



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 06:00 PM JST

PDB ID : 7VVZ
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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

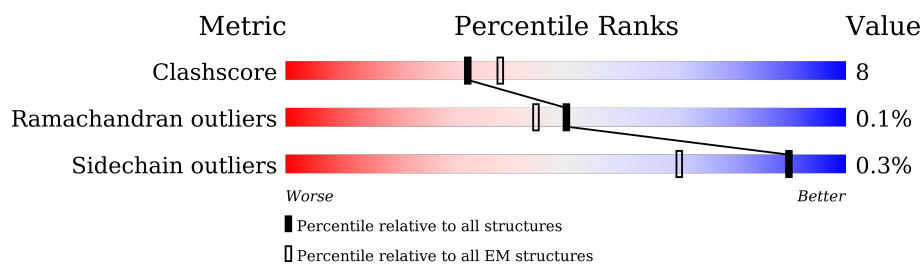
1 Overall quality at a glance

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.






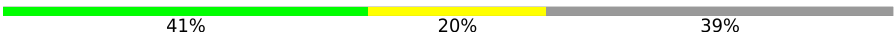
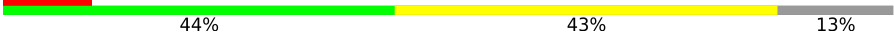
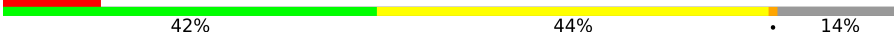






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
2	V	282	
3	H	832	
3	T	832	
4	A	136	
4	O	136	
5	B	103	
5	Q	103	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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		

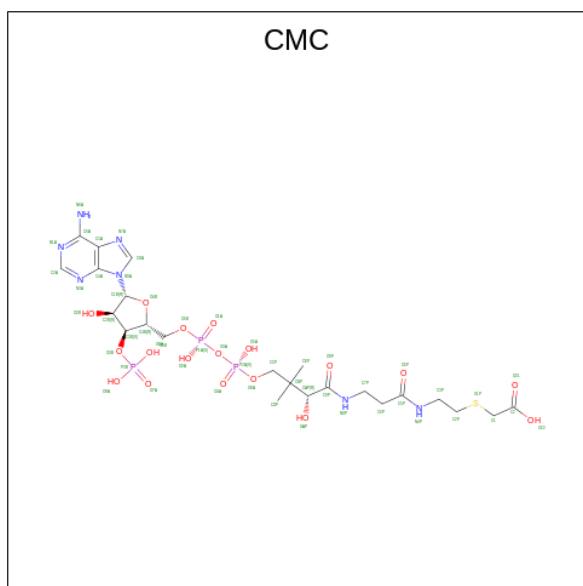
- Molecule 15 is a protein called SWR1-complex protein 4.

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 (three-letter code: CMC) (formula: $C_{23}H_{38}N_7O_{18}P_3S$) (labeled as "Ligand of Interest" by depositor).

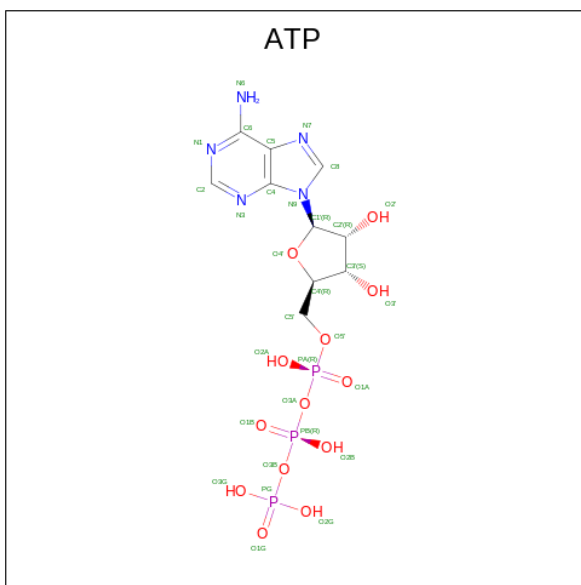


Mol	Chain	Residues	Atoms						AltConf
17	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 18 is MAGNESIUM ION (three-letter code: 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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

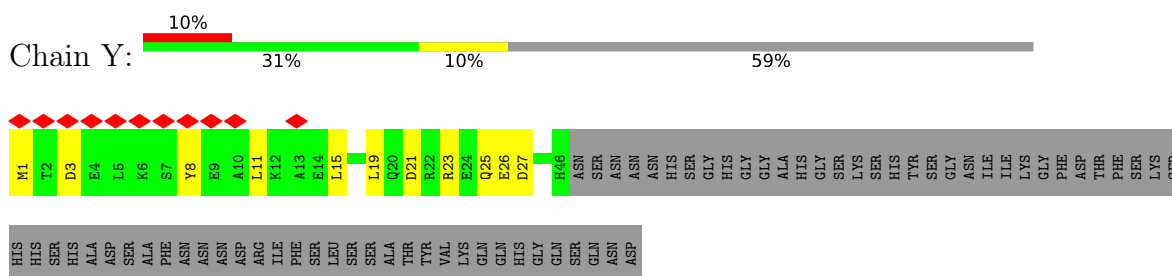


Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total 31	C 10	N 5	O 13	P 3	0
19	G	1	Total 31	C 10	N 5	O 13	P 3	0

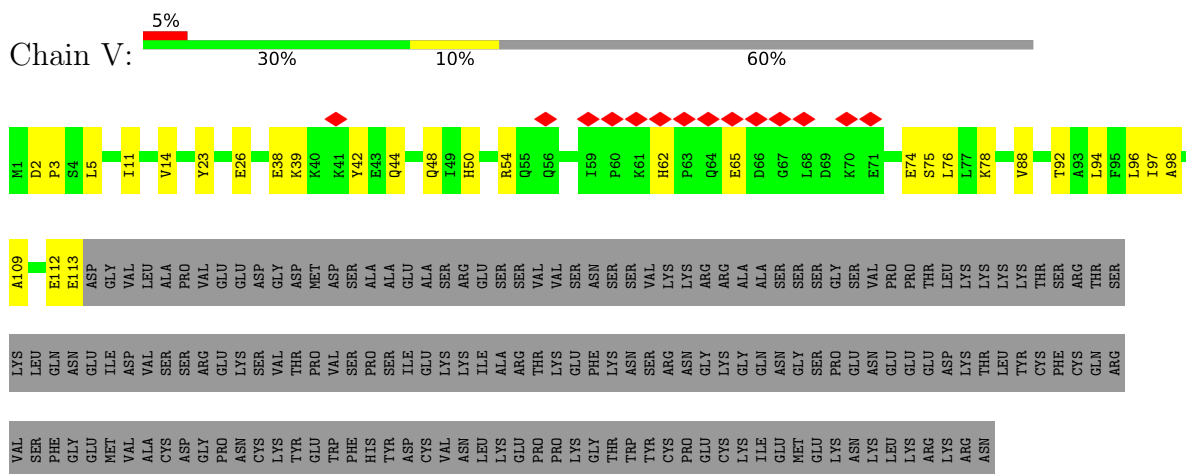
3 Residue-property plots [i](#)

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.

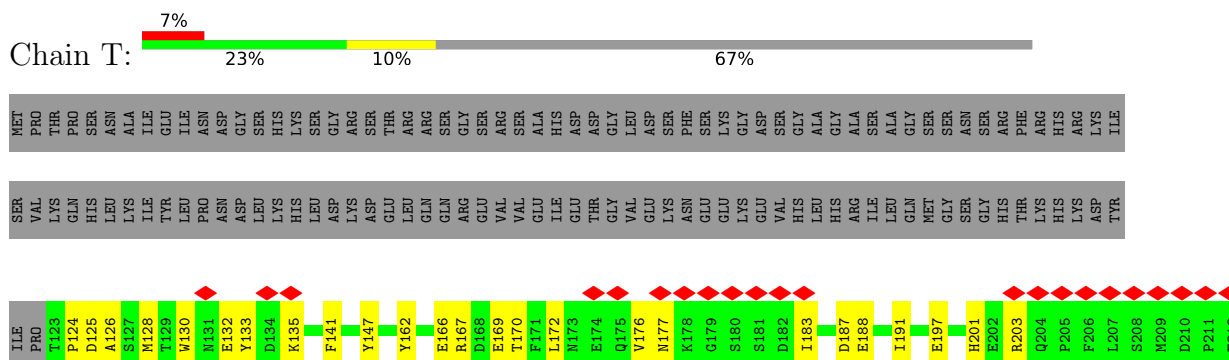
- Molecule 1: Chromatin modification-related protein EAF6

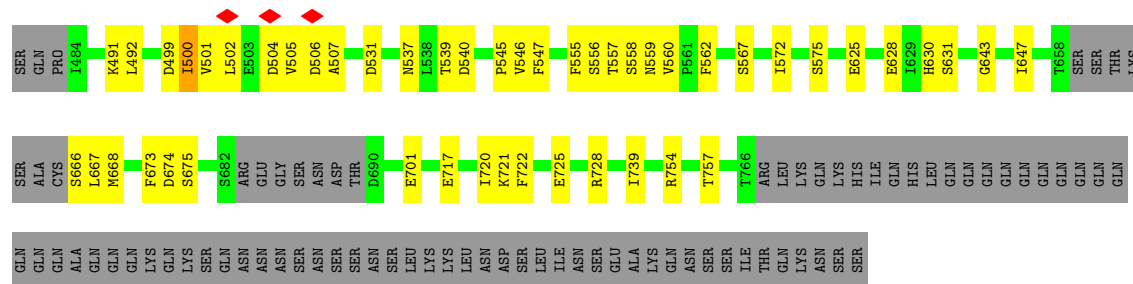


- Molecule 2: Chromatin modification-related protein YNG2



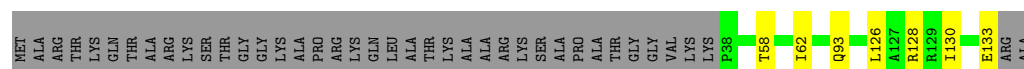
- Molecule 3: Enhancer of polycomb-like protein 1





