wwPDB EM Validation Summary Report (i)

Jul 3, 2024 – 06:47 am BST

PDB ID	:	7NPN
EMDB ID	:	EMD-12516
Title	:	B-brick bare in 5 mM Mg2+
Authors	:	Bertosin, E.; Stoemmer, P.; Feigl, E.; Wenig, M.; Honemann, M.; Dietz, H.
Deposited on	:	2021-02-27
Resolution	:	10.38 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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 10.38 Å.

There are no overall percentile quality scores available for this entry.

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 <=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	AA	2873	59% 34% 7%
2	AB	34	68% 29% •
3	AC	48	65% 29% 6%
4	AD	34	62% 35% •
5	AE	41	63% 32% 5%
6	AF	41	68% 29% •
7	AG	34	56% 35% 9%
8	AH	42	50% 43% 7%
9	AI	28	54% 46%
10	AJ	34	12% 47% 41% 12%
11	AK	42	57% 36% 7%
12	AL	42	57% 33% 10%
13	AM	42	57% 40% •
14	AN	42	64% 33% •
15	AO	49	61% 37% •
16	AP	49	73% 22% •
17	AQ	28	• 50% 50%

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Mol	Chain	Length	Quality of chain
18	AR	28	54% 43% •
19	AS	42	• 57% 38% 5%
20	AT	52	65% 33% •
21	AU	49	65% 22% 12%
22	AV	52	56% 42% •
23	AW	42	64% 33% •
24	AX	38	55% 45%
25	AY	31	71% 19% 10%
26	AZ	49	63% 29% 8%
27	Aa	41	71% 27% •
28	Ab	42	52% 43% 5%
29	Ac	42	64% 29% 7%
30	Ad	34	• 68% 29% •
31	Ae	41	• 66% 29% 5%
32	Af	42	64% 31% 5%
33	Ag	28	61% 36% •
34	Ah	34	50% 41% 9%
35	Ai	49	63% 35% •
36	Aj	42	81% 14% 5%
37	Ak	59	• 69% 25% 5%
38	Al	42	64% 29% 7%
39	Am	42	64% 24% 12%
40	An	42	62% 33% 5%
41	Ao	28	43% 50% 7%
42	Ap	28	46% 54%

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Mol	Chain	Length	Quality of chain
43	Aq	41	5% 66% 29% 5%
44	Ar	52	69% 25% 6%
45	As	49	59% 39% •
46	At	52	67% 31% •
47	Au	52	• 73% 23% •
48	Av	42	64% 31% 5%
49	Aw	42	69% 24% 7%
50	Ax	42	45% 45% 10%
51	Ay	41	56% 37% 7%
52	Az	35	57% 37% 6%
53	A0	41	76% 22% •
54	A1	45	7% 62% 31% 7%
55	A2	34	• 53% 44% •
56	A3	41	56% 32% 12%
57	A4	42	74% 24% •
58	A5	31	61% 35% •
59	A6	28	68% 25% 7%
60	A7	34	• 62% 38%
61	A8	34	68% 32%
62	A9	42	64% 33% •
63	BA	35	63% 26% 11%
64	BB	45	58% 38% •
65	BC	35	57% 34% 9%
66	BD	28	• 71% 25% •
67	BE	28	64% 36%

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Mol	Chain	Length	Quality of chain
68	BF	41	5% 51% 44% 5%
69	BG	35	54% 40% 6%
70	BH	42	76% 21% •
71	BI	42	69% 26% 5%
72	BJ	45	62% 36% •
73	BK	31	77% 23%
74	BL	42	67% 31% •
75	BM	49	59% 29% 12%
76	BN	41	59% 29% 12%
77	BO	42	71% 24% 5%
78	BP	34	• 59% 38% •
79	BQ	37	62% 35% •

2 Entry composition (i)

There are 79 unique types of molecules in this entry. The entry contains 122511 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 DNA chain called SCAFFOLD STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	2873	58849	28004	10702	17271	2872	0	0

- Molecule 2 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	34	691	331	125	202	33	0	0

- Molecule 3 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AC	48	967	464	160	296	47	0	0

- Molecule 4 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	AD	34	702	337	134	198	33	0	0

- Molecule 5 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	AE	41	838	400	155	243	40	0	0

- Molecule 6 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	AF	41	831	398	145	248	40	0	0

- Molecule 7 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	AG	34	688	331	119	205	33	0	0

- Molecule 8 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	AH	42	857	409	149	258	41	0	0

- Molecule 9 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AI	28	575	275	109	164	27	0	0

- Molecule 10 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	AJ	34	674	329	94	218	33	0	0

- Molecule 11 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AK	42	859	413	151	254	41	0	0

- Molecule 12 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
12	AL	42	865	411	162	251	41	0	0

- Molecule 13 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
13	AM	42	864	412	161	250	41	0	0

- Molecule 14 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
14	AN	42	877	410	184	242	41	0	0

- Molecule 15 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	AO	49	1007	478	194	287	48	0	0

- Molecule 16 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
16	AP	49	999	479	178	294	48	0	0

- Molecule 17 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
17	AQ	28	561	271	86	177	27	0	0

- Molecule 18 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
18	AR	28	564	273	90	174	27	0	0

- Molecule 19 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
19	AS	42	857	412	143	261	41	0	0

- Molecule 20 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	AT	52	1049	503	181	314	51	0	0

- Molecule 21 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	AU	49	1011	479	187	297	48	0	0

- Molecule 22 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	AV	52	1064	507	195	311	51	0	0

- Molecule 23 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	AW	42	860	408	165	246	41	0	0

- Molecule 24 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
24	AX	38	762	369	117	239	37	0	0

- Molecule 25 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	AY	31	628	304	107	187	30	0	0

- Molecule 26 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	AZ	49	1000	478	185	289	48	0	0

- Molecule 27 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	Aa	41	832	398	163	231	40	0	0

- Molecule 28 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
28	Ab	42	856	407	163	245	41	0	0

- Molecule 29 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
29	Ac	42	860	410	154	255	41	0	0

- Molecule 30 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	Ad	34	697	337	116	211	33	0	0

- Molecule 31 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	Ae	41	826	401	130	255	40	0	0

- Molecule 32 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	Af	42	865	415	155	254	41	0	0

- Molecule 33 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
33	Ag	28	569	275	94	173	27	0	0

- Molecule 34 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	Ah	34	688	336	105	214	33	0	0

- Molecule 35 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
35	Ai	49	1007	481	194	284	48	0	0

- Molecule 36 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
36	Aj	42	851	407	154	249	41	0	0

- Molecule 37 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
37	Ak	59	1199	574	203	364	58	0	0

- Molecule 38 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	Al	42	861	409	170	241	41	0	0

- Molecule 39 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	Am	42	862	410	163	248	41	0	0

- Molecule 40 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	An	42	862	411	159	251	41	0	0

- Molecule 41 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	Ao	28	573	274	104	168	27	0	0

- Molecule 42 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	Ap	28	569	276	90	176	27	0	0

- Molecule 43 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
43	Aq	41	832	400	140	252	40	0	0

- Molecule 44 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	Ar	52	1052	510	165	326	51	0	0

- Molecule 45 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
45	As	49	985	470	169	298	48	0	0

- Molecule 46 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	At	52	1067	507	192	317	51	0	0

- Molecule 47 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	Au	52	1063	507	198	307	51	0	0

- Molecule 48 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	Av	42	849	404	160	244	41	0	0

- Molecule 49 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	Aw	42	872	409	179	243	41	0	0

- Molecule 50 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	Ax	42	859	407	163	248	41	0	0

- Molecule 51 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
51	Ay	41	841	402	150	249	40	0	0

- Molecule 52 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	Az	35	717	339	141	203	34	0	0

- Molecule 53 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	A0	41	840	401	151	248	40	0	0

- Molecule 54 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	A1	45	923	439	167	273	44	0	0

- Molecule 55 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	A2	34	697	338	115	211	33	0	0

- Molecule 56 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	A3	41	835	404	136	255	40	0	0

- Molecule 57 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	A4	42	852	409	158	244	41	0	0

- Molecule 58 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	A5	31	627	302	115	180	30	0	0

- Molecule 59 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	A6	28	573	277	95	174	27	0	0

- Molecule 60 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
60	A7	34	682	331	104	214	33	0	0

- Molecule 61 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
61	A8	34	697	335	127	202	33	0	0

- Molecule 62 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
62	A9	42	867	413	166	247	41	0	0

- Molecule 63 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
63	BA	35	708	337	137	200	34	0	0

- Molecule 64 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
64	BB	45	909	441	153	271	44	0	0

- Molecule 65 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
65	BC	35	725	346	137	208	34	0	0

- Molecule 66 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
66	BD	28	570	277	92	174	27	0	0

- Molecule 67 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
67	BE	28	573	280	86	180	27	0	0

- Molecule 68 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
68	BF	41	827	401	124	262	40	0	0

- Molecule 69 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
69	BG	35	712	344	124	210	34	0	0

- Molecule 70 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
70	BH	42	863	413	160	249	41	0	0

- Molecule 71 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
71	BI	42	873	415	182	235	41	0	0

- Molecule 72 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
72	BJ	45	924	445	161	274	44	0	0

- Molecule 73 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
73	BK	31	633	305	112	186	30	0	0

- Molecule 74 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
74	BL	42	852	405	153	253	41	0	0

- Molecule 75 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
75	BM	49	1002	477	195	282	48	0	0

- Molecule 76 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
76	BN	41	840	401	151	248	40	0	0

- Molecule 77 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
77	BO	42	852	412	143	256	41	0	0

- Molecule 78 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
78	BP	34	687	335	103	216	33	0	0

- Molecule 79 is a DNA chain called STAPLE STRAND.

