	18	32,33,33	0.54	0	48,52,52	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	CMC	B	501	5	-	7/50/67/68	0/3/3/3
19	ATP	F	1002	18	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ATP	G	502	18	-	0/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
17	B	501	CMC	P3B-O3B-C3B	-5.41	108.99	123.43

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

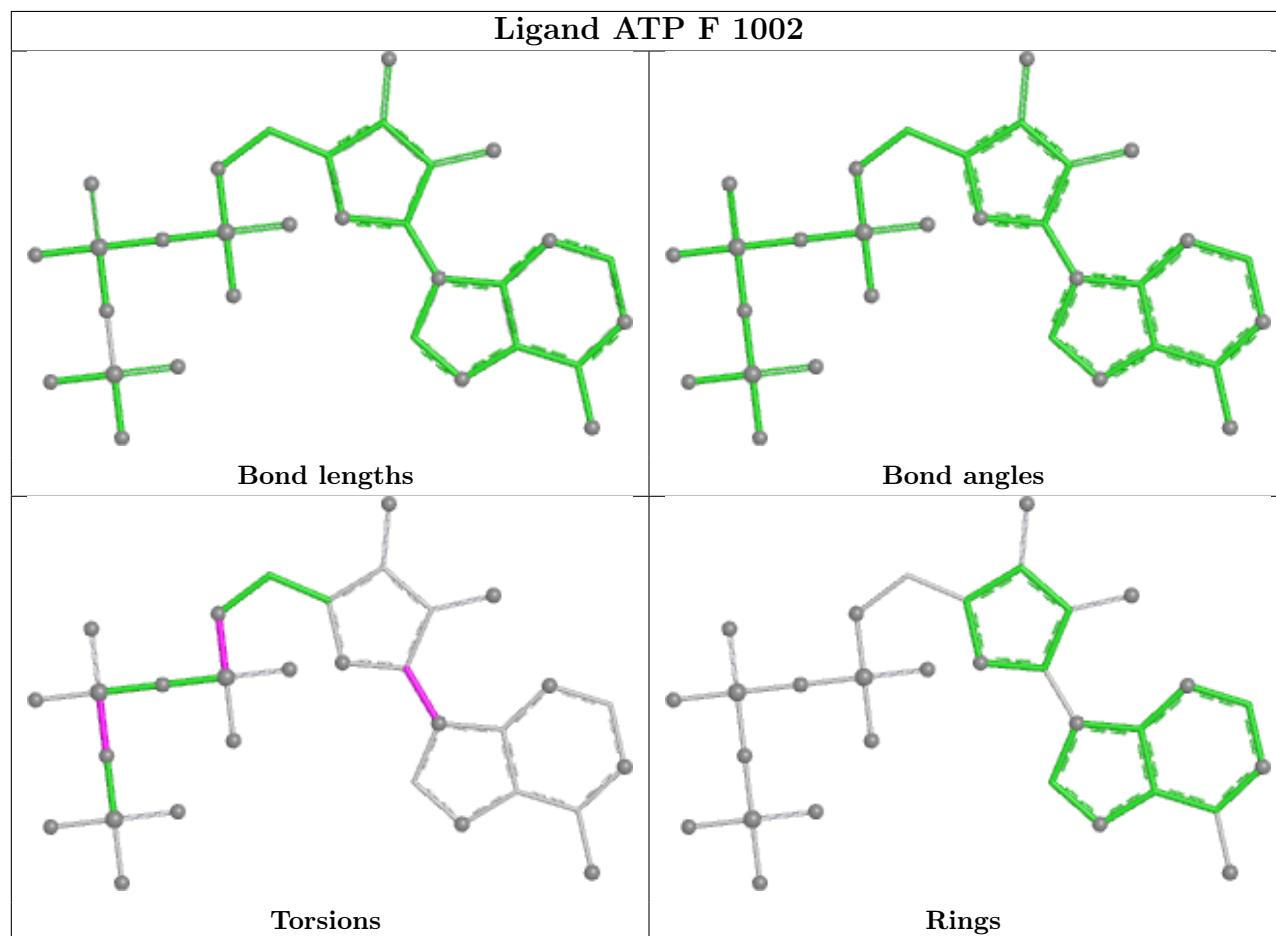
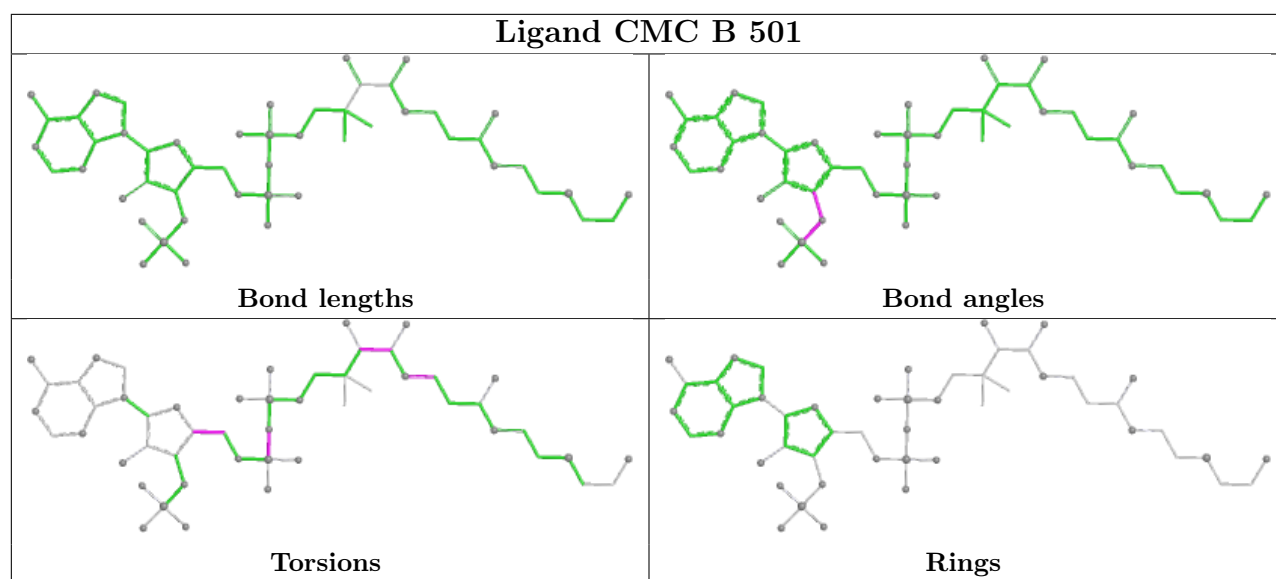
Mol	Chain	Res	Type	Atoms
19	F	1002	ATP	C5'-O5'-PA-O2A
19	F	1002	ATP	C5'-O5'-PA-O3A
17	B	501	CMC	C3B-C4B-C5B-O5B
17	B	501	CMC	O4B-C4B-C5B-O5B
17	B	501	CMC	P2A-O3A-P1A-O1A