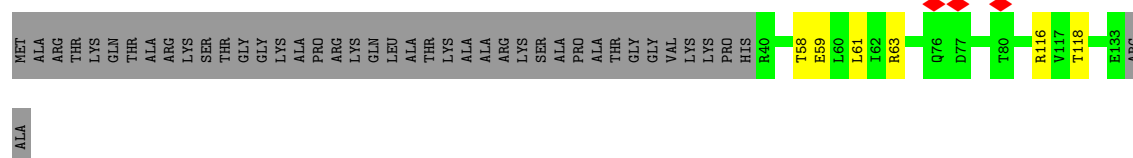
• Molecule 4: Histone H3

Chain O: 65% 5% 29%



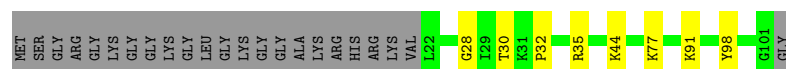
• Molecule 4: Histone H3

Chain A: 65% 31%



• Molecule 5: Histone H4

Chain Q: 70% 8% 22%



• Molecule 5: Histone H4

Chain B: 5% 69% 16% 16%




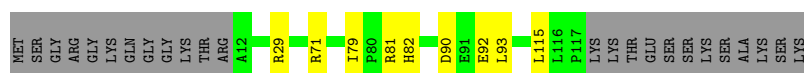
• Molecule 6: Histone H2A

Chain S: 77% 5% 18%



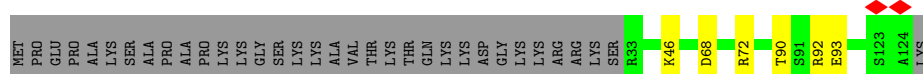
• Molecule 6: Histone H2A

Chain N: 



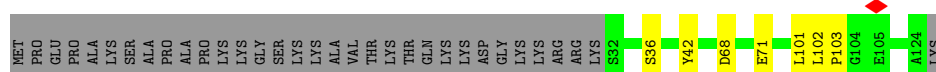
• Molecule 7: Histone H2B 1.1

Chain U: 



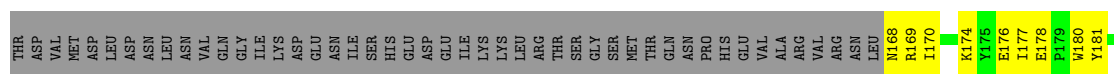
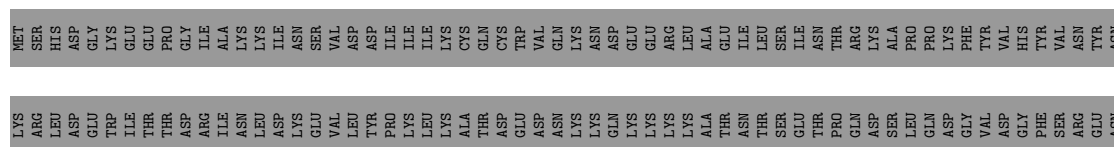
• Molecule 7: Histone H2B 1.1

Chain D: 




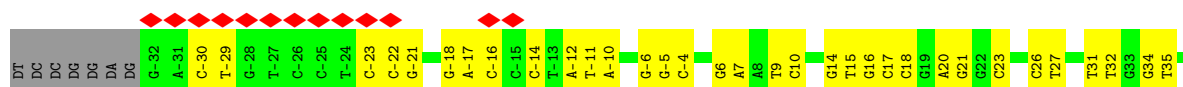
• Molecule 8: Histone acetyltransferase ESA1

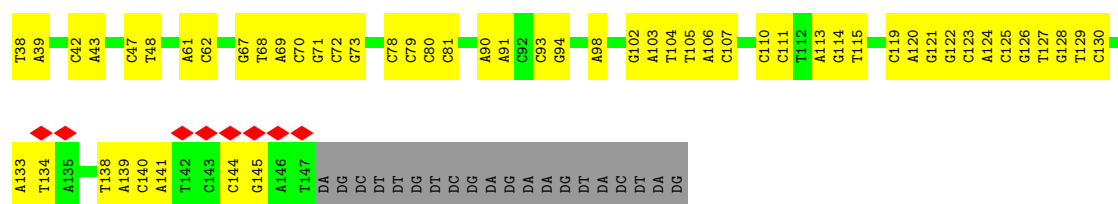
Chain P: 



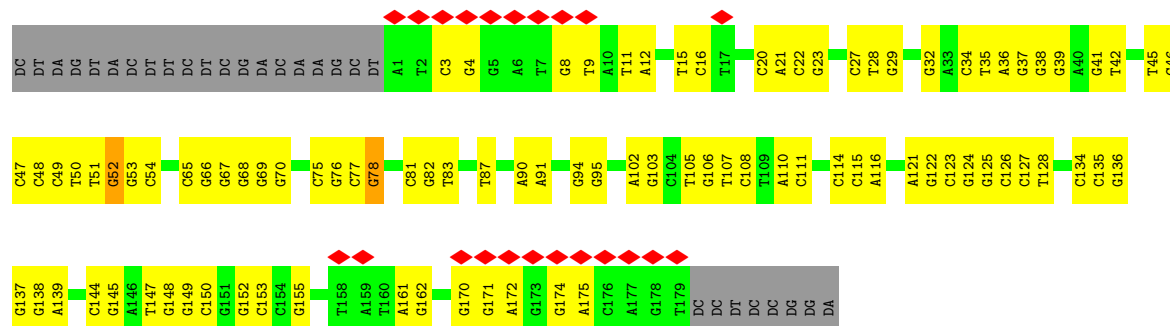
• Molecule 9: DNA (207-mer)

Chain W: 

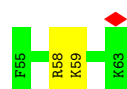
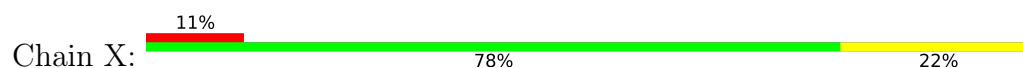




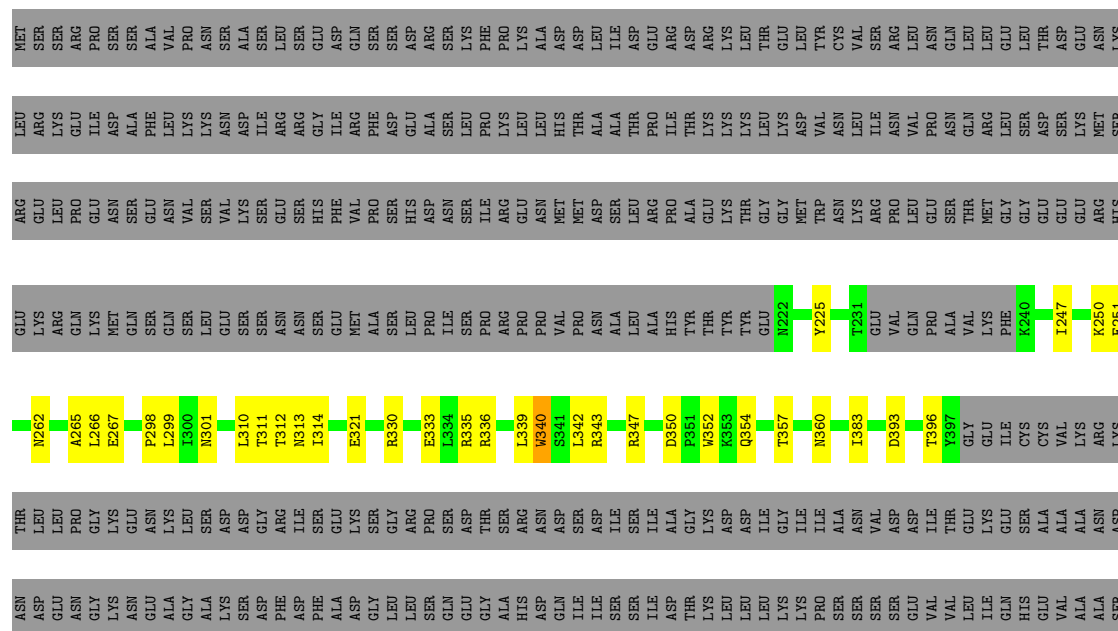
• Molecule 10: DNA (207-mer)