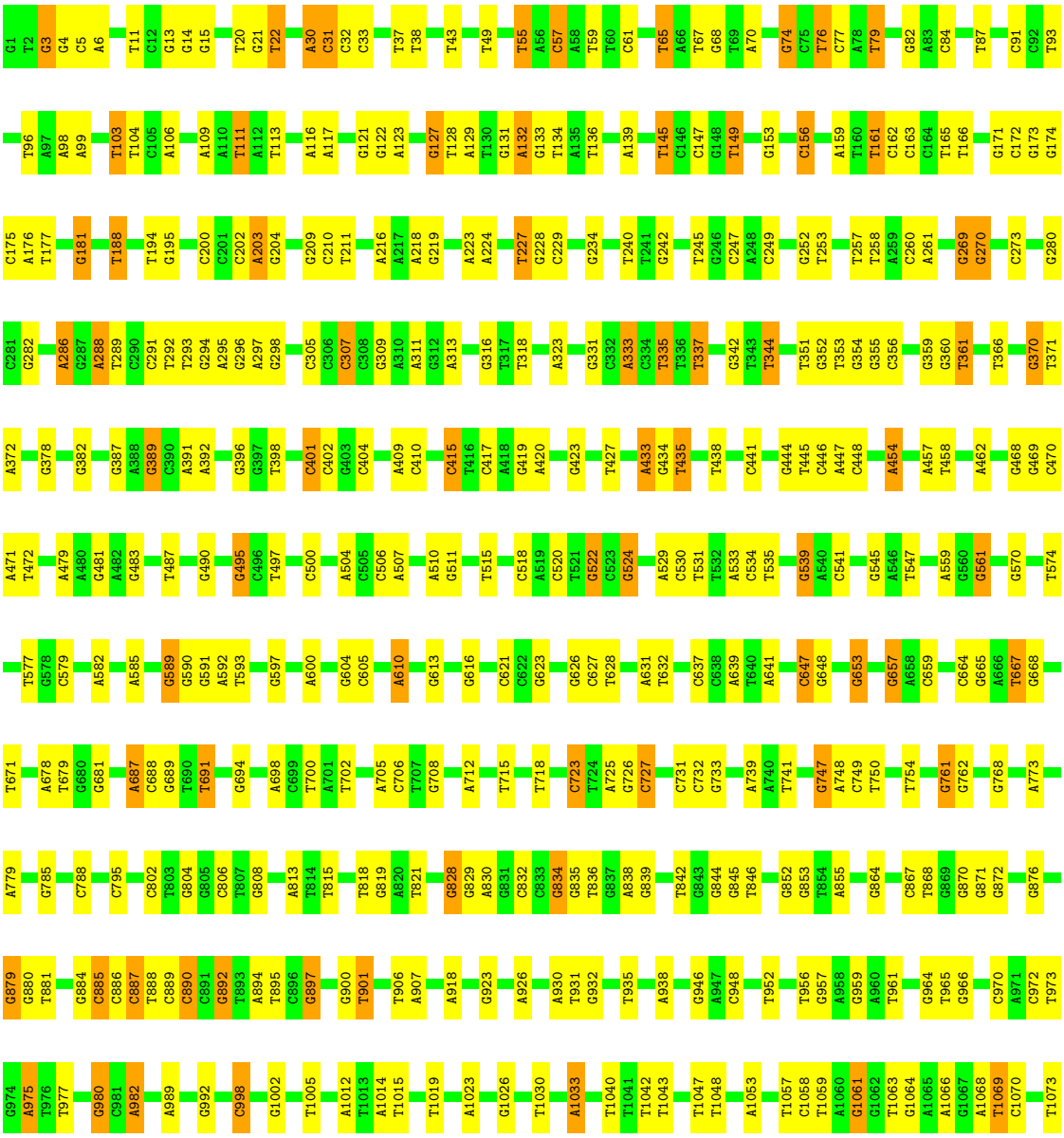
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
79	BQ	37	755	362	133	224	36	0	0

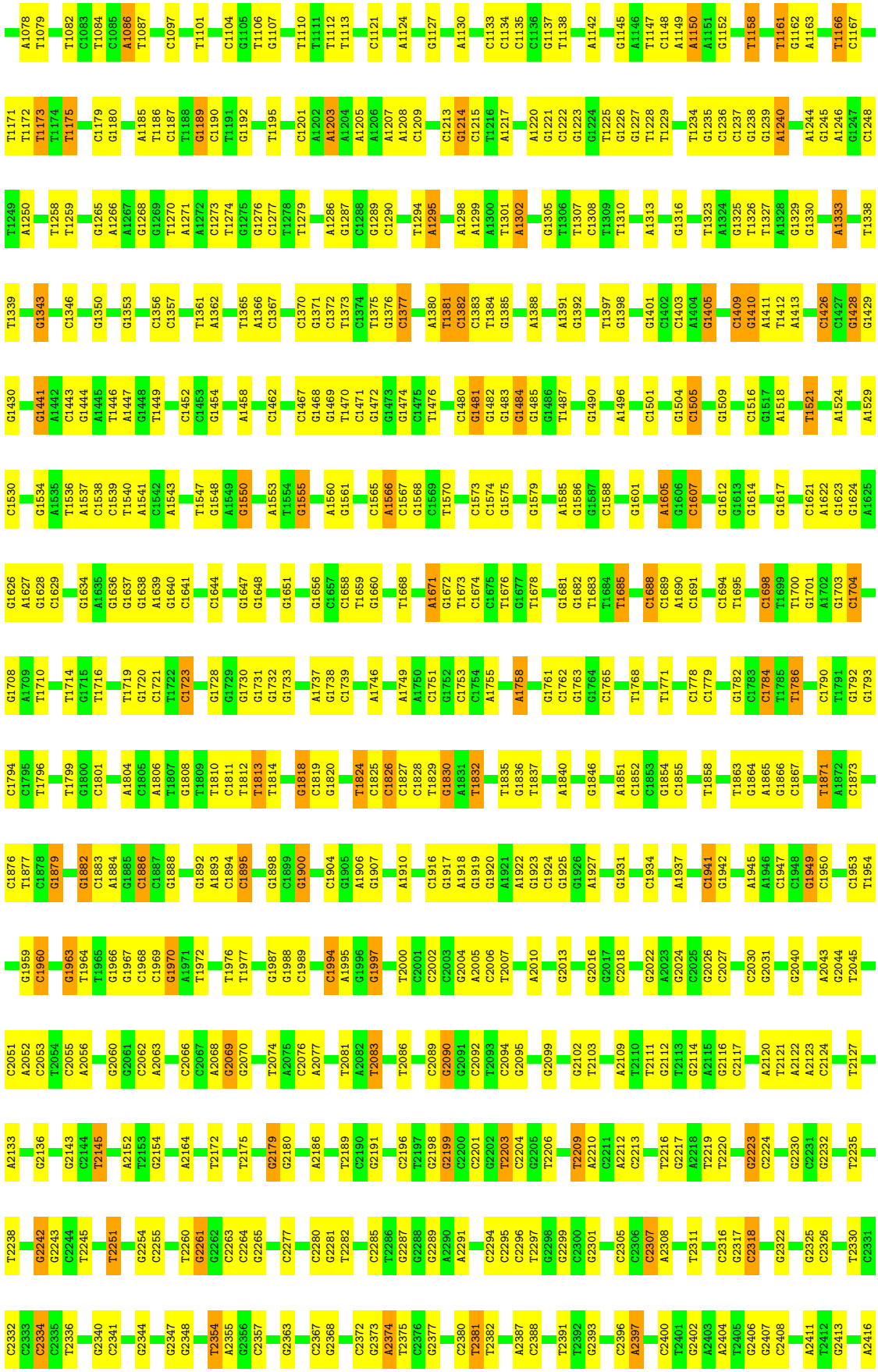
3 Residue-property plots (i)