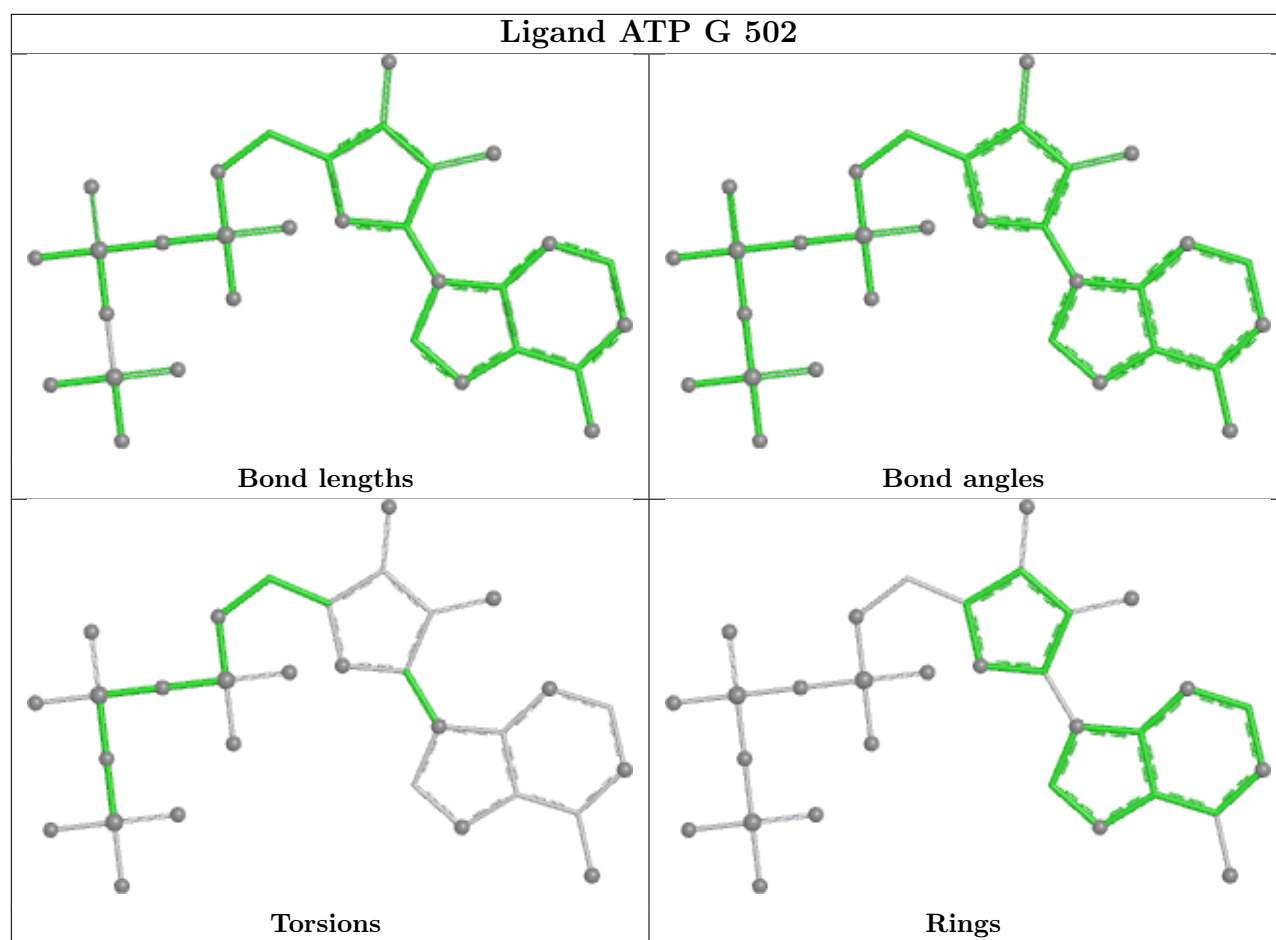
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	501	CMC	3	0
19	F	1002	ATP	1	0
19	G	502	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