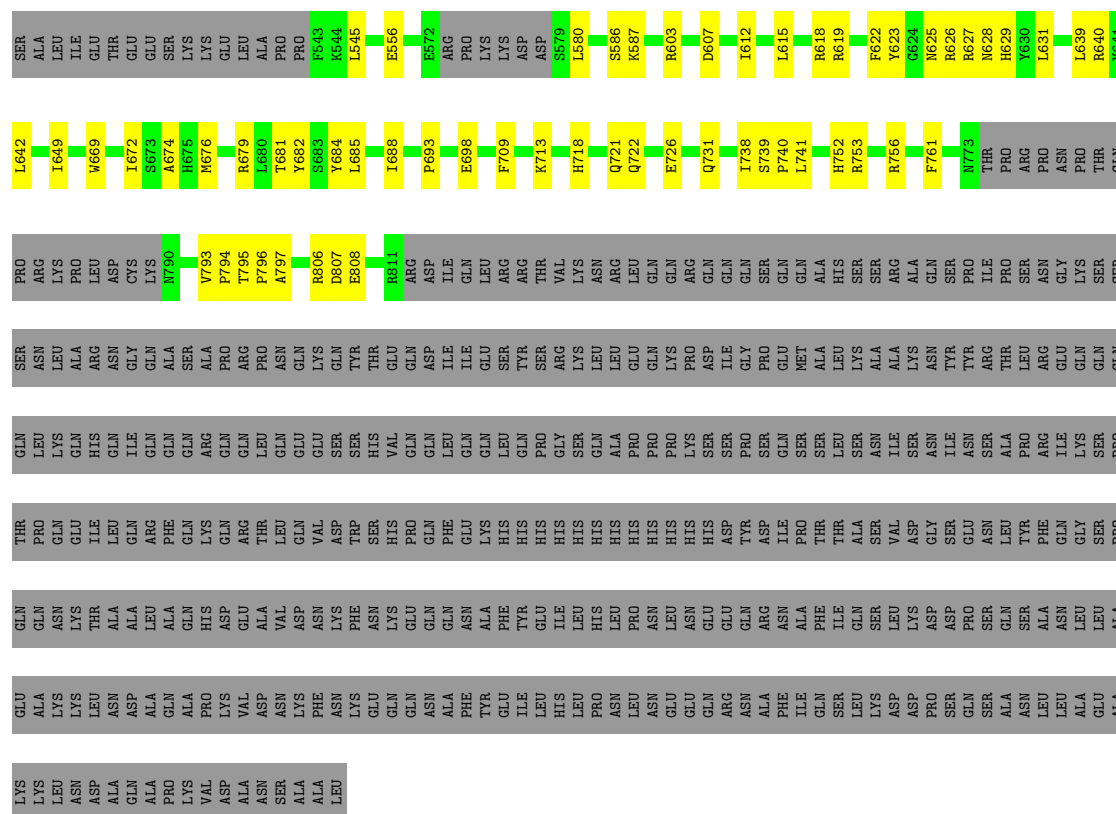


• Molecule 11: Epl1 arginine anchor



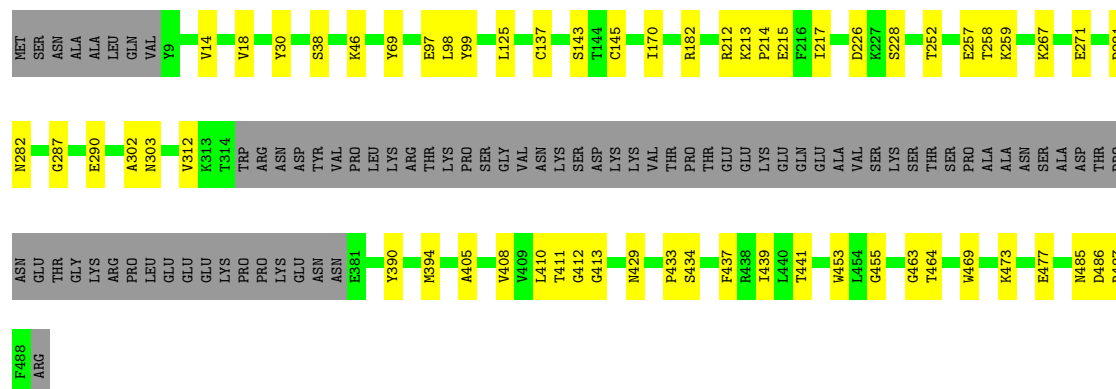
• Molecule 12: Chromatin modification-related protein EAF1





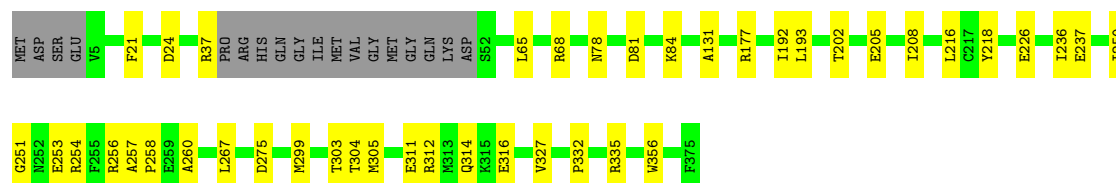
• Molecule 13: Actin-related protein 4

Chain F: 73% 12% 15%



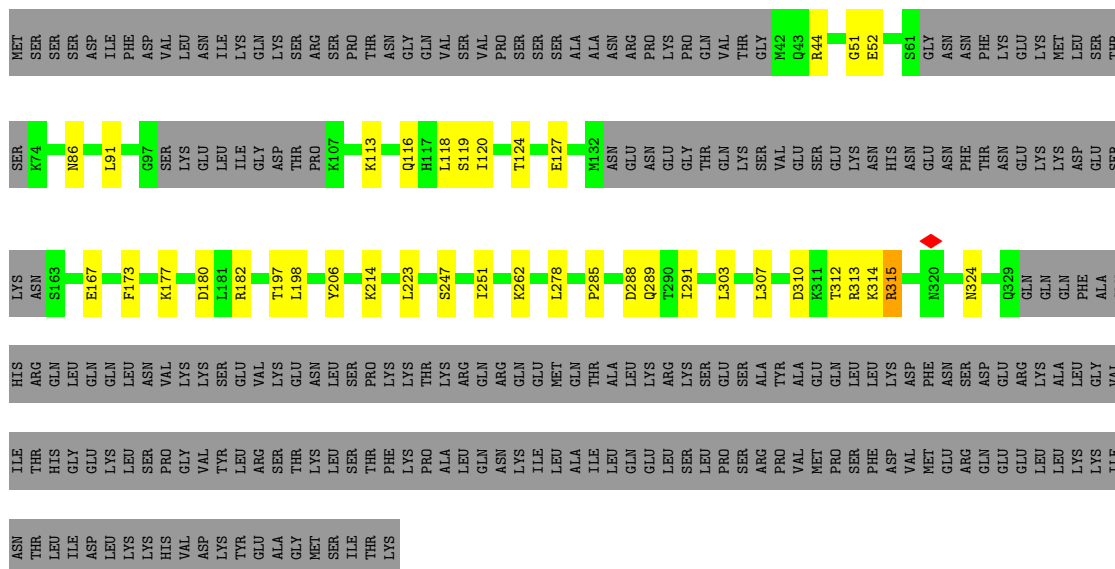
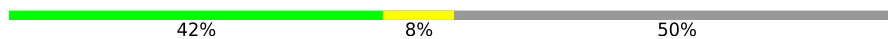
• Molecule 14: Actin

Chain G: 84% 11% 5%



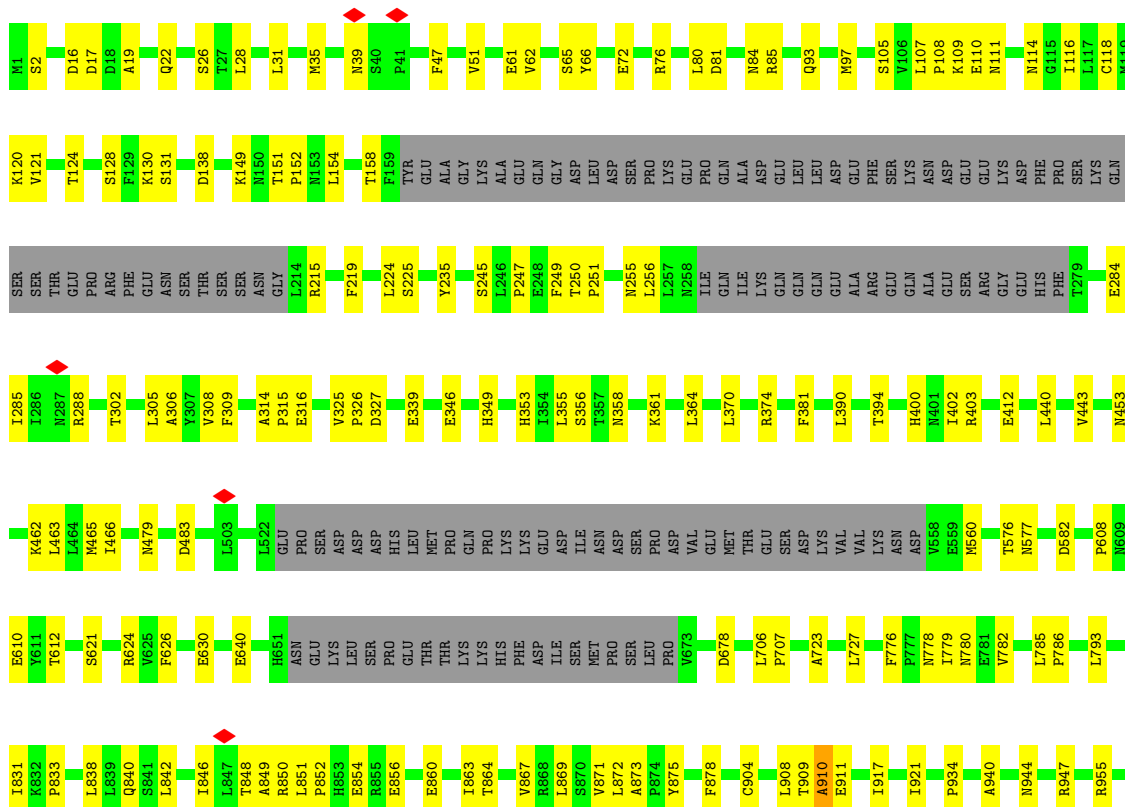
- Molecule 15: SWR1-complex protein 4

Chain K:

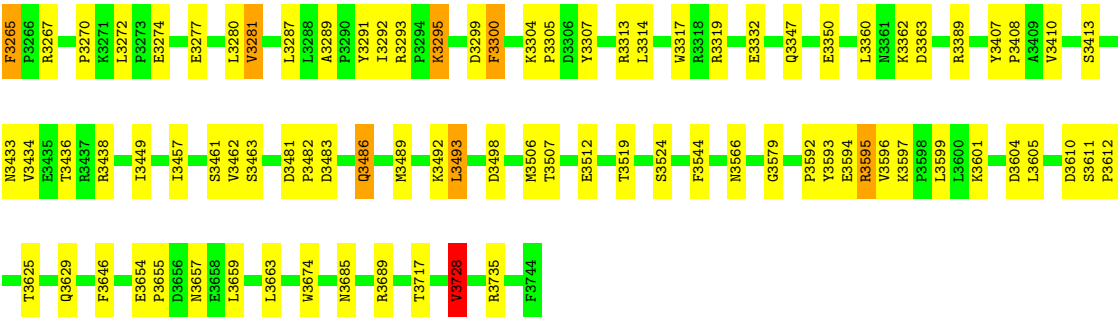


- Molecule 16: Transcription-associated protein 1

Chain L:



F3121	L2936	E2444	L2310	M2605	F2765	L2310	Y2169	VAL	E1976	S1818	E1683	L1507	Y993
I3128	T2972	R2450	K2313	I2613	T2756	K2313	F2172	GLU	Q1981	G1819	V1684	E1508	Y1007
W3131	F2982	R2456	Y2316	S2615	D2757	Y2316	K2177	ASP	F1988	Y1824	I1320	L1509	H1012
Y3132	F2982	D2457	L2320	L2616	C2762	L2320	E2178	THR	L1989	V1826	D1327	Y1513	H1014
F3136	E2998	E2461	S2328	L2618	D2768	S2328	W2179	ALA	H1992	E1827	S1329	V1532	R1014
L3140	T3001	P2620	P2620	P2619	W2769	P2620	I2180	ILE	P1993	D1828	K1330	D1536	M1028
M3151	Q3018	S2771	L2339	H2821	S2771	L2339	M2181	VAL	M2011	P1830	Q1331	T1029	K1030
V3152	V2623	D2772	L2622	L2623	D2772	L2622	L2184	ASP	F2016	K1832	S1335	S1032	S1031
R3153	K2624	D2774	D2341	K2624	D2774	D2341	L2198	ASN	MET	W1833	P1336	S1032	A1033
R3158	L2625	E2483	M2344	E2483	E2483	M2344	H2199	ASN	SER	L1834	P1548	M1547	K1044
Q3182	L2626	K2484	D2345	K2484	K2484	D2345	H2199	ASN	ASN	H1838	I1558	P1548	K1044
ARG	A2627	E2485	Q2347	E2485	E2485	Q2347	H2200	PRO	SER	E1734	L1345	I1558	K1044
GLN	L2628	L2488	F2348	L2488	L2488	F2348	Q2203	ILE	ASN	I1841	L1562	L1562	V1047
THR	N2631	T2491	R2349	T2491	T2491	R2349	E2204	ASN	S2022	N1844	P1563	P1563	N1048
THR	W2633	Y2492	L2350	Y2492	Y2492	L2350	A2205	THR	A2028	A1847	T1367	Q1564	K1051
MET	W2633	C2493	V2353	C2493	C2493	V2353	L2206	THR	D2030	I1849	L1368	Q1565	L1052
ALA	L2643	L2494	V2369	L2494	L2494	V2369	V2209	THR	L2031	F1750	F1370	R1582	I1055
VAL	N2651	I2499	A2373	I2499	I2499	A2373	I2236	ASN	K2041	I1850	R1601	N1601	D1062
MET	T2652	Q2501	R2385	Q2501	Q2501	R2385	I2243	HIS	L2035	Y1851	R1602	R1602	L1063
GLY	K2653	E2502	R2385	E2502	E2502	R2385	Q2248	ARG	L2036	D1852	F1603	F1603	L1377
LYS	E2656	L2504	F2394	L2504	L2504	F2394	Q2249	ALA	Y2037	V1853	H1604	H1604	L1378
ASP	W2658	L2504	F2394	L2504	L2504	F2394	Q2249	ILE	W2038	F1767	N1605	N1605	K1093
ASN	E2658	N2521	I2397	N2521	N2521	I2397	T2250	GLU	K2041	H1857	P1606	P1606	E1094
ASP	E2664	K2524	F2402	K2524	K2524	F2402	T2251	THR	L2042	I1771	V1607	V1607	D1098
ARG	L2665	K2524	F2402	K2524	K2524	F2402	S2252	ILE	L2043	A1772	D1386	D1386	N1105
GLY	W2679	S2529	E2405	S2529	S2529	E2405	S2252	THR	GLU	S1774	Q1397	Q1397	L1133
ARG	Y2685	Q2531	H2406	Q2531	Q2531	H2406	P2272	ASN	VAL	E1777	T1400	T1400	P1136
R2879	K2713	R2535	N2408	R2535	R2535	N2408	L2274	ASN	ASN	D1898	N1137	N1137	P1136
W2884	A2714	D2540	N2409	D2540	D2540	N2409	L2275	THR	THR	Q1629	R1412	R1412	D1141
W2904	R2715	F2541	T2410	R2715	R2715	T2410	P2277	LYS	LYS	P1631	E1426	E1426	L1144
L2917	L2719	I2546	E2411	L2719	L2719	E2411	L2278	THR	THR	E1632	E1427	E1427	Y1156
P2918	P2720	I2546	T2412	P2720	P2720	T2412	P2279	ASN	SER	E1638	F1444	F1444	I1171
Q2924	Y2721	H2557	V2414	Y2721	Y2721	V2414	K2284	VAL	ASP	K1642	L1463	L1463	L1171
GLN	Q2722	Y2568	N2416	Q2722	Q2722	N2416	C2286	ASN	ASP	L1788	L1478	L1478	Q1234
SER	Q2723	Y2568	E2417	Q2723	Q2723	E2417	D2287	VAL	VAL	F1789	L1473	L1473	L1193
ASN	Y2726	K2573	Q2418	Y2726	Y2726	Q2418	D2288	VAL	VAL	L1791	P1474	P1474	Q1234
ASN	W2729	N2574	F2420	W2729	W2729	F2420	Q2294	MET	MET	K1794	L1478	L1478	T1271
ASN	W2729	N2574	L2421	W2729	W2729	L2421	P2295	SER	SER	C1795	S1490	S1490	E1277
SER	D2744	H2591	V2422	D2744	D2744	V2422	K2296	GLN	SER	L1796	D1491	D1491	E1278
ASN	W2745	H2592	I2429	W2745	W2745	I2429	D2297	ASP	LYS	D1797	H1492	H1492	D1279
ILE	E2748	T2593	I2429	E2748	E2748	I2429	A2298	LEU	SER	A1798	L1503	L1503	L1280
THR	H2752	I2596	R2434	H2752	H2752	R2434	M2299	ASP	ASN	R1799	S1504	S1504	N1298
HIS			T2437			T2437	L2301	ASN	PRQ	K1804			



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 (\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 (\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: CMC, ATP, MG

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	0.25	0/401	0.36	0/535
2	V	0.25	0/934	0.37	0/1251
3	H	0.71	0/2298	0.63	0/3093
3	T	0.25	0/2341	0.42	0/3153
4	A	0.31	0/784	0.40	0/1052
4	O	0.31	0/803	0.39	0/1078
5	B	0.32	0/711	0.45	0/948
5	Q	0.33	0/648	0.45	0/868
6	N	0.30	0/824	0.42	0/1113
6	S	0.30	0/824	0.42	0/1113
7	D	0.32	0/736	0.41	0/991
7	U	0.31	0/730	0.41	0/983
8	P	0.27	0/2347	0.44	0/3171
9	W	0.69	0/4107	0.98	0/6330
10	I	0.69	0/4150	0.96	2/6410 (0.0%)
11	X	0.24	0/83	0.51	0/107
12	E	0.67	0/3527	0.62	0/4769
13	F	0.69	0/3350	0.57	0/4544
14	G	0.57	0/2849	0.54	0/3859
15	K	0.70	0/2036	0.57	0/2739
16	L	0.58	3/29358 (0.0%)	0.58	2/39779 (0.0%)
All	All	0.58	3/63841 (0.0%)	0.63	4/87886 (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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	L	2755	PHE	CB-CG	-5.67	1.41	1.51
16	L	3728	VAL	CB-CG2	-5.26	1.41	1.52
16	L	3512	GLU	CB-CG	-5.12	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	2626	LEU	CB-CG-CD2	-6.70	99.61	111.00
10	I	78	DG	O4'-C4'-C3'	-6.18	102.03	104.50
16	L	3263	LEU	CA-CB-CG	5.95	129.00	115.30
10	I	52	DG	O4'-C1'-N9	5.29	111.70	108.00

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	55	0
3	T	2294	0	2236	75	0
4	A	774	0	813	5	0
4	O	791	0	828	4	0
5	B	703	0	753	13	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	71	0
9	W	3666	0	2018	71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	3695	0	2007	67	0
11	X	82	0	92	2	0
12	E	3448	0	3448	95	0
13	F	3278	0	3238	33	0
14	G	2788	0	2760	28	0
15	K	1989	0	1961	39	0
16	L	28729	0	29144	490	0
17	B	51	0	33	3	0
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	999	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 8.