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: SCAFFOLD STRAND

Chain AA: 59% 34% 7%

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T1082 C1083 T1084 C1085 A1086 T1087
C1097
T1101
C1104 G1105 T1106 G1107
T1110 T1111 T1112 T1113
C1121
A1124
G1127
A1130
C1133 C1134 C1135 C1136 G1137 T1138
A1142
G1145 A1146 T1147 C1148 A1149 A1150 A1151 G1152
T1158
T1161 G1162 A1163
T1166 C1167
T1171 T1172 T1173 T1174 T1175
C1179 G1180
A1185 T1186 C1187 T1188 G1189 C1190
T1191 G1192
T1195
C1201 A1202 A1203 A1204 A1205 A1206 A1207 A1208 C1209
C1213 G1214 C1215
T1216 A1217
A1220 G1221 C1222 G1223 G1224 T1225 G1226 G1227 T1228 T1229
T1234 G1235 C1236 C1237 G1238 G1239
A1240
A1244 G1245 A1246 G1247 C1248
T1249 A1250
T1258 T1259
G1265 A1266 A1267 G1268 G1269 T1270 A1271 A1272 C1273 T1274 G1275 G1276 C1277 T1278 T1279
A1286 A1287 C1288 G1289 C1290
T1294 A1295
A1298 A1299 A1300 T1301 A1302
G1305 T1306 T1307 C1308 T1309 T1310
A1313
G1316
T1323 A1324 G1325 T1326 T1327 A1328 G1329 G1330
A1333
T1338
T1339 G1343
C1346
G1350
G1353
C1356 C1357
T1361 A1362
T1365 A1366 C1367
C1370 G1371 C1372 T1373 C1374 T1375 G1376 C1377
A1380 T1381 C1382 C1383 T1384 G1385
A1388
A1391 G1392
T1397 G1398
G1401 C1402 C1403 A1404 G1405
C1409 G1410 A1411 T1412 A1413
C1426 C1427 G1428 G1429
G1430 G1441 A1442 C1443 G1444 A1445 T1446 A1447 G1448 T1449
C1452 C1453 G1454
A1458
C1462
C1467 G1468 G1469 T1470 C1471 G1472 G1473 G1474 C1475 T1476
C1480 G1481 G1482 G1483 G1484 G1485 G1486 T1487
G1490
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G1504 C1505
G1509
C1516 G1517 A1518
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A1524
A1529
C1530 G1534 A1535 T1536 A1537 C1538 C1539 T1540 A1541 C1542 A1543
T1547 G1548 A1549 G1550
A1553 T1554 G1555
A1560 G1561
C1565 A1566 C1567 G1568 C1569 T1570
C1573 C1574 G1575
G1579
A1585 G1586 G1587 C1588
G1601
A1605 G1606 C1607
G1612 G1613 G1614
G1617
C1621 A1622 G1623 G1624 A1625
G1626 A1627 G1628 C1629
G1634 A1635 G1636 G1637 G1638 A1639 G1640 C1641
C1644
G1647 G1648
G1651
G1656 C1657 C1658 T1659 G1660
T1668
A1671 G1672 T1673 C1674 C1675 T1676 G1677 T1678
G1681 G1682 T1683 T1684 T1685
C1688 C1689 A1690 C1691
C1694 T1695
C1698 T1699 T1700 G1701 A1702 G1703 C1704
G1708 A1709 T1710
T1714 G1715 T1716
T1719 G1720 C1721 T1722 C1723
G1728 G1729 G1730 G1731 G1732 G1733
A1737 G1738 C1739
A1746
A1749 A1750 C1751 G1752 C1753 C1754 A1755
A1758
G1761 C1762 G1763 G1764 C1765
T1768
T1771
C1778 C1779
G1782 C1783 C1784 T1785 T1786
C1790 T1791 G1792 G1793
C1794 C1795 T1796
T1799 G1800 C1801
A1804 C1805 A1806 T1807 G1808 T1809 T1810 C1811 T1812 T1813 T1814
G1818 C1819 G1820
T1824 C1825 C1826
C1827 C1828 T1829 G1830 A1831 T1832
T1835 G1836 T1837
A1840
G1846
A1851 C1852 C1853 G1854 C1855
T1858
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C1876 T1877 C1878 G1879
G1882 C1883 A1884 C1885 C1886 C1887 G1888
G1892 A1893 C1894 C1895
G1898 C1899 G1900
C1904 C1905 A1906 G1907
A1910
C1916 G1917 A1918 G1919 G1920 A1921 A1922 G1923 C1924 G1925 G1926 A1927
G1931
C1934
A1937
C1941 G1942
A1945 A1946 C1947 C1948 G1949 C1950
C1953 T1954
G1959 C1960
G1963 T1964 T1965 G1966 G1967 G1968 C1969 G1970 A1971 T1972
T1976 T1977
G1987 G1988 C1989
C1994 A1995 G1996 G1997
T2000 C2001 C2002 C2003 G2004 A2005 C2006 T2007
A2010
G2013
G2016 G2017 C2018
G2022 A2023 G2024 C2025 G2026 C2027
C2030 G2031
G2040
A2043 G2044 T2045
C2051 A2052 C2053 T2054 C2055 A2056
G2060 G2061 C2062 A2063
C2066 C2067 A2068 G2069 G2070
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T2081 A2082 T2083
T2086
C2089 G2090 G2091 C2092 T2093 C2094 G2095
G2099
G2102 T2103
A2109 T2110 T2111 G2112 T2113 G2114 A2115 G2116 C2117
A2120 T2121 A2122 A2123 C2124
T2127
A2133 G2136
G2143 C2144 T2145
A2152 T2153 G2154
A2164
T2172
T2175
G2179 G2180
A2186
T2189 C2190 G2191
C2196 T2197 G2198 G2199 C2200 C2201 G2202 T2203 C2204 G2205 T2206
T2209 A2210 C2211 A2212 C2213
T2216 G2217 A2218 T2219 T2220
G2223 C2224
G2230 C2231 G2232
T2235
T2238 G2242 G2243 C2244 T2245
T2251
G2254 C2255
T2260 G2261 G2262 C2263 C2264 G2265
C2277
C2280 G2281 T2282
C2285 T2286 G2287 G2288 G2289 A2290 A2291
C2294 C2295 C2296 T2297 G2298 G2299 C2300 G2301
C2305 C2306 C2307 A2308
T2311
C2316 G2317 C2318
G2322
G2325 C2326
T2330 G2331
C2332 G2333 C2334 C2335 T2336
G2340 C2341
G2344
G2347 G2348
T2354 A2355 G2356 C2357
G2363
C2367 G2368
C2372 G2373 A2374 T2375 C2376 G2377
C2380 T2381 T2382
A2387 C2388
T2391 T2392 G2393
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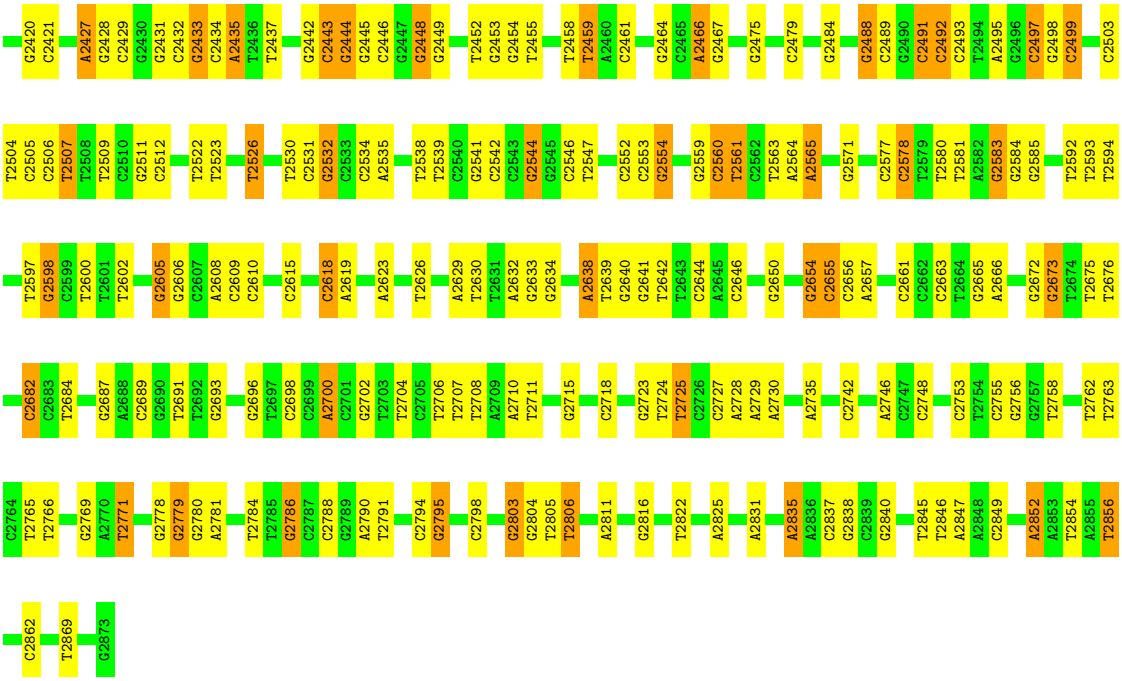
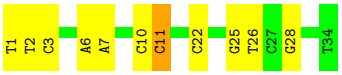
A2411 T2412 G2413
A2416



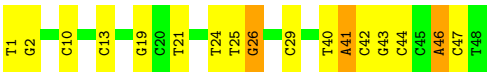
- Molecule 2: STAPLE STRAND

Chain AB:



- Molecule 3: STAPLE STRAND

Chain AC:

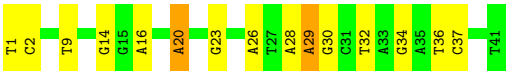


- Molecule 4: STAPLE STRAND

Chain AD:

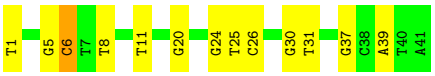
- Molecule 5: STAPLE STRAND

Chain AE:



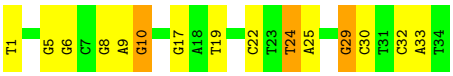
- Molecule 6: STAPLE STRAND

Chain AF: 68% 29% •



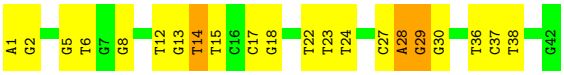
• Molecule 7: STAPLE STRAND

Chain AG: 56% 35% 9%



• Molecule 8: STAPLE STRAND

Chain AH: 50% 43% 7%

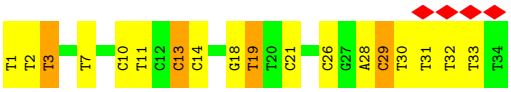


• Molecule 9: STAPLE STRAND

Chain AI: 54% 46%

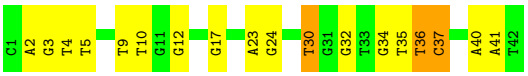
• Molecule 10: STAPLE STRAND

Chain AJ: 12% 47% 41% 12%



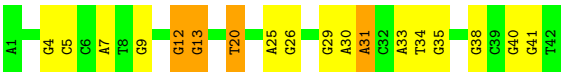
• Molecule 11: STAPLE STRAND

Chain AK: 57% 36% 7%



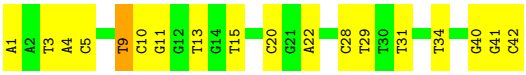
• Molecule 12: STAPLE STRAND

Chain AL: 57% 33% 10%



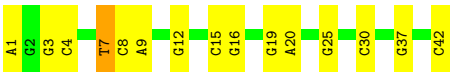
• Molecule 13: STAPLE STRAND

Chain AM: 57% 40% •



• Molecule 14: STAPLE STRAND

Chain AN:

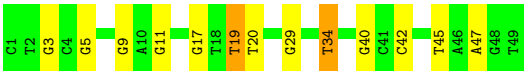


• Molecule 15: STAPLE STRAND

Chain AO:

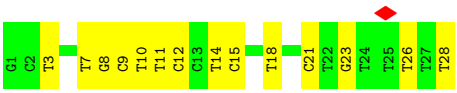
• Molecule 16: STAPLE STRAND

Chain AP:



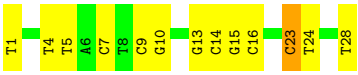
• Molecule 17: STAPLE STRAND

Chain AQ:



• Molecule 18: STAPLE STRAND

Chain AR:

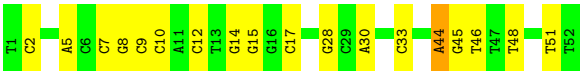


• Molecule 19: STAPLE STRAND

Chain AS:

• Molecule 20: STAPLE STRAND

Chain AT:



• Molecule 21: STAPLE STRAND

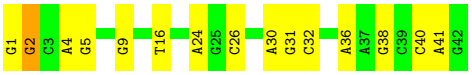
Chain AU:

• Molecule 22: STAPLE STRAND

Chain AV:

• Molecule 23: STAPLE STRAND

Chain AW:



• Molecule 24: STAPLE STRAND

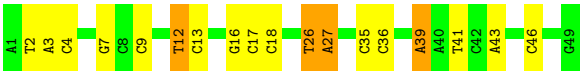
Chain AX:

• Molecule 25: STAPLE STRAND

Chain AY:

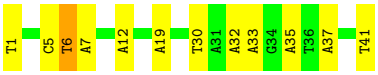
• Molecule 26: STAPLE STRAND

Chain AZ:



• Molecule 27: STAPLE STRAND

Chain Aa:



- Molecule 28: STAPLE STRAND

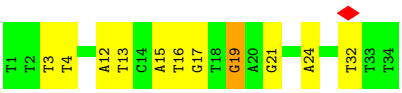
Chain Ab:

- Molecule 29: STAPLE STRAND

Chain Ac:

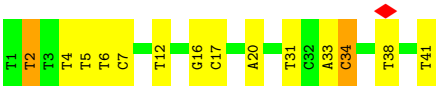
- Molecule 30: STAPLE STRAND

Chain Ad:



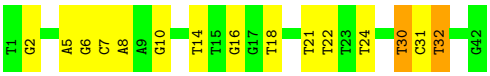
- Molecule 31: STAPLE STRAND

Chain Ae:



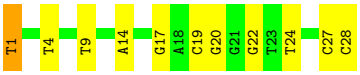
- Molecule 32: STAPLE STRAND

Chain Af:



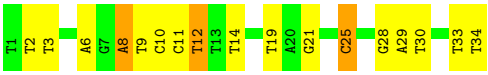
- Molecule 33: STAPLE STRAND

Chain Ag:



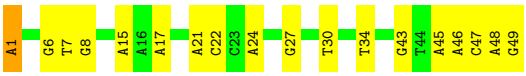
- Molecule 34: STAPLE STRAND

Chain Ah:



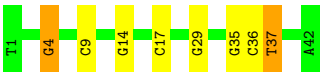
• Molecule 35: STAPLE STRAND

Chain Ai:



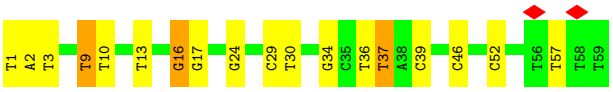
• Molecule 36: STAPLE STRAND

Chain Aj:



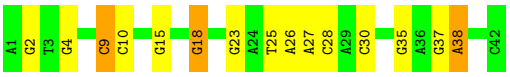
• Molecule 37: STAPLE STRAND

Chain Ak:



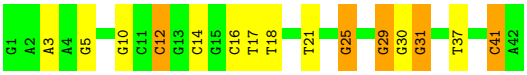
• Molecule 38: STAPLE STRAND

Chain Al:



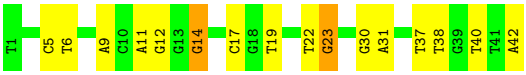
• Molecule 39: STAPLE STRAND

Chain Am:



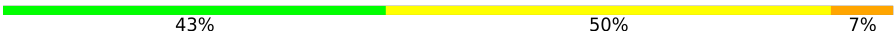
• Molecule 40: STAPLE STRAND

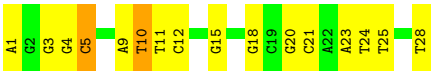
Chain An:



• Molecule 41: STAPLE STRAND

Chain Ao:



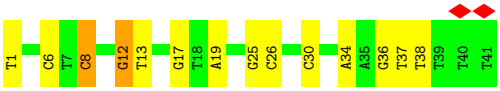


• Molecule 42: STAPLE STRAND

Chain Ap: 46% 54%

• Molecule 43: STAPLE STRAND

Chain Aq: 5% 66% 29% 5%

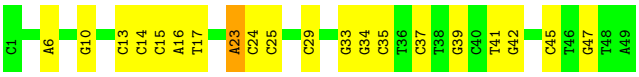


• Molecule 44: STAPLE STRAND

Chain Ar: 69% 25% 6%

• Molecule 45: STAPLE STRAND

Chain As: 59% 39% •

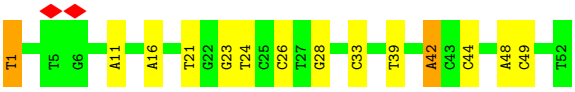


• Molecule 46: STAPLE STRAND

Chain At: 67% 31% •

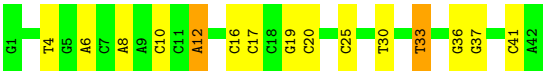
• Molecule 47: STAPLE STRAND

Chain Au: • 73% 23% •



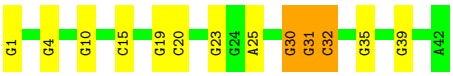
• Molecule 48: STAPLE STRAND

Chain Av: 64% 31% 5%



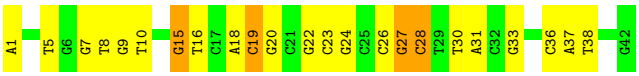
- Molecule 49: STAPLE STRAND

Chain Aw:



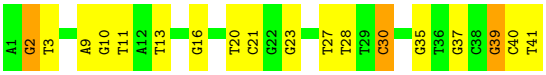
- Molecule 50: STAPLE STRAND

Chain Ax:



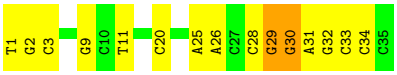
- Molecule 51: STAPLE STRAND

Chain Ay:



- Molecule 52: STAPLE STRAND

Chain Az:

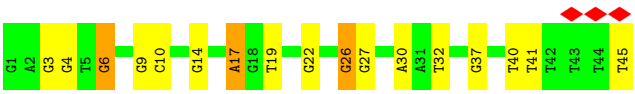


- Molecule 53: STAPLE STRAND

Chain A0:

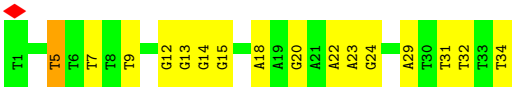
- Molecule 54: STAPLE STRAND

Chain A1:



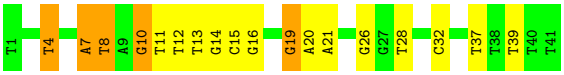
- Molecule 55: STAPLE STRAND

Chain A2:



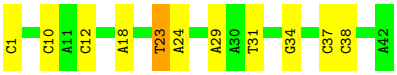
• Molecule 56: STAPLE STRAND

Chain A3:



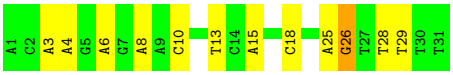
• Molecule 57: STAPLE STRAND

Chain A4:



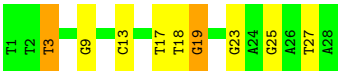
• Molecule 58: STAPLE STRAND

Chain A5:



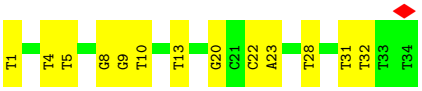
• Molecule 59: STAPLE STRAND

Chain A6:



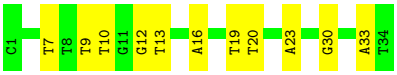
• Molecule 60: STAPLE STRAND

Chain A7:



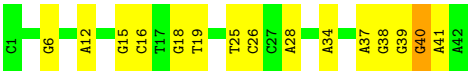
• Molecule 61: STAPLE STRAND

Chain A8:



• Molecule 62: STAPLE STRAND

Chain A9:

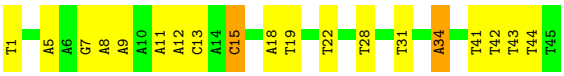


• Molecule 63: STAPLE STRAND

Chain BA: 63% 26% 11%

• Molecule 64: STAPLE STRAND

Chain BB: 58% 38%

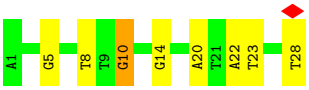


• Molecule 65: STAPLE STRAND

Chain BC: 57% 34% 9%

• Molecule 66: STAPLE STRAND

Chain BD: 71% 25%

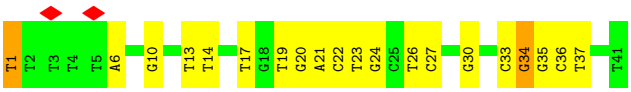


• Molecule 67: STAPLE STRAND

Chain BE: 64% 36%

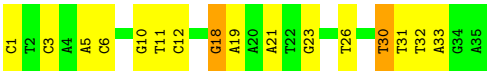
• Molecule 68: STAPLE STRAND

Chain BF: 5% 51% 44% 5%



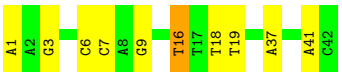
• Molecule 69: STAPLE STRAND

Chain BG: 54% 40% 6%



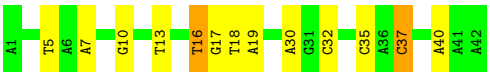
- Molecule 70: STAPLE STRAND

Chain BH:



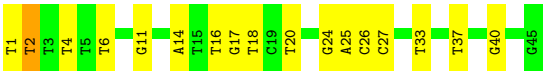
- Molecule 71: STAPLE STRAND

Chain BI:



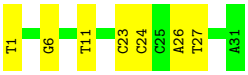
- Molecule 72: STAPLE STRAND

Chain BJ:



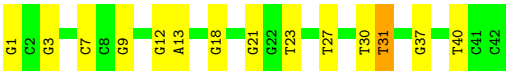
- Molecule 73: STAPLE STRAND

Chain BK:



- Molecule 74: STAPLE STRAND

Chain BL:

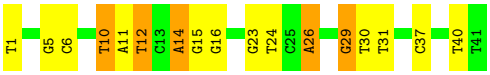


- Molecule 75: STAPLE STRAND

Chain BM:

- Molecule 76: STAPLE STRAND

Chain BN:

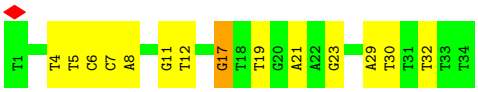


• Molecule 77: STAPLE STRAND

Chain BO:

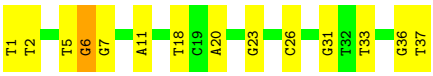
• Molecule 78: STAPLE STRAND

Chain BP:



• Molecule 79: STAPLE STRAND

Chain BQ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.372	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0628	Depositor
Map size (Å)	695.7, 695.7, 695.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.319, 2.319, 2.319	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	AA	1.23	5/66004 (0.0%)	1.43	971/101868 (1.0%)
2	AB	1.27	0/774	1.37	5/1192 (0.4%)
3	AC	1.22	0/1078	1.46	19/1660 (1.1%)
4	AD	1.19	0/790	1.49	11/1219 (0.9%)
5	AE	1.25	0/940	1.42	8/1449 (0.6%)
6	AF	1.22	0/929	1.41	11/1431 (0.8%)
7	AG	1.20	0/769	1.48	12/1184 (1.0%)
8	AH	1.27	0/958	1.47	18/1478 (1.2%)
9	AI	1.22	0/646	1.31	6/996 (0.6%)
10	AJ	1.22	0/746	1.68	24/1147 (2.1%)
11	AK	1.22	0/962	1.35	9/1484 (0.6%)
12	AL	1.22	0/971	1.36	11/1499 (0.7%)
13	AM	1.24	0/970	1.45	17/1497 (1.1%)
14	AN	1.31	0/990	1.38	11/1530 (0.7%)
15	AO	1.26	0/1132	1.43	17/1746 (1.0%)
16	AP	1.23	0/1119	1.33	10/1725 (0.6%)
17	AQ	1.23	0/623	1.42	5/959 (0.5%)
18	AR	1.23	0/628	1.56	16/967 (1.7%)
19	AS	1.22	0/957	1.38	13/1477 (0.9%)
20	AT	1.21	0/1172	1.28	3/1804 (0.2%)
21	AU	1.31	0/1134	1.44	12/1752 (0.7%)
22	AV	1.26	0/1193	1.52	27/1840 (1.5%)
23	AW	1.22	0/966	1.37	10/1489 (0.7%)
24	AX	1.21	0/847	1.35	7/1304 (0.5%)
25	AY	1.21	0/702	1.32	8/1081 (0.7%)
26	AZ	1.22	0/1122	1.38	11/1729 (0.6%)
27	Aa	1.16	0/936	1.37	10/1439 (0.7%)
28	Ab	1.31	1/961 (0.1%)	1.64	25/1480 (1.7%)
29	Ac	1.26	0/963	1.43	11/1486 (0.7%)
30	Ad	1.20	1/779 (0.1%)	1.21	3/1203 (0.2%)
31	Ae	1.22	1/920 (0.1%)	1.42	9/1417 (0.6%)
32	Af	1.24	0/970	1.42	16/1498 (1.1%)
33	Ag	1.19	0/635	1.29	7/979 (0.7%)
34	Ah	1.24	0/766	1.62	17/1181 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
35	Ai	1.22	0/1133	1.37	15/1747 (0.9%)
36	Aj	1.25	0/953	1.33	5/1467 (0.3%)
37	Ak	1.23	0/1339	1.34	13/2065 (0.6%)
38	Al	1.26	0/969	1.40	11/1493 (0.7%)
39	Am	1.28	0/968	1.46	14/1493 (0.9%)
40	An	1.28	1/967 (0.1%)	1.34	10/1492 (0.7%)
41	Ao	1.19	0/642	1.47	13/990 (1.3%)
42	Ap	1.21	0/634	1.60	19/978 (1.9%)
43	Aq	1.21	0/929	1.34	9/1432 (0.6%)
44	Ar	1.18	0/1172	1.30	12/1807 (0.7%)
45	As	1.26	0/1099	1.47	16/1691 (0.9%)
46	At	1.26	0/1195	1.45	15/1845 (0.8%)
47	Au	1.22	0/1193	1.25	8/1839 (0.4%)
48	Av	1.21	0/952	1.34	9/1464 (0.6%)
49	Aw	1.28	0/983	1.41	14/1518 (0.9%)
50	Ax	1.31	1/964 (0.1%)	1.38	13/1486 (0.9%)
51	Ay	1.26	0/942	1.40	12/1454 (0.8%)
52	Az	1.29	1/806 (0.1%)	1.46	16/1242 (1.3%)
53	A0	1.20	0/941	1.33	6/1452 (0.4%)
54	A1	1.27	0/1034	1.44	13/1596 (0.8%)
55	A2	1.21	0/779	1.40	8/1203 (0.7%)
56	A3	1.23	0/932	1.42	17/1438 (1.2%)
57	A4	1.21	0/956	1.32	2/1471 (0.1%)
58	A5	1.17	0/703	1.35	8/1081 (0.7%)
59	A6	1.23	0/640	1.47	9/988 (0.9%)
60	A7	1.22	1/758 (0.1%)	1.40	7/1167 (0.6%)
61	A8	1.20	0/782	1.40	11/1206 (0.9%)
62	A9	1.26	0/975	1.37	7/1505 (0.5%)
63	BA	1.27	0/795	1.48	16/1222 (1.3%)
64	BB	1.17	0/1016	1.30	10/1564 (0.6%)
65	BC	1.26	0/815	1.49	19/1259 (1.5%)
66	BD	1.18	0/636	1.20	3/981 (0.3%)
67	BE	1.18	0/638	1.23	7/986 (0.7%)
68	BF	1.24	0/919	1.40	16/1417 (1.1%)
69	BG	1.18	0/797	1.41	11/1228 (0.9%)
70	BH	1.24	0/969	1.38	8/1495 (0.5%)
71	BI	1.19	0/987	1.35	12/1523 (0.8%)
72	BJ	1.25	0/1035	1.41	16/1598 (1.0%)
73	BK	1.22	0/709	1.30	6/1093 (0.5%)
74	BL	1.24	0/953	1.41	15/1468 (1.0%)
75	BM	1.30	0/1127	1.47	16/1736 (0.9%)
76	BN	1.28	0/941	1.39	15/1452 (1.0%)
77	BO	1.20	1/952 (0.1%)	1.34	7/1467 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
78	BP	1.21	0/764	1.66	21/1178 (1.8%)
79	BQ	1.18	0/845	1.45	12/1303 (0.9%)
All	All	1.23	13/137290 (0.0%)	1.42	1892/211770 (0.9%)

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
1	AA	10	739
2	AB	0	8
3	AC	0	9
4	AD	0	8
5	AE	0	10
6	AF	0	8
7	AG	0	10
8	AH	0	12
9	AI	0	9
10	AJ	0	10
11	AK	0	13
12	AL	0	13
13	AM	0	10
14	AN	0	11
15	AO	0	9
16	AP	0	8
17	AQ	0	10
18	AR	0	7
19	AS	1	11
20	AT	0	16
21	AU	0	13
22	AV	0	8
23	AW	0	9
24	AX	0	10
25	AY	1	5
26	AZ	0	13
27	Aa	0	7
28	Ab	0	8
29	Ac	0	10
30	Ad	0	9
31	Ae	0	10
32	Af	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	Ag	0	6
34	Ah	0	11
35	Ai	0	9
36	Aj	0	6
37	Ak	0	11
38	Al	0	11
39	Am	0	12
40	An	0	12
41	Ao	0	10
42	Ap	0	6
43	Aq	0	8
44	Ar	0	12
45	As	0	11
46	At	0	9
47	Au	0	9
48	Av	0	9
49	Aw	0	9
50	Ax	0	19
51	Ay	0	13
52	Az	0	5
53	A0	0	6
54	A1	0	10
55	A2	0	13
56	A3	0	11
57	A4	0	10
58	A5	0	7
59	A6	0	5
60	A7	0	6
61	A8	0	4
62	A9	0	10
63	BA	0	8
64	BB	0	13
65	BC	0	8
66	BD	0	6
67	BE	0	6
68	BF	0	10
69	BG	0	11
70	BH	0	6
71	BI	0	7
72	BJ	0	10
73	BK	0	4
74	BL	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
75	BM	0	14
76	BN	0	10
77	BO	0	9
78	BP	0	3
79	BQ	0	6
All	All	12	1459

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1302	DA	C5'-C4'	5.50	1.57	1.51
30	Ad	32	DT	C5'-C4'	5.45	1.57	1.51
50	Ax	15	DG	C2-N2	-5.25	1.29	1.34
1	AA	2655	DC	C5'-C4'	5.23	1.57	1.51
1	AA	1452	DC	C5'-C4'	5.23	1.57	1.51

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Ah	12	DT	P-O3'-C3'	15.81	138.68	119.70
1	AA	1873	DC	P-O3'-C3'	15.25	138.00	119.70
1	AA	175	DC	P-O3'-C3'	15.17	137.90	119.70
54	A1	9	DG	P-O3'-C3'	15.13	137.85	119.70
1	AA	409	DA	P-O3'-C3'	14.92	137.60	119.70

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	342	DG	C3'
1	AA	738	DC	C3'
1	AA	1302	DA	C3'
1	AA	1360	DC	C3'
1	AA	1774	DG	C3'

5 of 1459 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	DG	Sidechain
1	AA	14	DG	Sidechain
1	AA	21	DG	Sidechain
1	AA	3	DG	Sidechain
1	AA	5	DC	Sidechain

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein molecules in this entry.

5.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

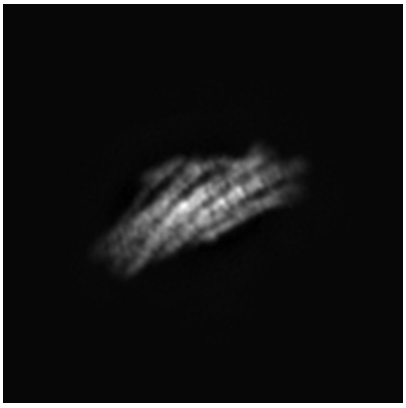
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12516. These allow visual inspection of the internal detail of the map and identification of artifacts.

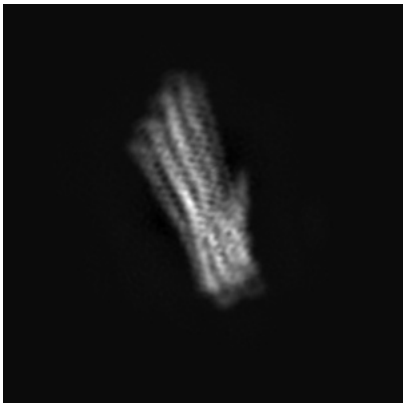
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

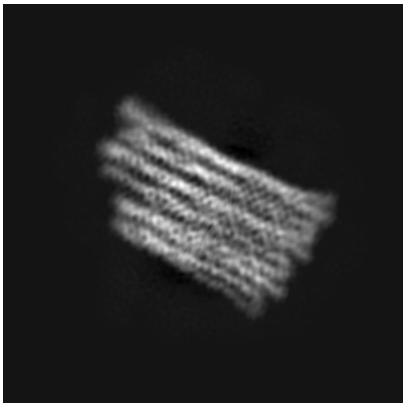
6.1.1 Primary map



X



Y



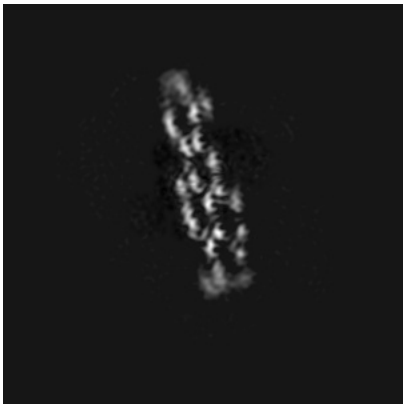
Z

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

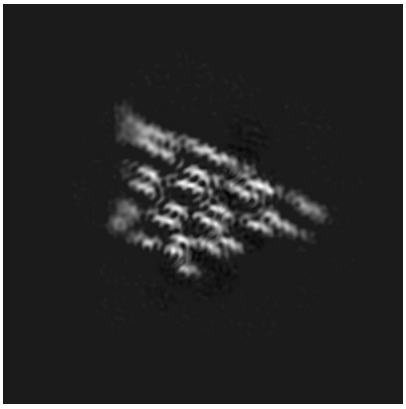
6.2 Central slices (i)

6.2.1 Primary map

X Index: 150



Y Index: 150

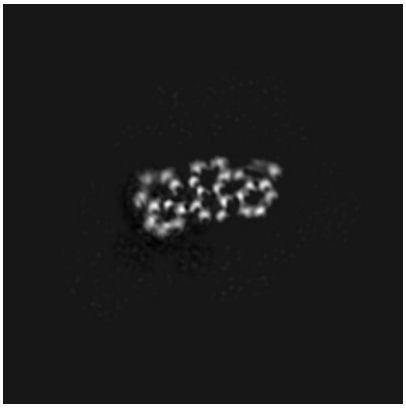


Z Index: 150

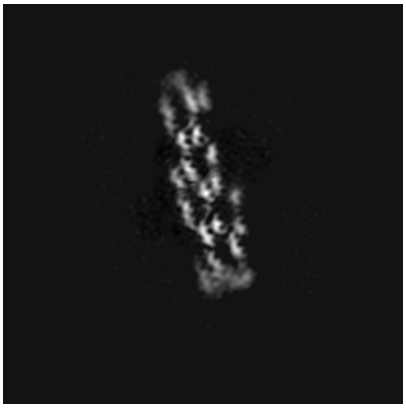
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