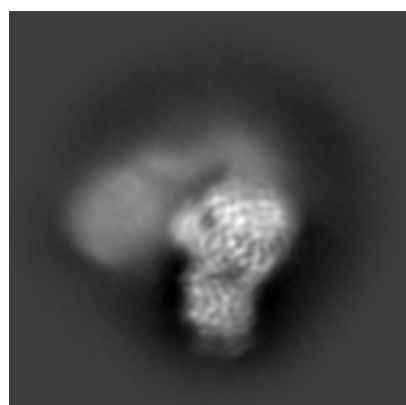
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32150. These allow visual inspection of the internal detail of the map and identification of artifacts.

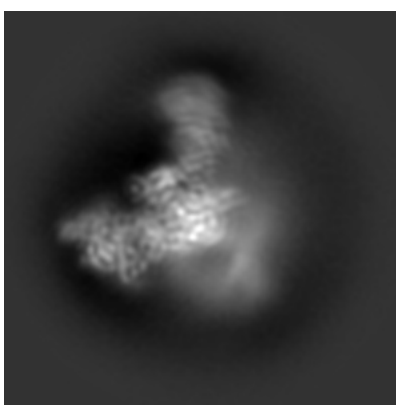
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

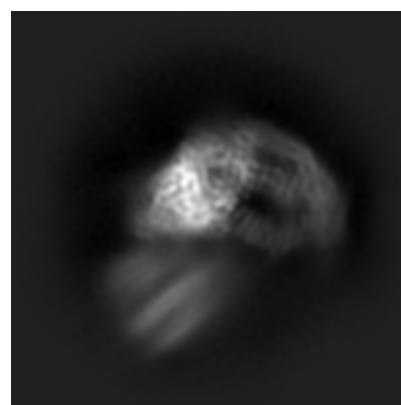
6.1.1 Primary map



X



Y

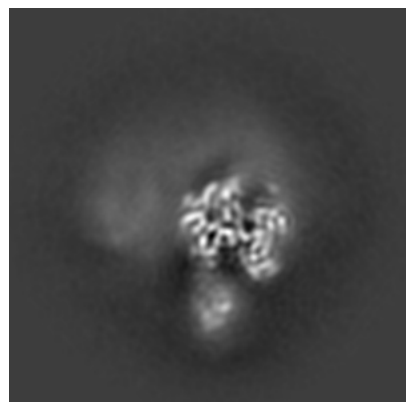


Z

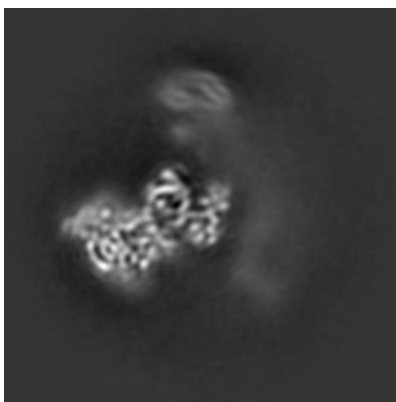
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