The worst 5 of 999 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	68
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
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%)	44	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	68
16	L	3489/3744 (93%)	3203 (92%)	284 (8%)	2 (0%)	48	83
All	All	6589/9755 (68%)	6155 (93%)	429 (6%)	5 (0%)	50	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
3	H	256/769 (33%)	256 (100%)	0	100	100
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%)	72 (100%)	0	100	100
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%)	79 (100%)	0	100	100
7	U	78/106 (74%)	78 (100%)	0	100	100
8	P	253/414 (61%)	253 (100%)	0	100	100
11	X	9/9 (100%)	9 (100%)	0	100	100
12	E	379/1054 (36%)	379 (100%)	0	100	100
13	F	367/434 (85%)	367 (100%)	0	100	100
14	G	305/320 (95%)	305 (100%)	0	100	100
15	K	221/441 (50%)	221 (100%)	0	100	100
16	L	3238/3452 (94%)	3218 (99%)	20 (1%)	84	88
All	All	6064/8816 (69%)	6044 (100%)	20 (0%)	90	92

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	L	3486	GLN
16	L	3506	MET
16	L	3728	VAL
16	L	3595	ARG
16	L	3263	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
16	L	2913	ASN
16	L	2941	HIS
16	L	2992	HIS
16	L	1605	ASN
12	E	222	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	$\# Z > 2$
19	ATP	G	502	18	26,33,33	0.69	0	31,52,52	0.82	1 (3%)
17	CMC	B	501	5	45,53,54	0.58	0	55,78,80	0.77	1 (1%)
19	ATP	F	1002	18	26,33,33	0.74	0	31,52,52	0.76	1 (3%)

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
19	ATP	G	502	18	-	0/18/38/38	0/3/3/3
17	CMC	B	501	5	-	6/46/67/68	0/3/3/3
19	ATP	F	1002	18	-	4/18/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	B	501	CMC	C5A-C6A-N6A	2.35	123.93	120.35
19	G	502	ATP	C5-C6-N6	2.27	123.80	120.35
19	F	1002	ATP	C5-C6-N6	2.26	123.79	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

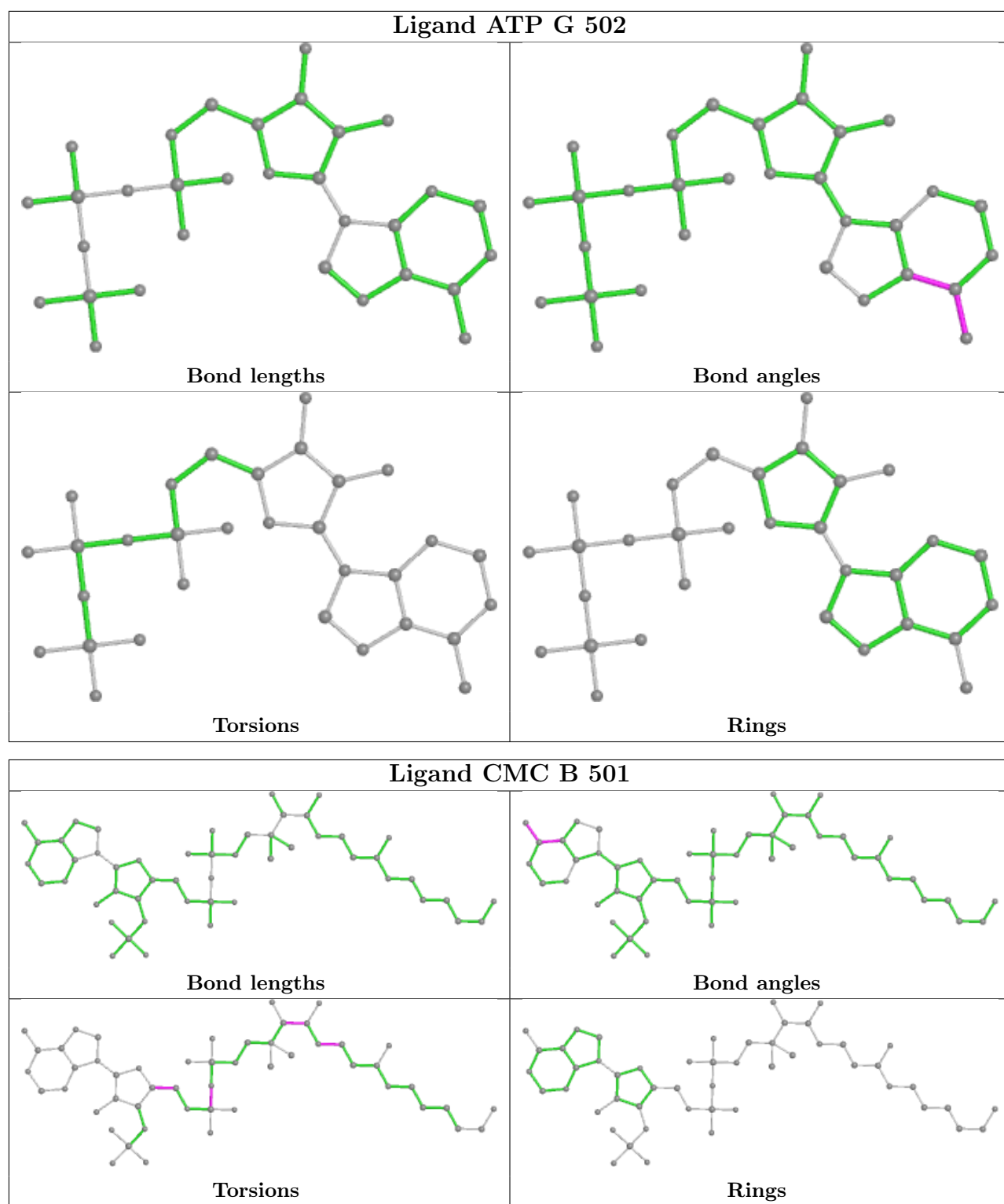
Mol	Chain	Res	Type	Atoms
17	B	501	CMC	O4B-C4B-C5B-O5B
17	B	501	CMC	C3B-C4B-C5B-O5B
17	B	501	CMC	P2A-O3A-P1A-O1A
17	B	501	CMC	C6P-C7P-N8P-C9P
19	F	1002	ATP	C5'-O5'-PA-O3A

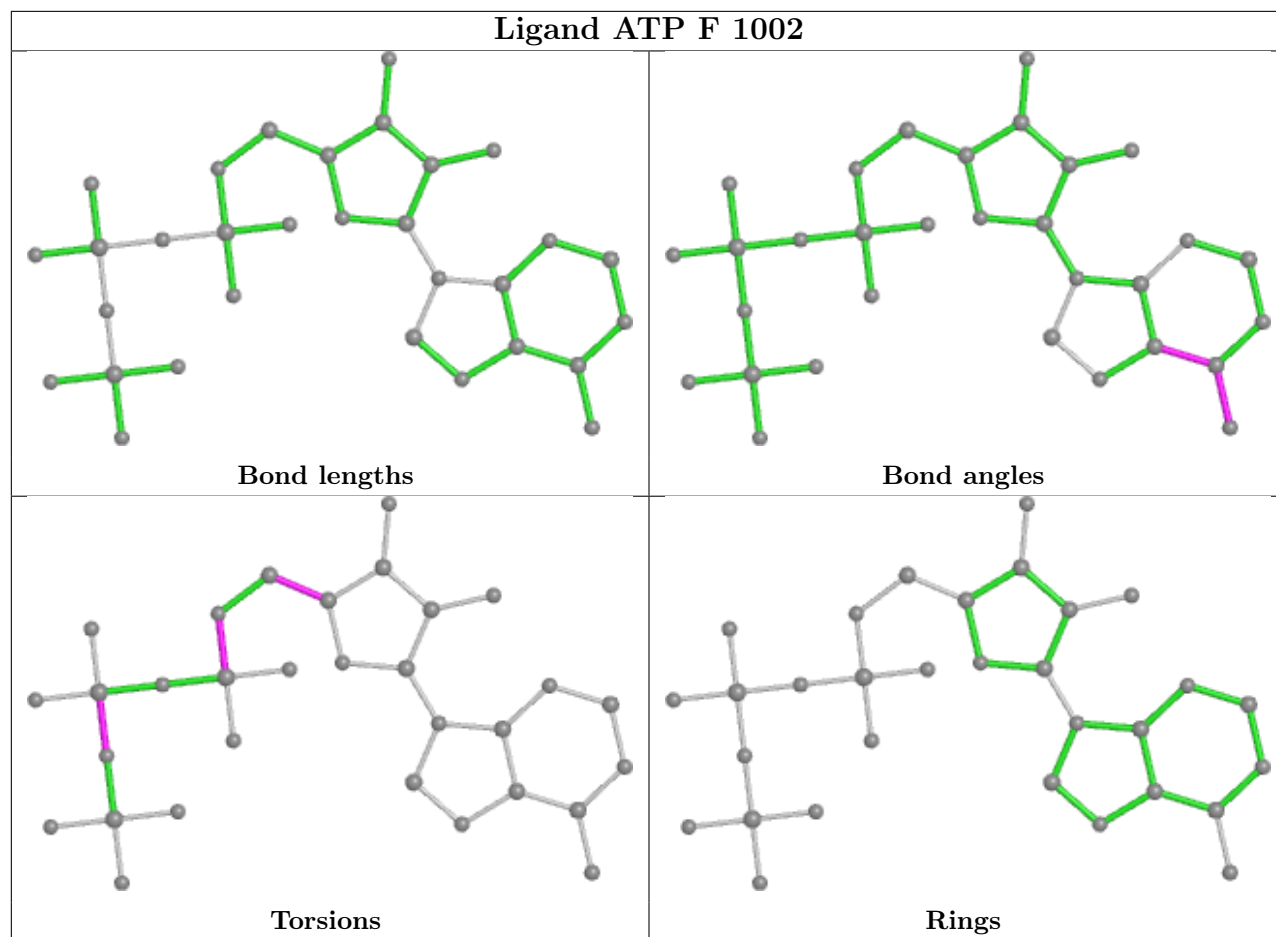
There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