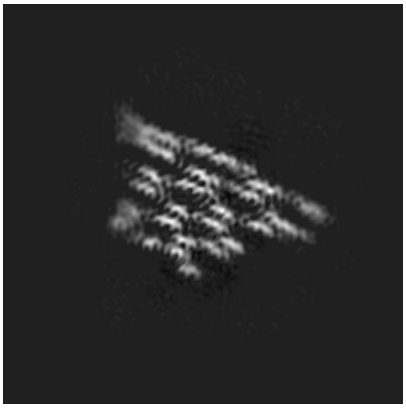
6.3.1 Primary map



X Index: 133



Y Index: 147

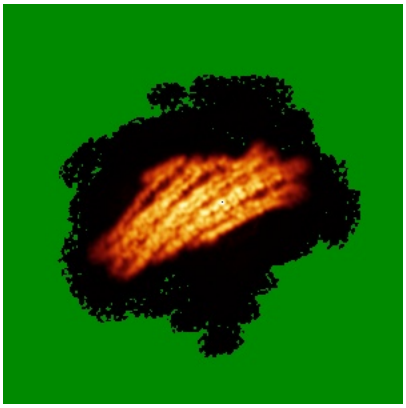


Z Index: 149

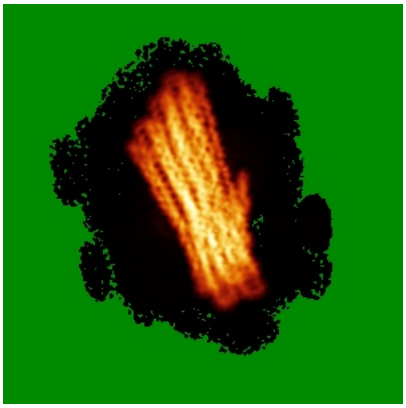
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

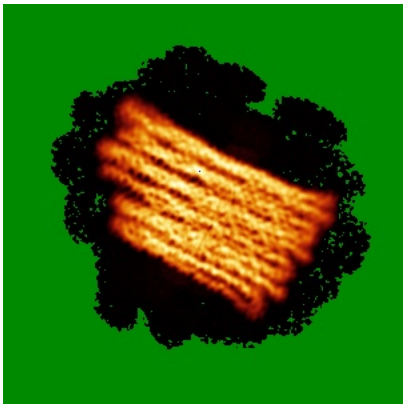
6.4.1 Primary map



X



Y

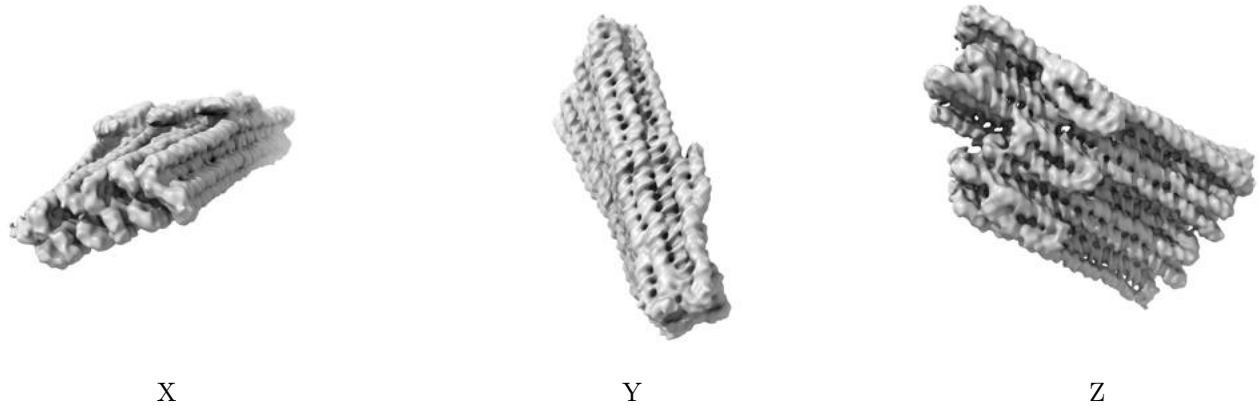


Z

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 0.0628. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

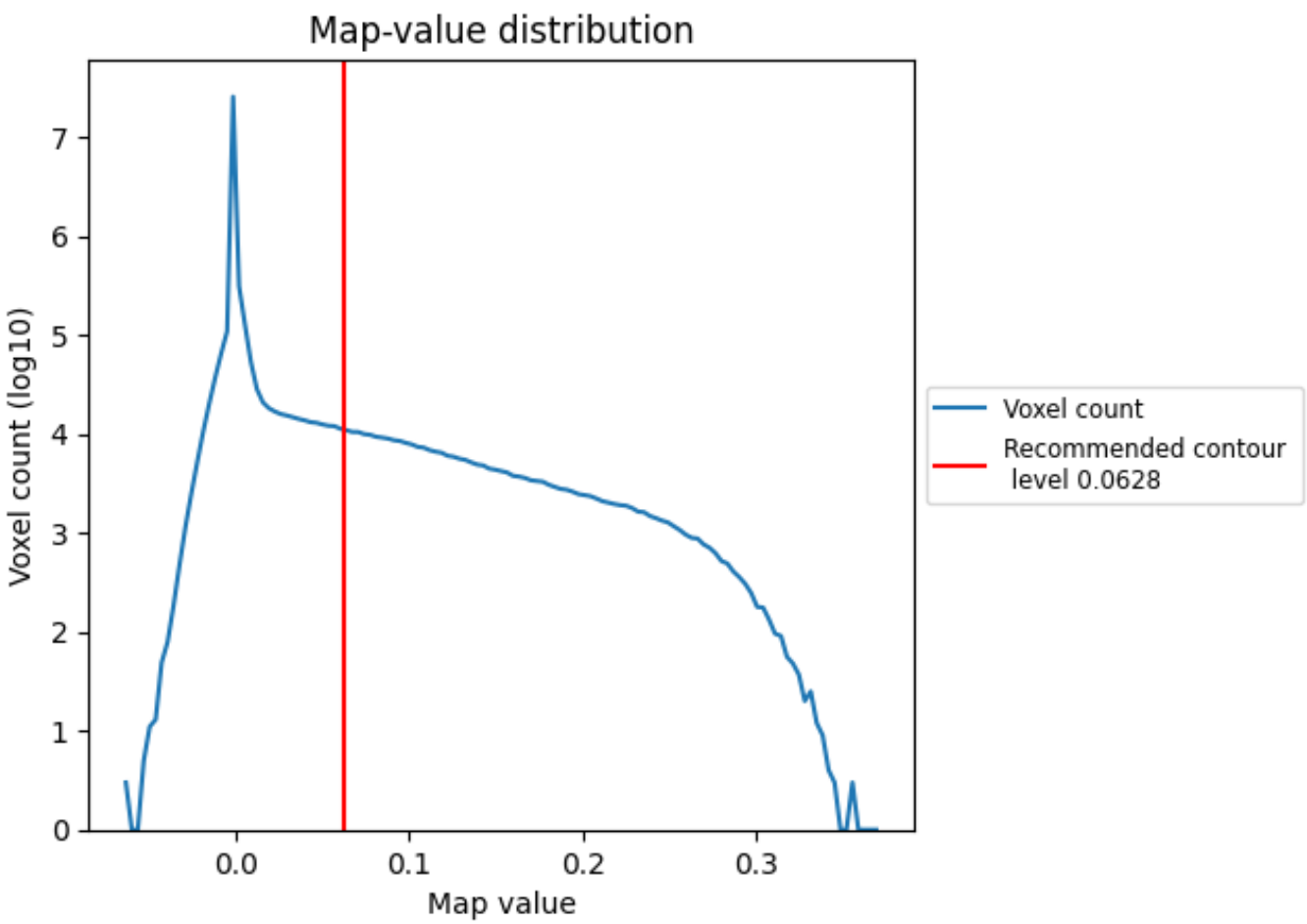
6.6 Mask visualisation (i)

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

7 Map analysis (i)

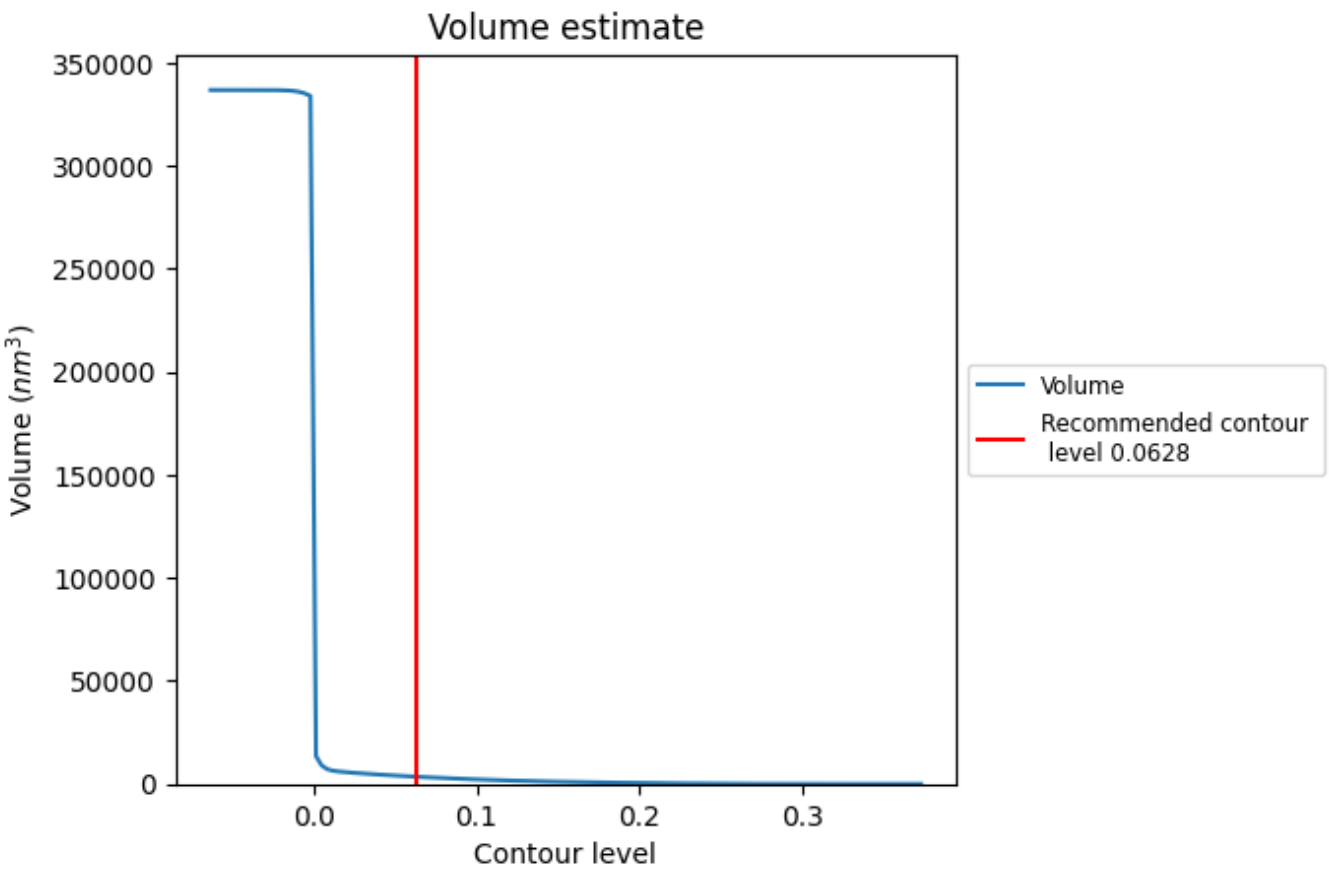
This section contains the results of statistical analysis of the map.