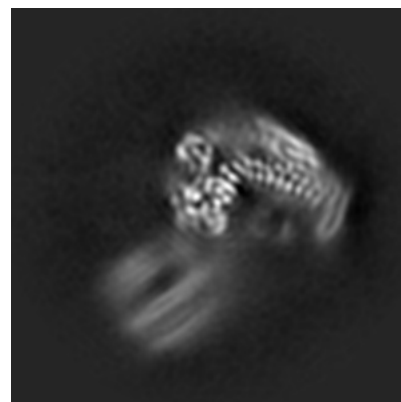
6.2.1 Primary map



X Index: 47



Y Index: 47

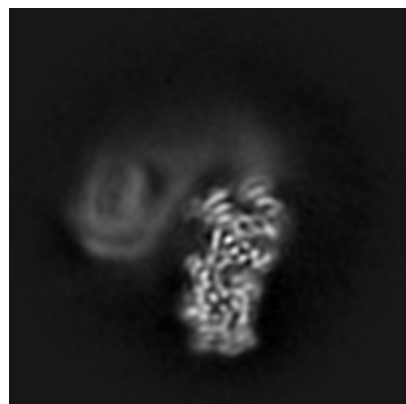


Z Index: 47

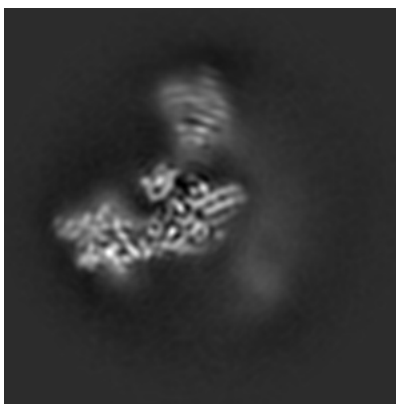
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

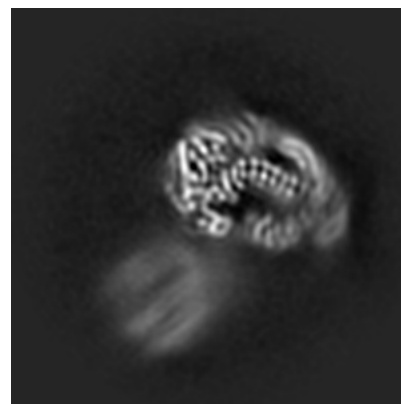
6.3.1 Primary map



X Index: 41



Y Index: 51

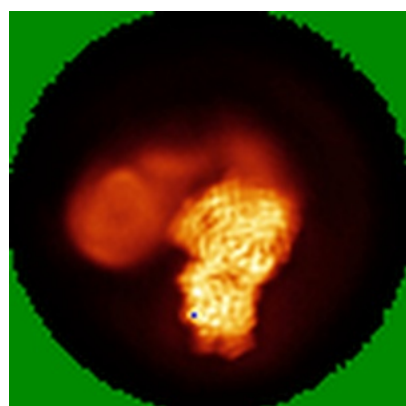


Z Index: 44

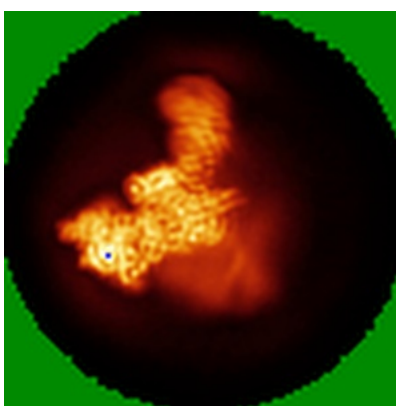
The images above show the largest variance slices of the map in three orthogonal directions.

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

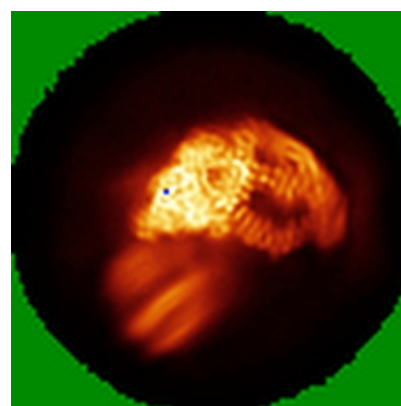
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