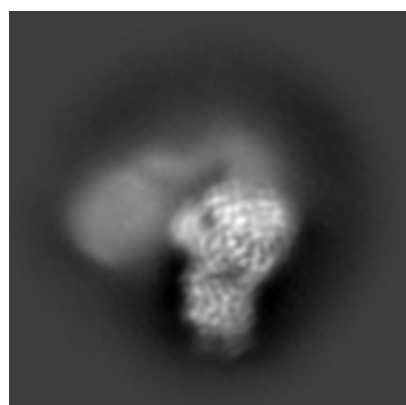
6 Map visualisation [i](#)

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.

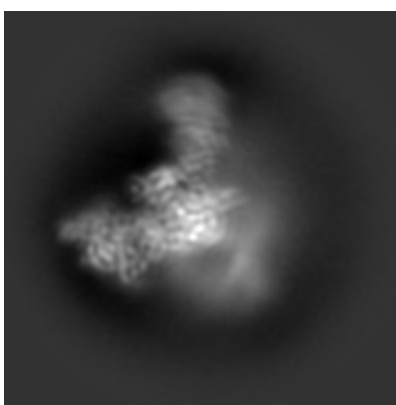
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

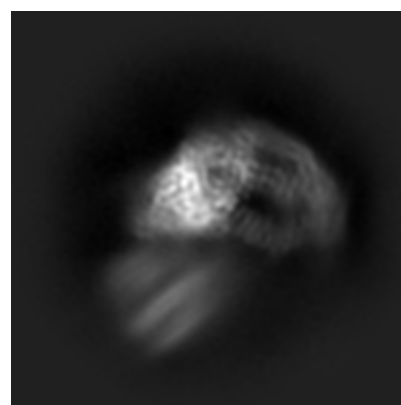
6.1.1 Primary map



X



Y

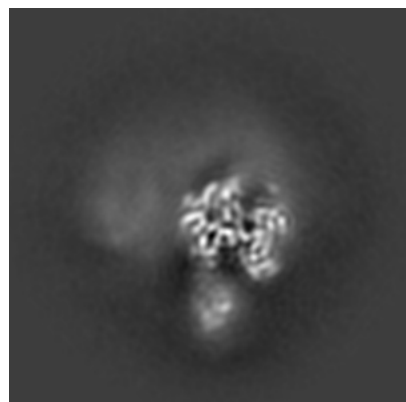


Z

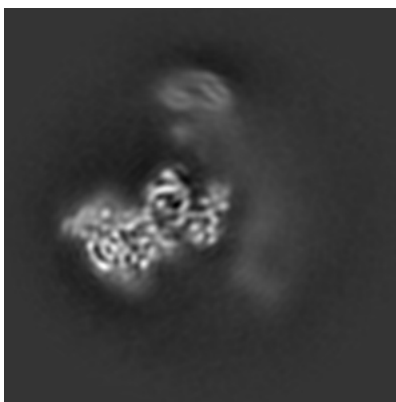
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

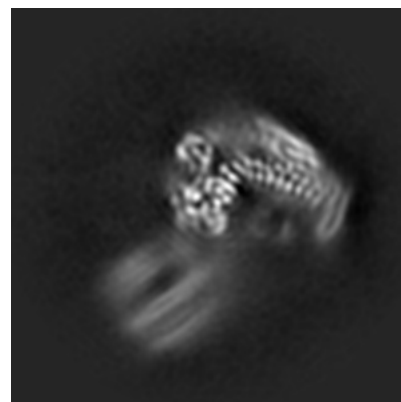
6.2.1 Primary map



X Index: 47



Y Index: 47

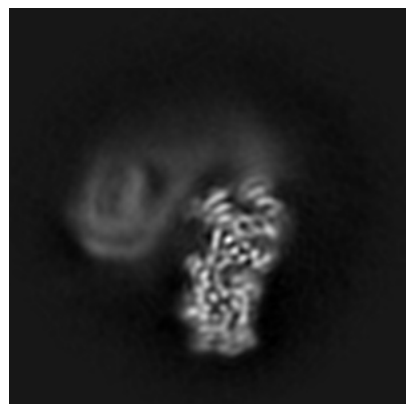


Z Index: 47

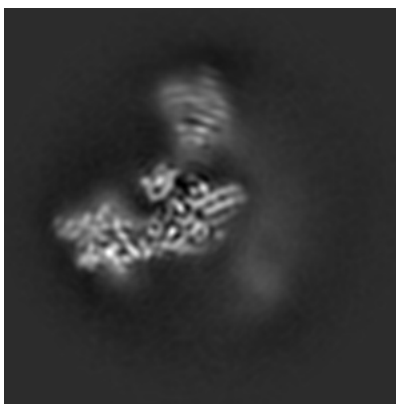
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

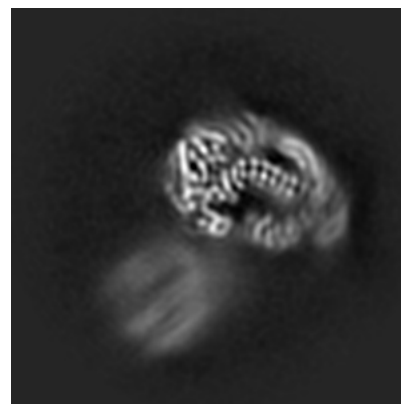
6.3.1 Primary map



X Index: 41



Y Index: 51

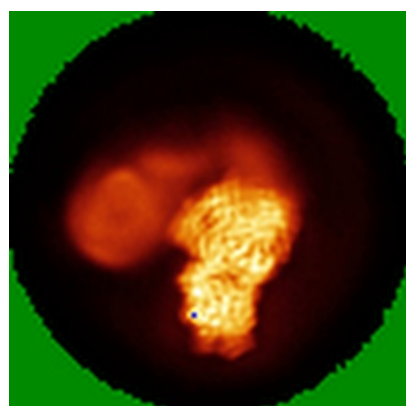


Z Index: 44

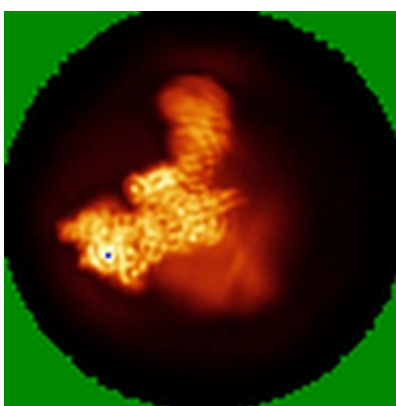
The images above show the largest variance slices of the map in three orthogonal directions.

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

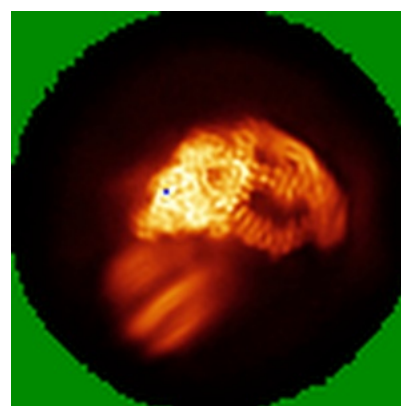
6.4.1 Primary map



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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