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.

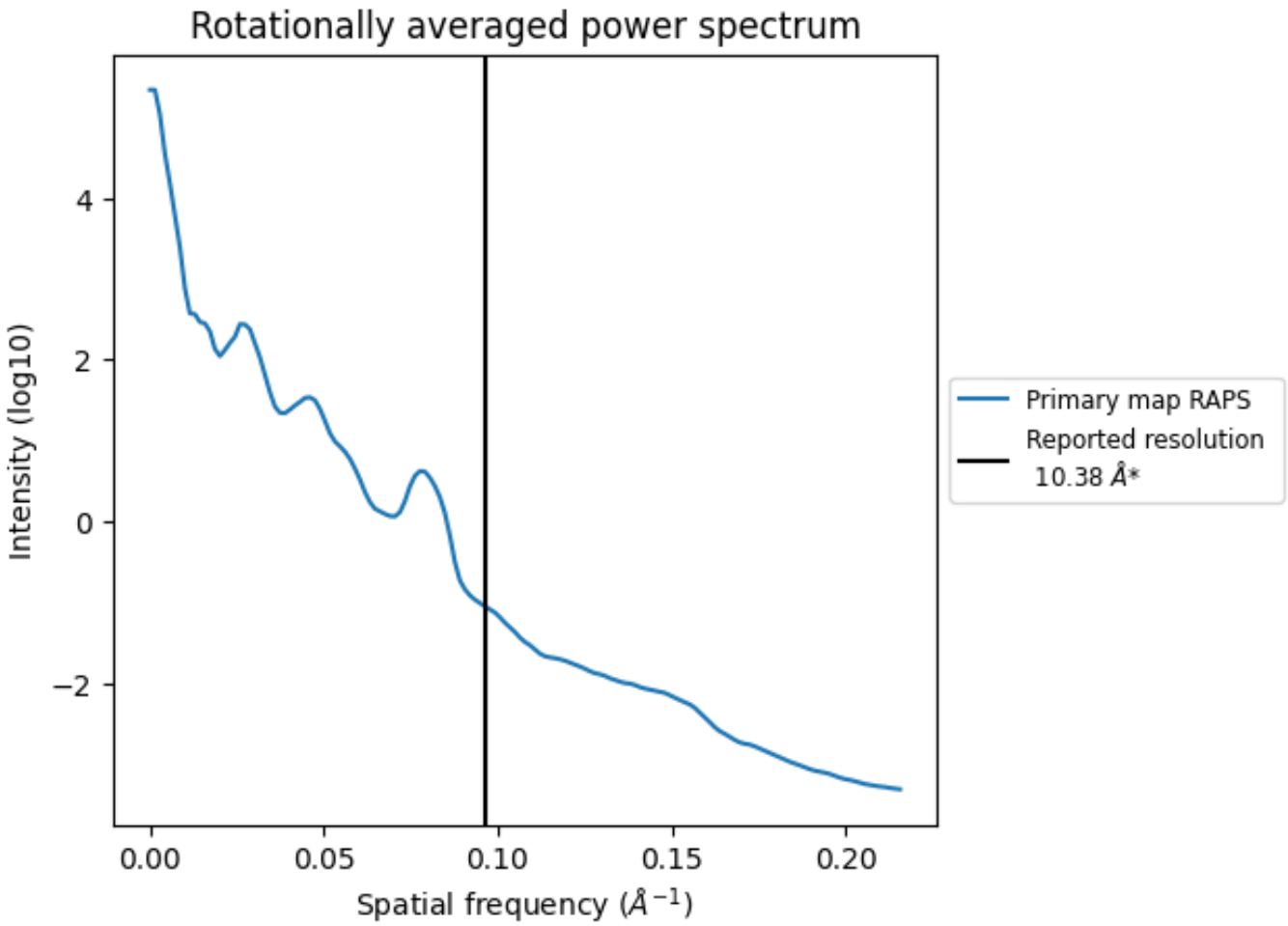
7.2 Volume estimate (i)



The volume at the recommended contour level is 3511 nm^3; this corresponds to an approximate mass of 3171 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

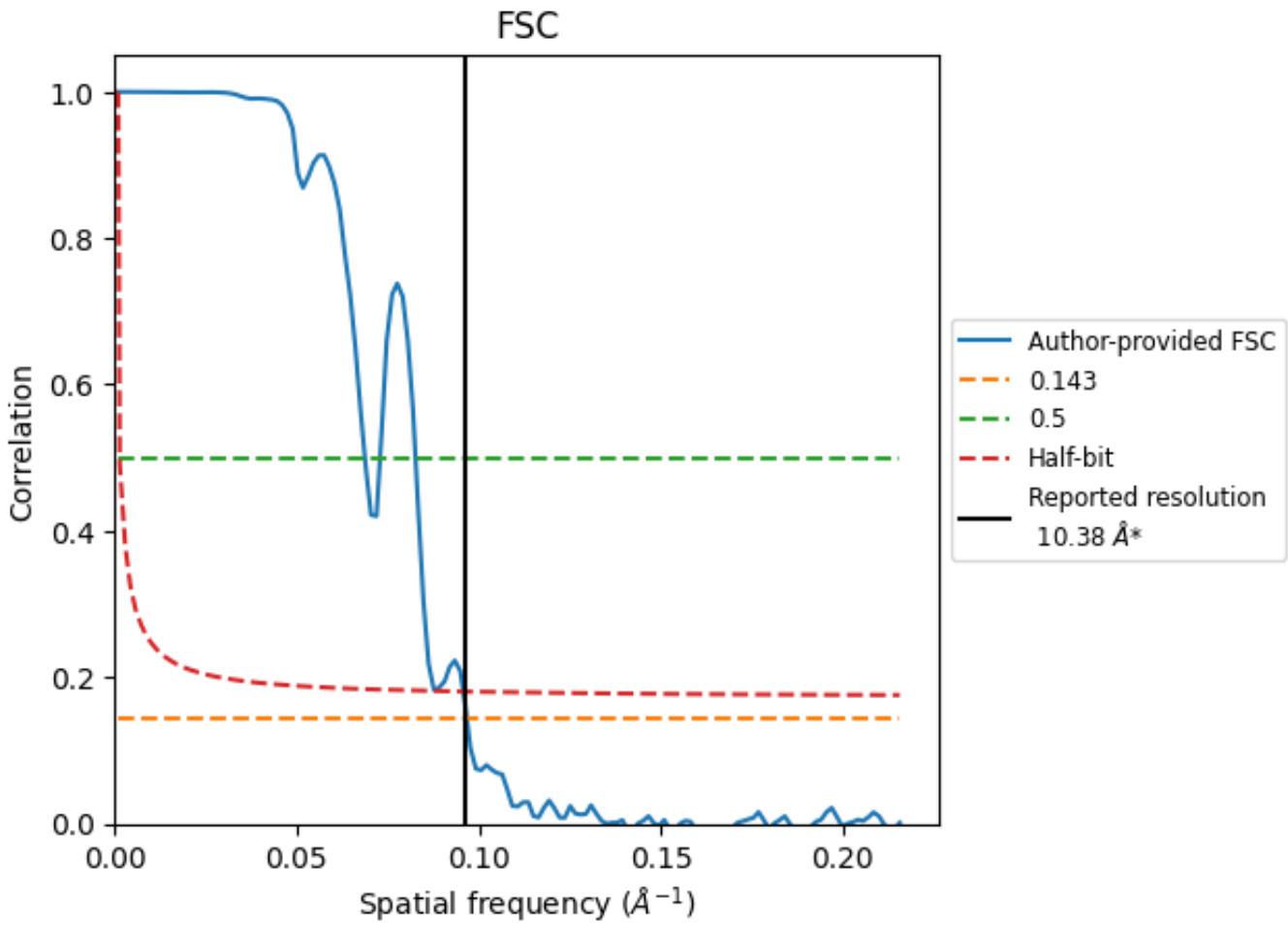


*Reported resolution corresponds to spatial frequency of 0.096 Å^{-1}

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 0.096 Å^{-1}

8.2 Resolution estimates (i)

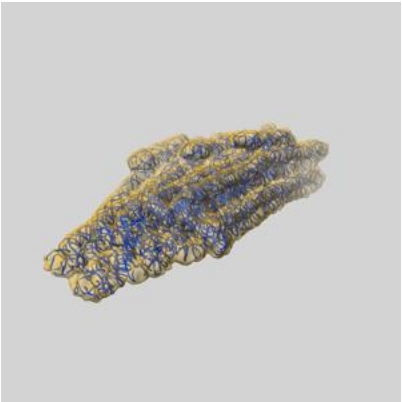
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.38	-	-
Author-provided FSC curve	10.34	14.56	10.45
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

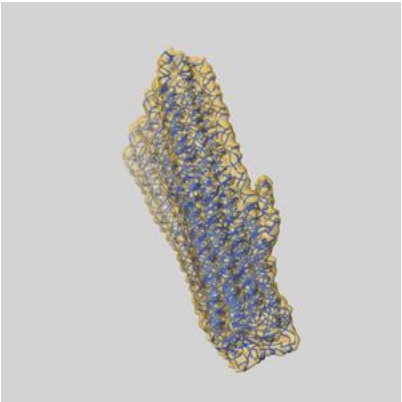
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12516 and PDB model 7NPN. Per-residue inclusion information can be found in section 3 on page 18.