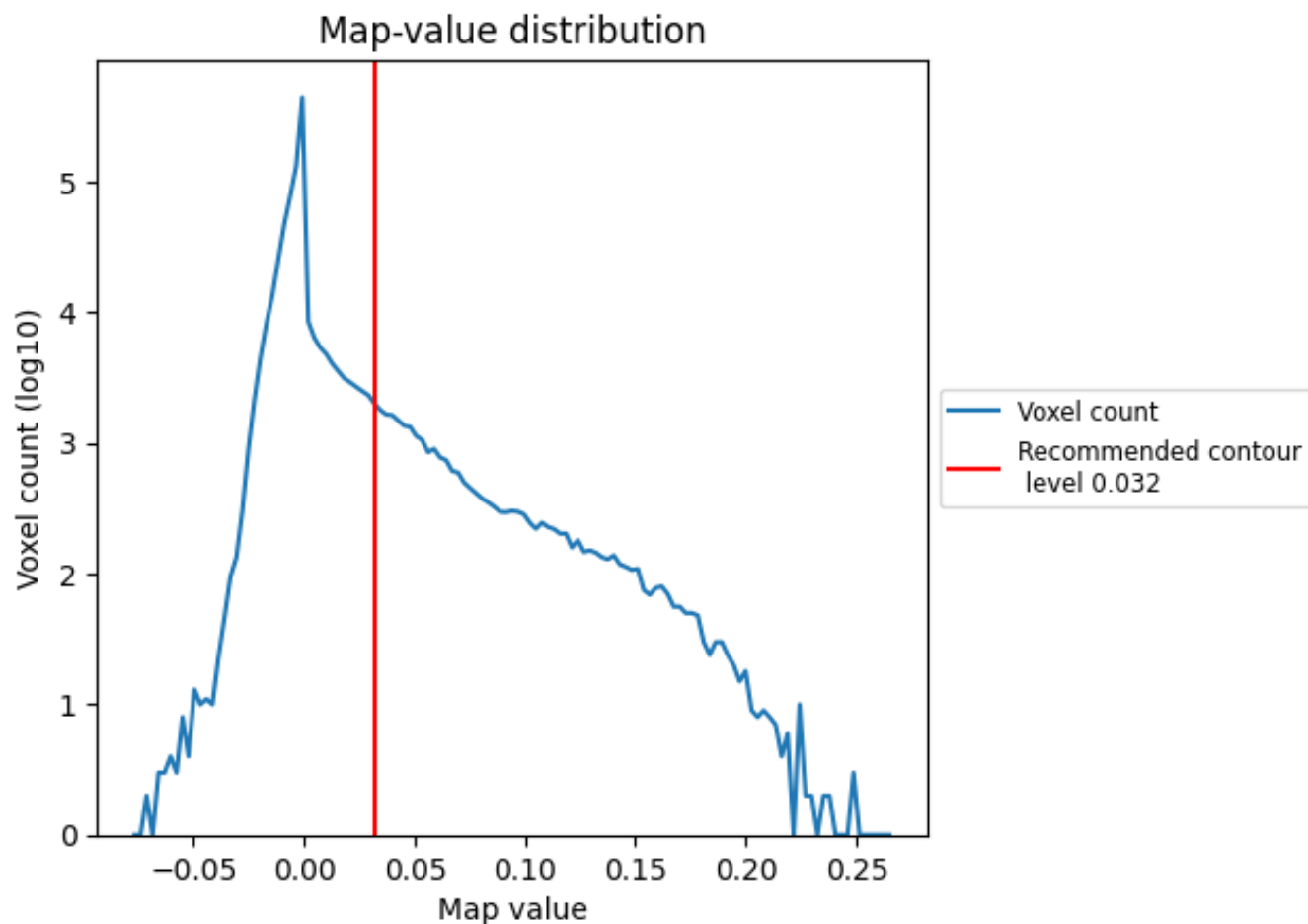
6.6 Mask visualisation

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

7 Map analysis [i](#)

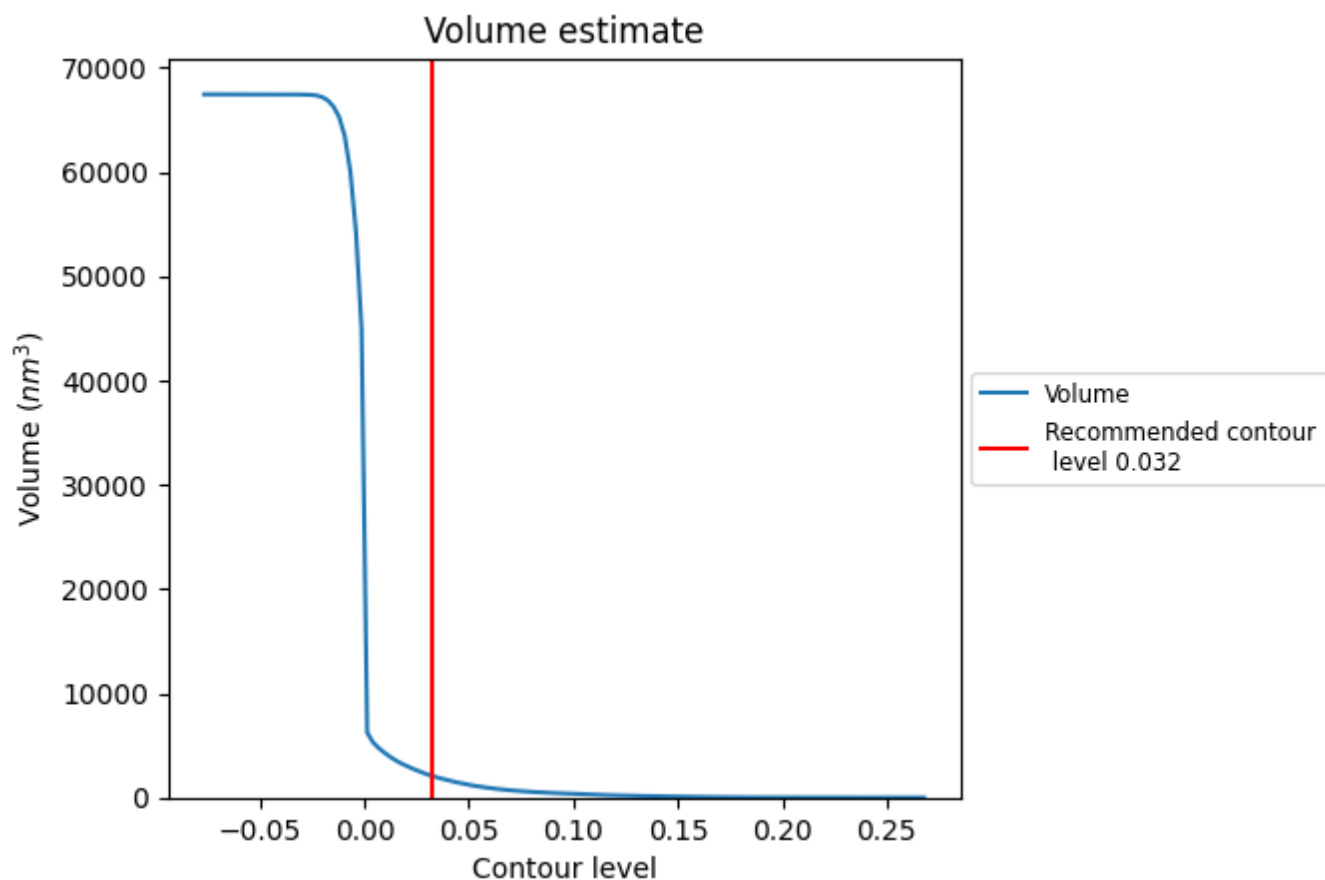
This section contains the results of statistical analysis of the map.