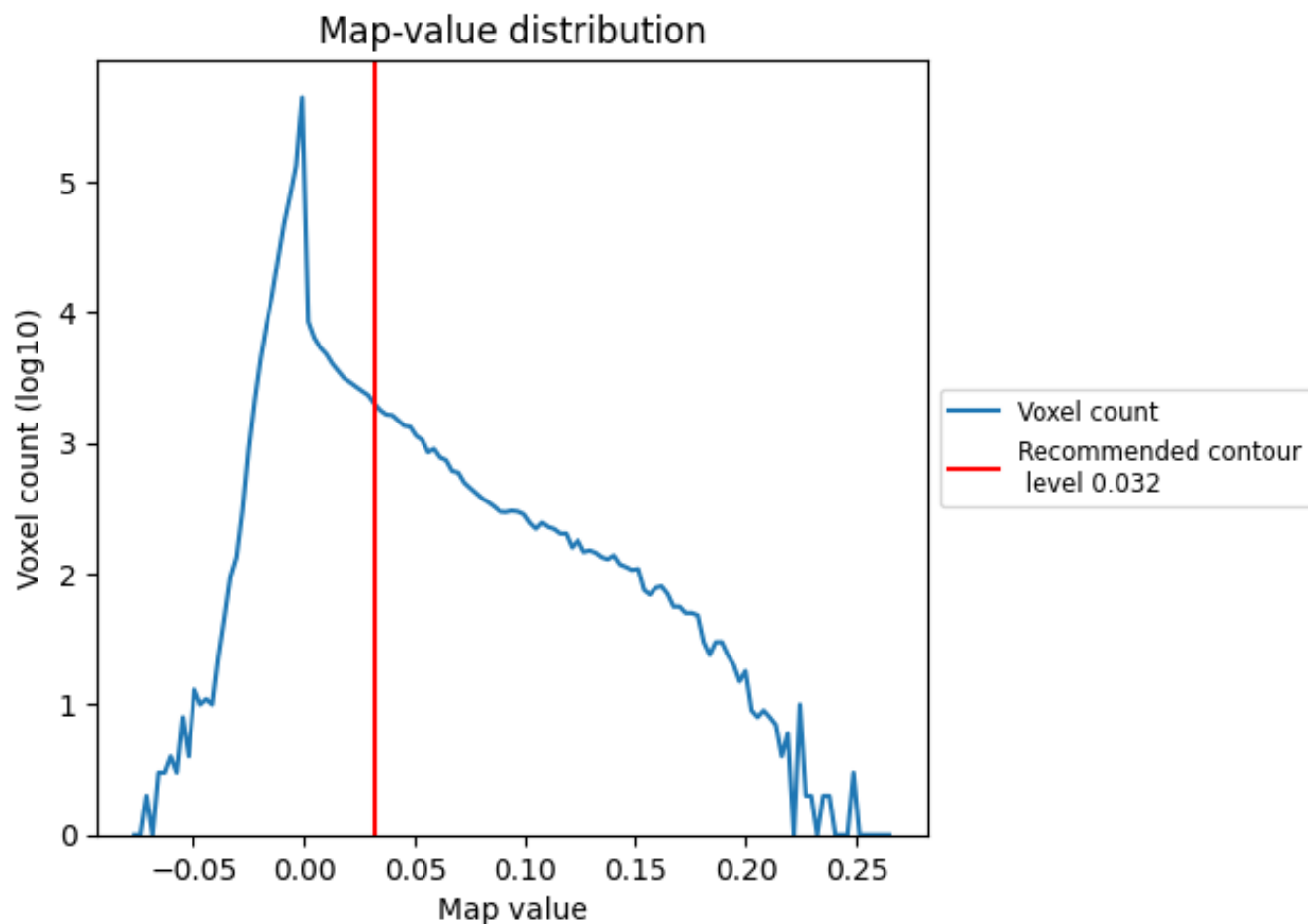
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

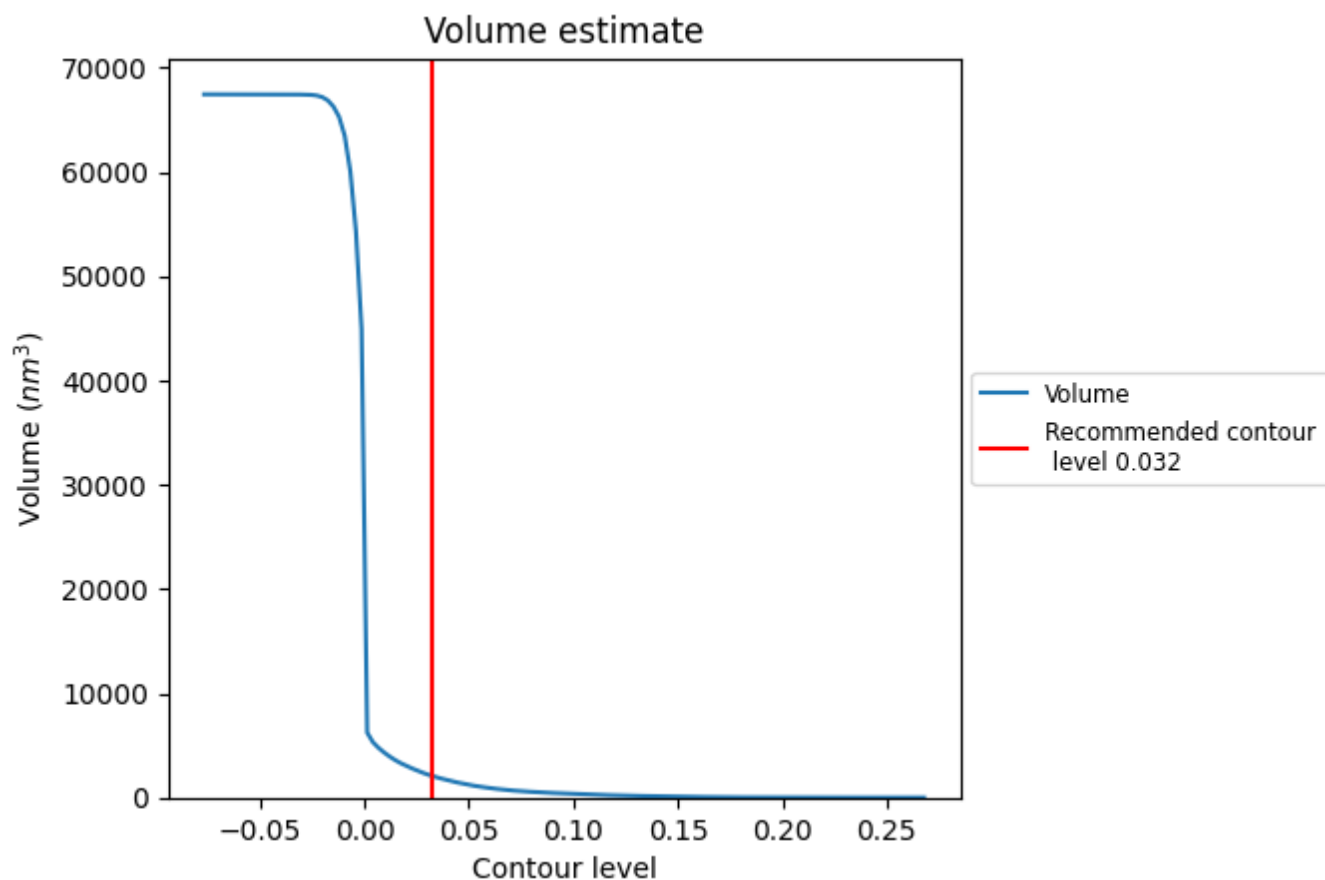
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

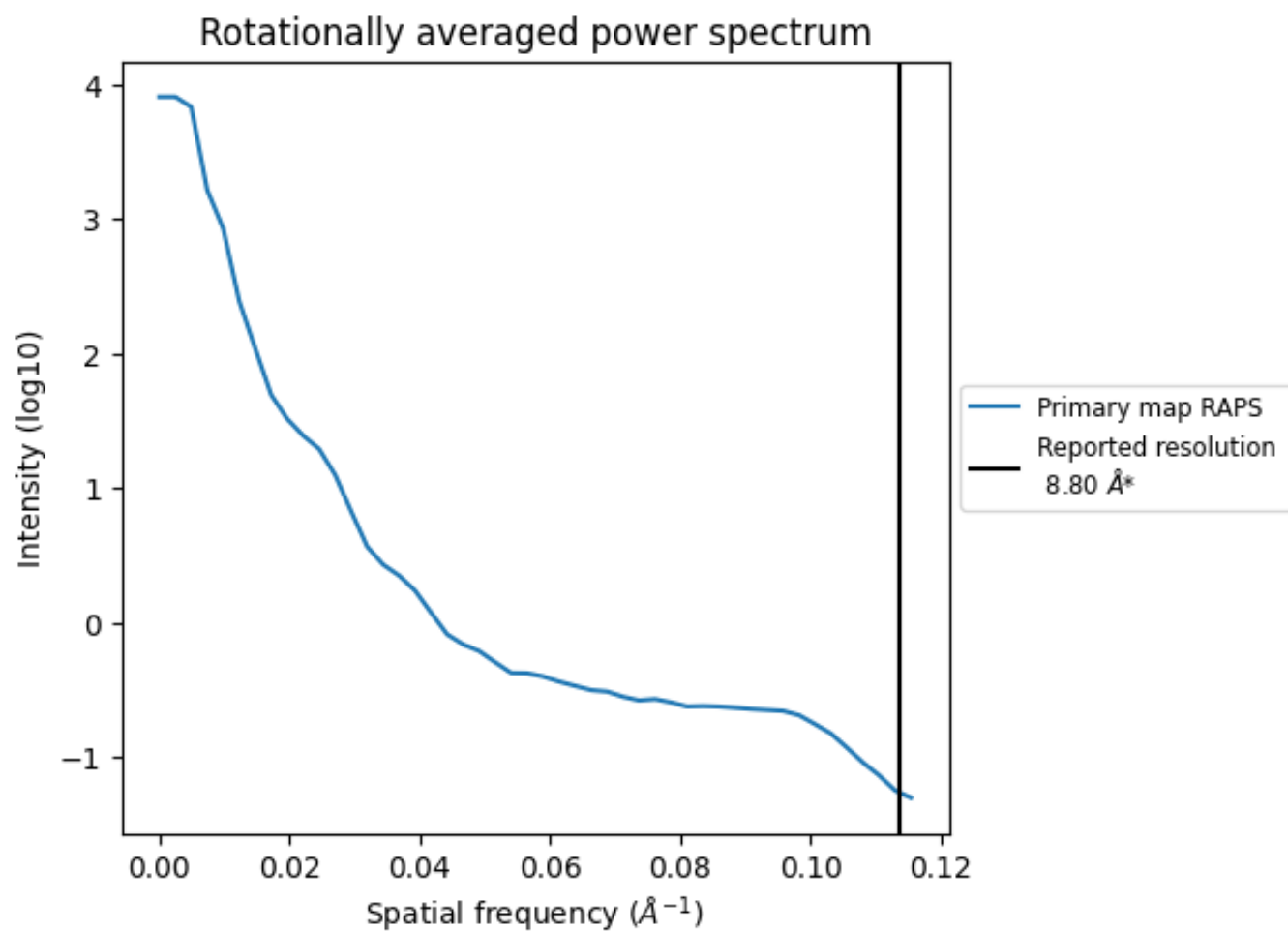
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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