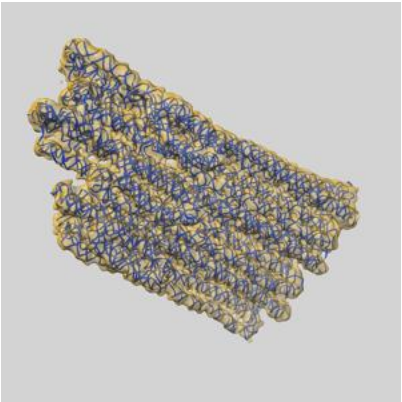
9.1 Map-model overlay (i)



X



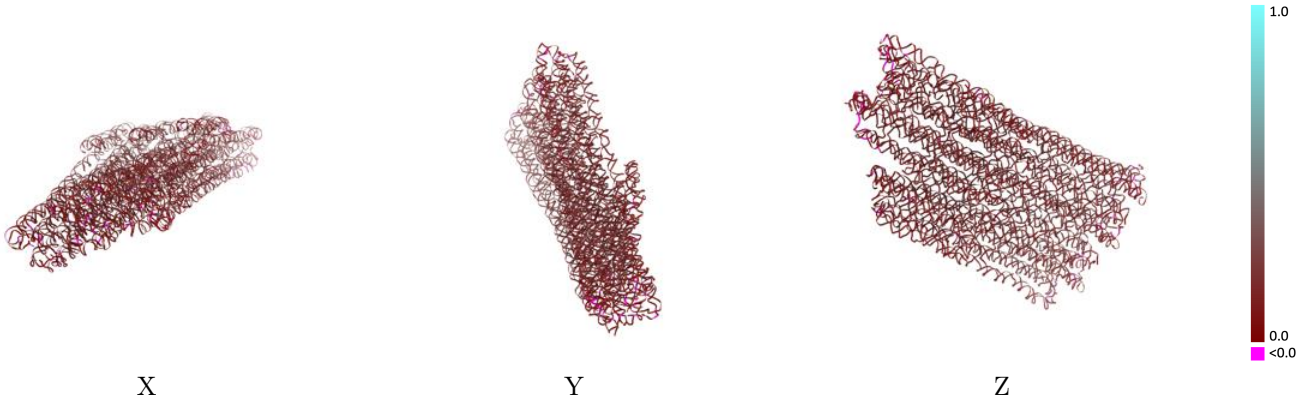
Y



Z

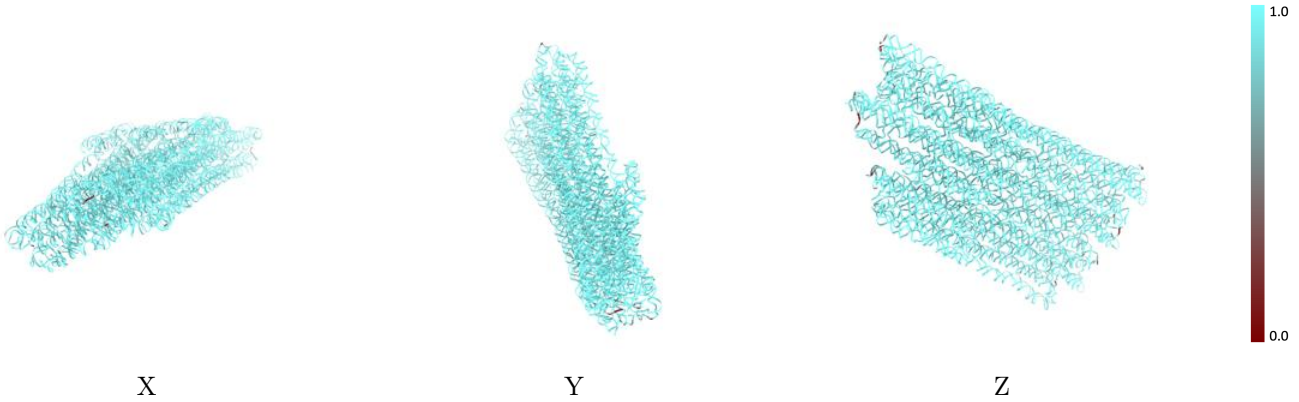
The images above show the 3D surface view of the map at the recommended contour level 0.0628 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



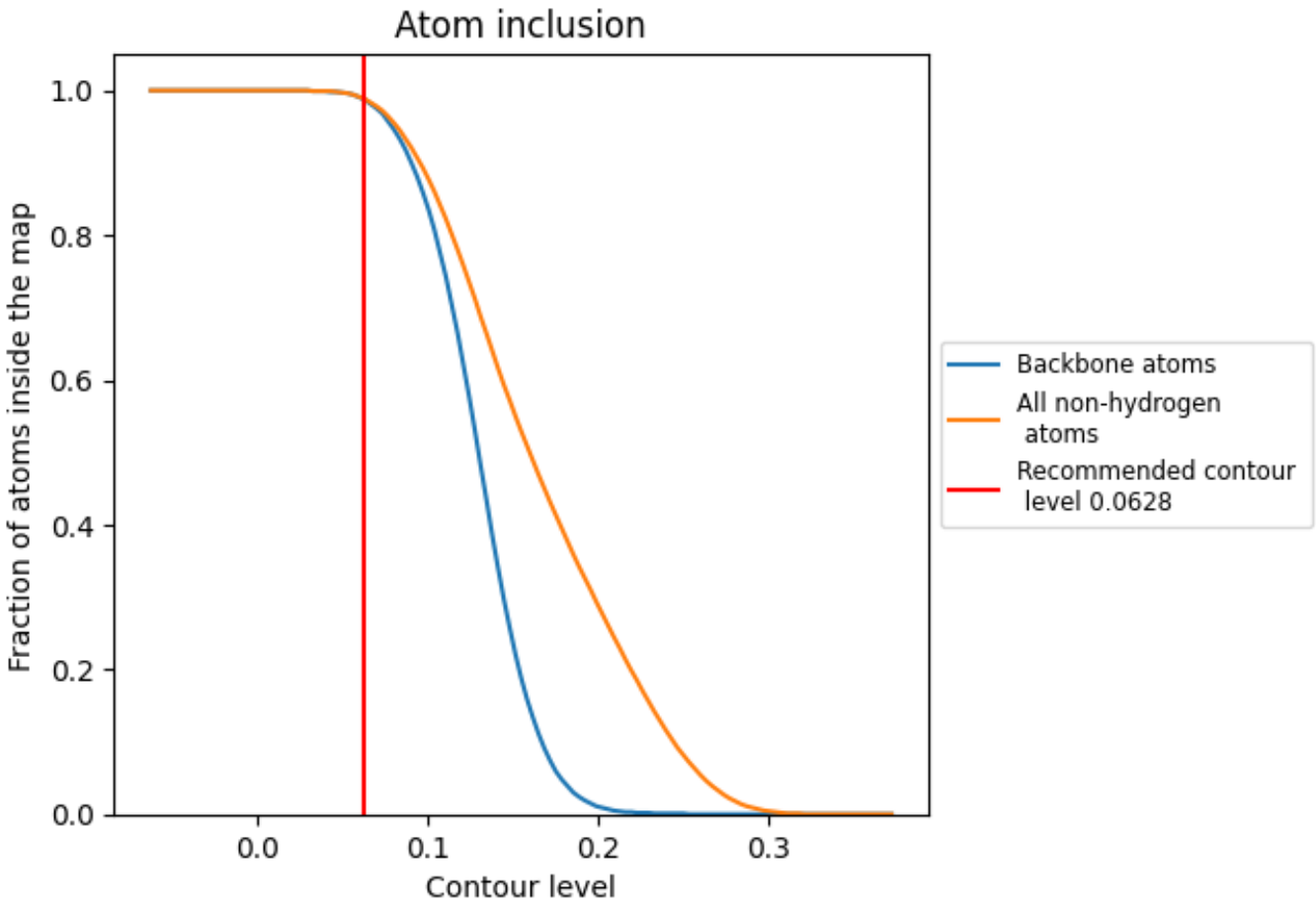
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0628).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0628) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9880	0.1650
A0	0.9980	0.1910
A1	0.9310	0.1530
A2	0.9600	0.1210
A3	0.9880	0.1620
A4	0.9980	0.1810
A5	0.9860	0.1520
A6	0.9840	0.1280
A7	0.9310	0.1230
A8	0.9990	0.1930
A9	1.0000	0.1800
AA	0.9950	0.1700
AB	0.9970	0.1520
AC	0.9870	0.1460
AD	0.9960	0.1910
AE	0.9910	0.1720
AF	0.9940	0.1810
AG	0.9900	0.1510
AH	1.0000	0.1630
AI	0.9790	0.1480
AJ	0.8720	0.1060
AK	1.0000	0.1910
AL	0.9990	0.1710
AM	1.0000	0.1920
AN	1.0000	0.1700
AO	1.0000	0.1700
AP	1.0000	0.1770
AQ	0.9220	0.1280
AR	0.9660	0.1080
AS	0.9480	0.0840
AT	0.9980	0.1780
AU	1.0000	0.1720
AV	0.9900	0.1510
AW	0.9980	0.1850
AX	0.9960	0.1330

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Chain	Atom inclusion	Q-score
AY	0.9520	0.1430
AZ	1.0000	0.1870
Aa	0.9980	0.1670
Ab	0.9980	0.1780
Ac	0.9990	0.1680
Ad	0.9600	0.1260
Ae	0.9530	0.1370
Af	1.0000	0.1850
Ag	0.9740	0.1330
Ah	0.9350	0.1090
Ai	1.0000	0.1750
Aj	1.0000	0.1670
Ak	0.9540	0.1480
Al	0.9970	0.1940
Am	0.9980	0.1710
An	0.9990	0.1740
Ao	0.9810	0.1430
Ap	0.9260	0.0890
Aq	0.9280	0.1090
Ar	0.9980	0.1790
As	1.0000	0.1880
At	0.9840	0.1500
Au	0.9210	0.1380
Av	0.9980	0.1940
Aw	0.9950	0.1890
Ax	0.9980	0.1800
Ay	0.9980	0.1610
Az	1.0000	0.1760
BA	0.9990	0.1670
BB	0.9600	0.1370
BC	1.0000	0.1650
BD	0.9510	0.1430
BE	0.9600	0.1340
BF	0.9300	0.1210
BG	0.9890	0.1660
BH	0.9990	0.1760
BI	1.0000	0.1960
BJ	0.9910	0.1620
BK	0.9560	0.1450
BL	1.0000	0.1710
BM	0.9980	0.1830
BN	0.9990	0.1710

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Chain	Atom inclusion	Q-score
BO	0.9990	0.1780
BP	0.9560	0.1420
BQ	0.9920	0.1530