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.

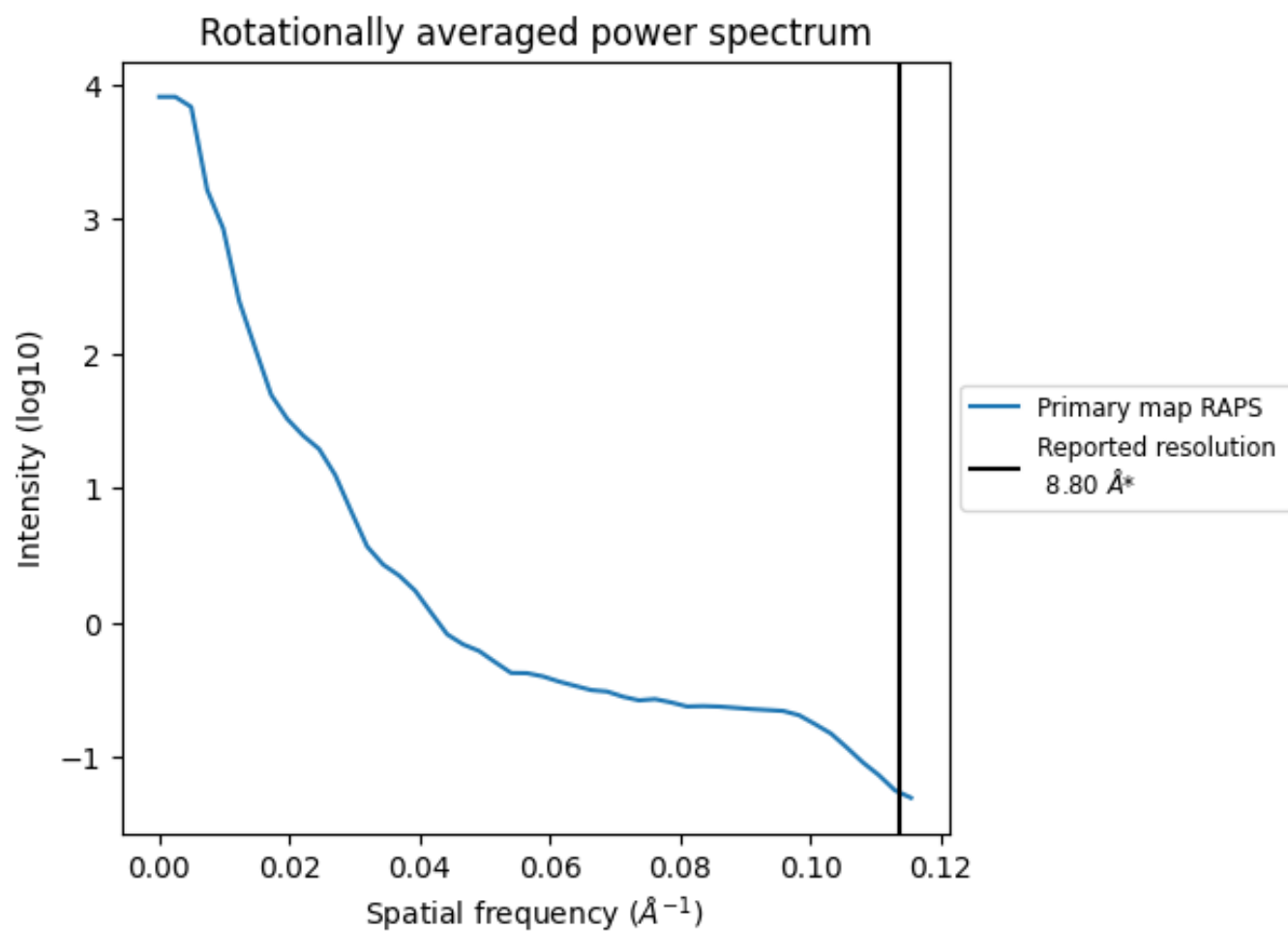
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2095 nm³; this corresponds to an approximate mass of 1893 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 0.114 Å⁻¹