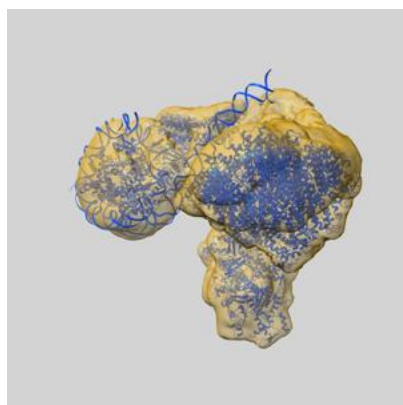
8 Fourier-Shell correlation

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

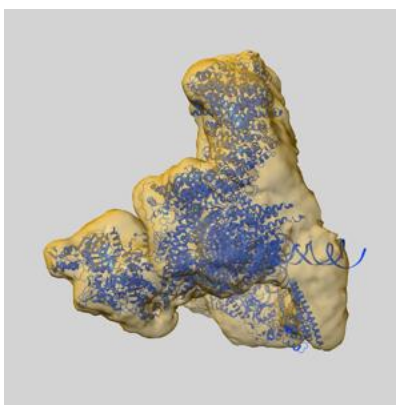
9 Map-model fit [i](#)

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.

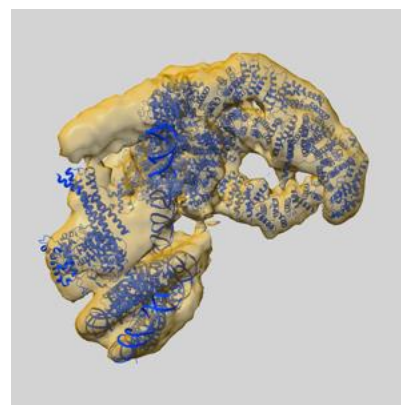
9.1 Map-model overlay [i](#)



X



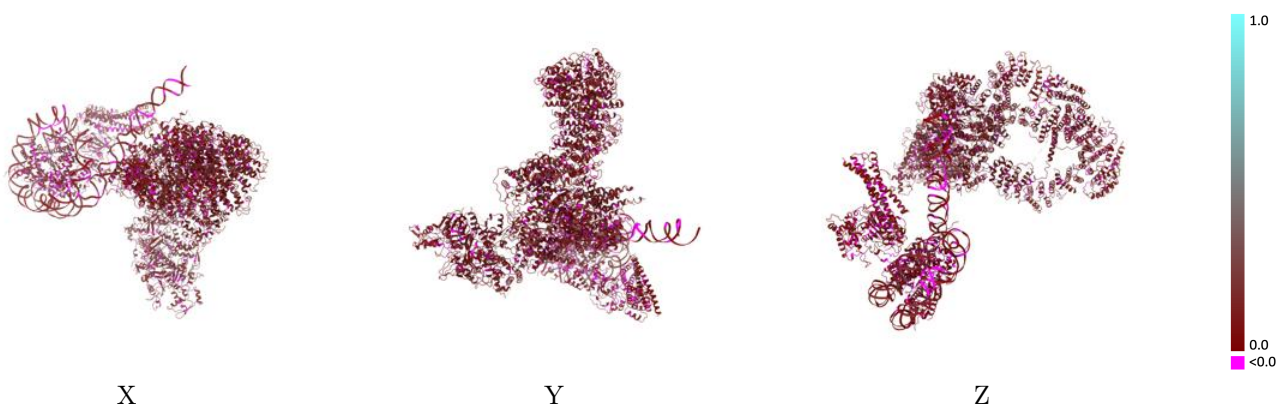
Y



Z

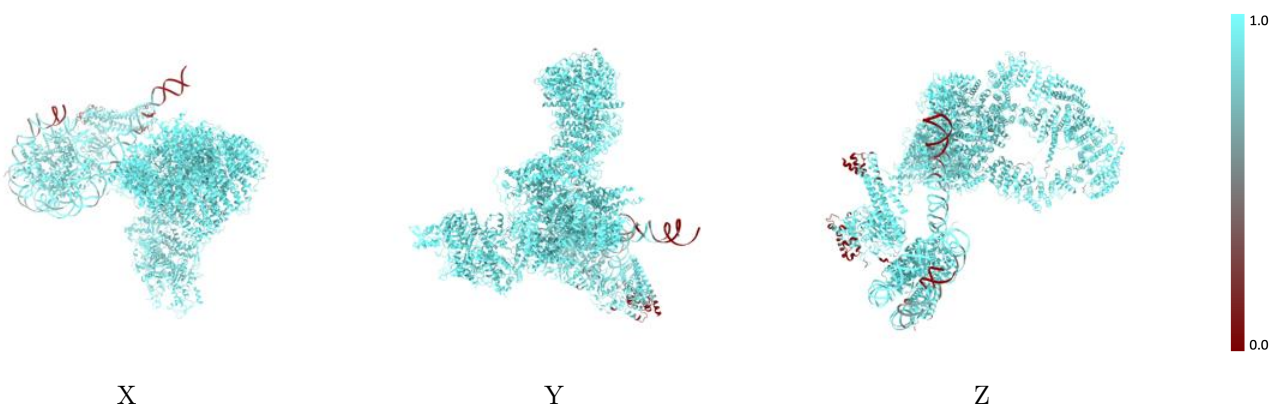
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



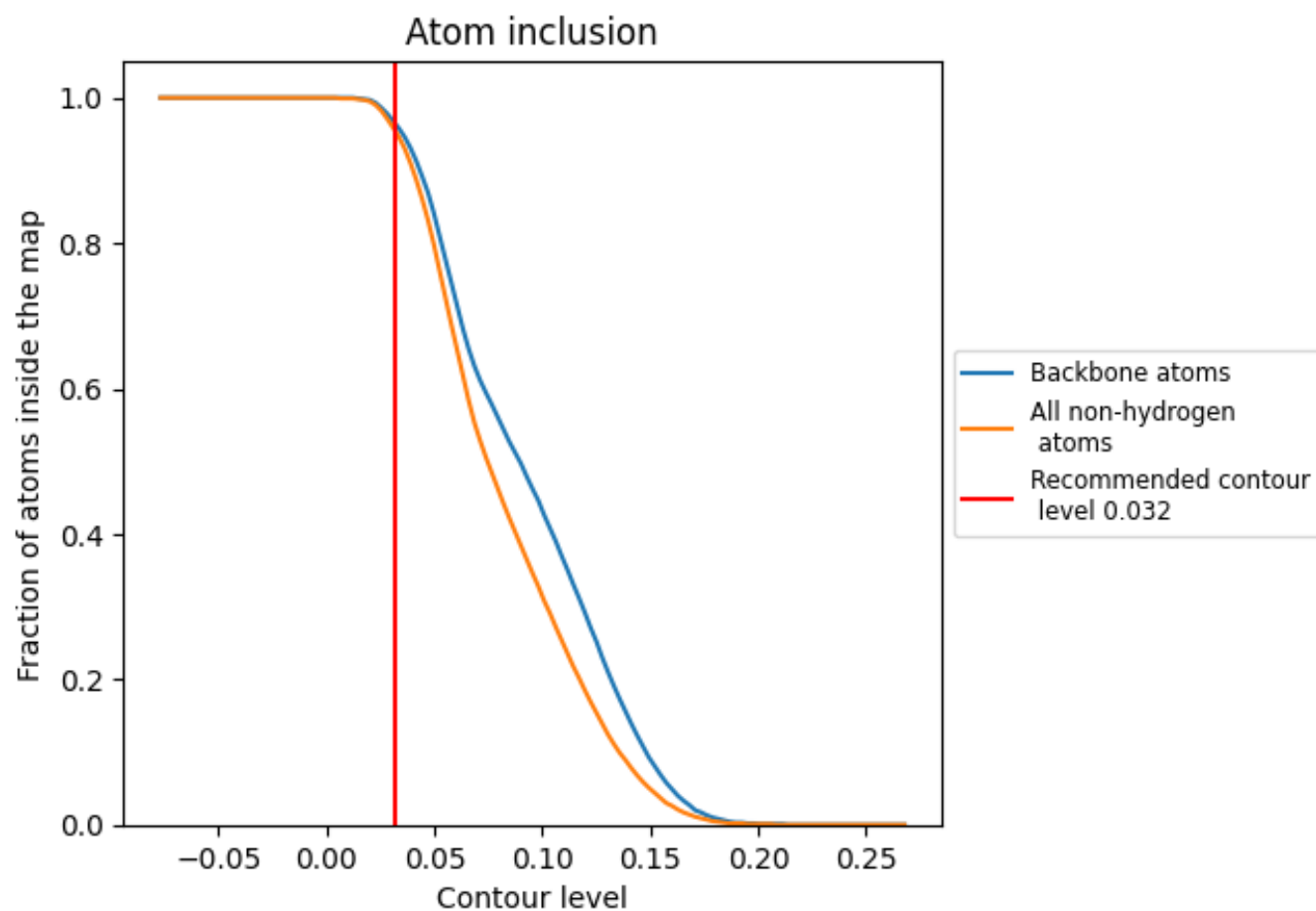
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