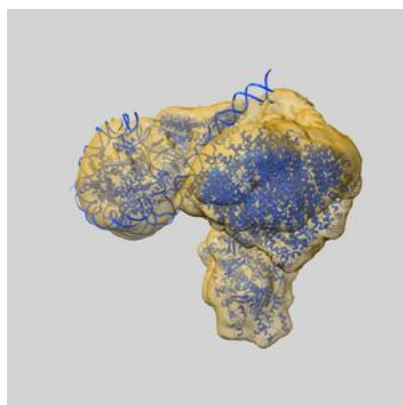
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

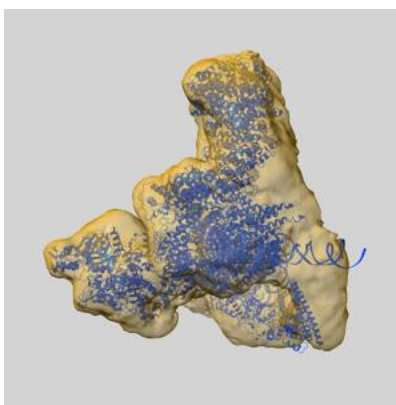
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32150 and PDB model 7VVZ. Per-residue inclusion information can be found in section 3 on page 13.

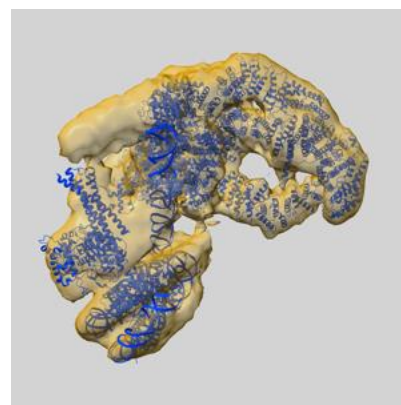
9.1 Map-model overlay [i](#)



X



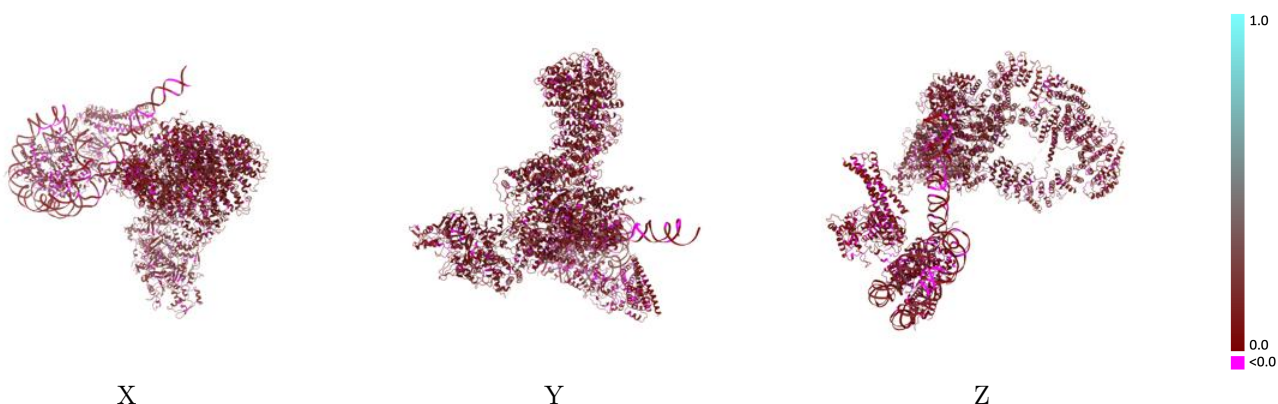
Y



Z

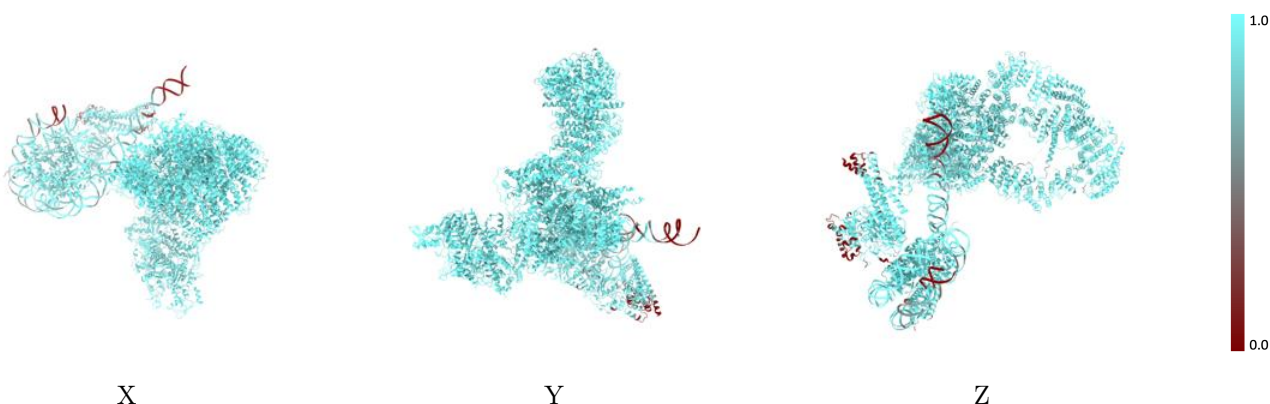
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



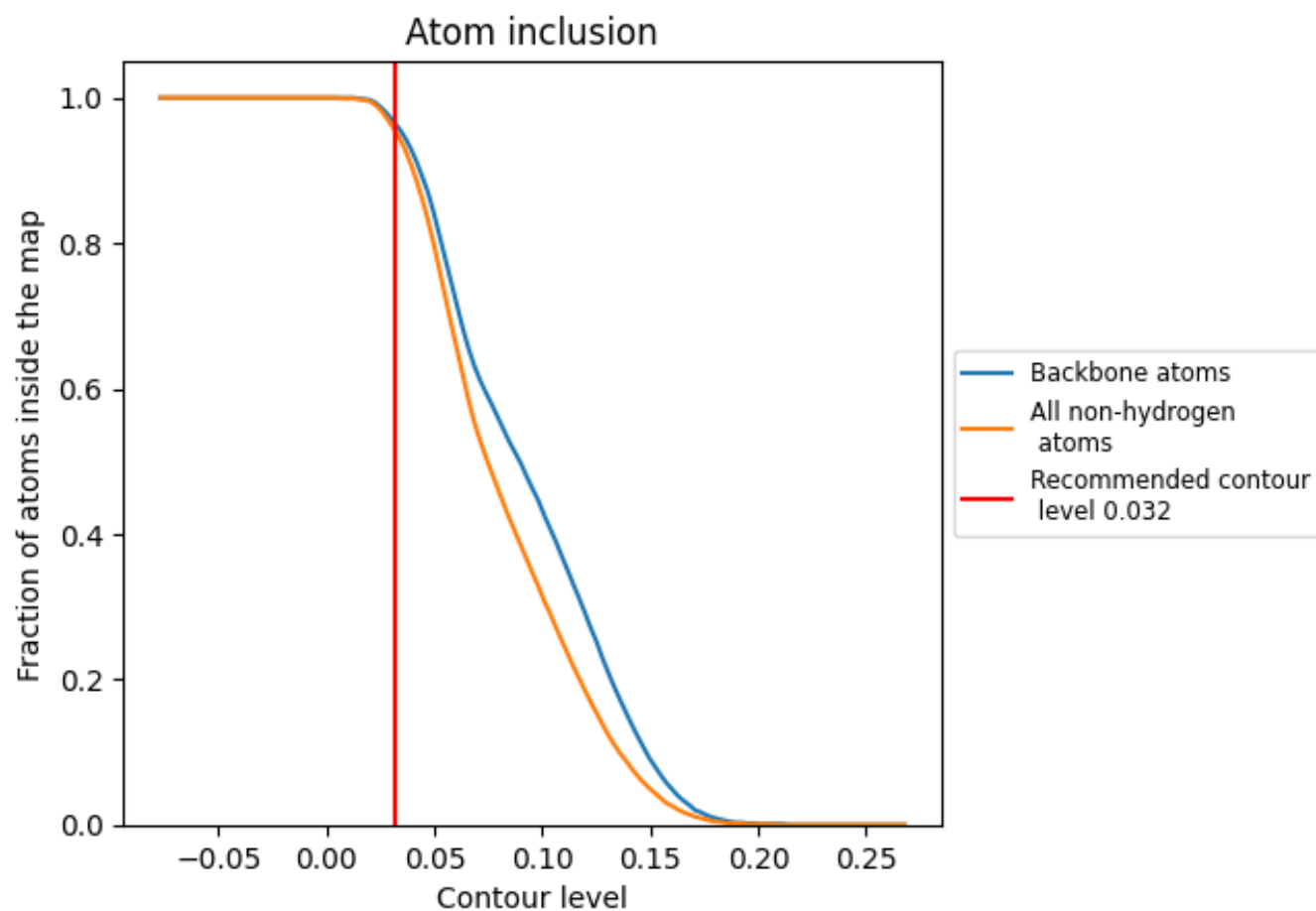
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9540	 0.1080
A	 0.9540	 0.0710
B	 0.9380	 0.0550
D	 0.9830	 0.0560
E	 0.9990	 0.1360
F	 1.0000	 0.1220
G	 0.9980	 0.1180
H	 0.9840	 0.1200
I	 0.8130	 0.0880
K	 0.9910	 0.1310
L	 0.9830	 0.1260
N	 0.9910	 0.0370
O	 1.0000	 0.0500
P	 0.9850	 0.0680
Q	 1.0000	 0.0320
S	 0.9730	 0.0490
T	 0.7880	 0.0650
U	 0.9830	 0.0670
V	 0.8430	 0.0470
W	 0.8130	 0.0750
X	 0.8850	 0.0650
Y	 0.7530	 0.0780

