



## wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 11:21 am GMT

PDB ID : 7NPN  
EMDB ID : EMD-12516  
Title : B-brick bare in 5 mM Mg<sup>2+</sup>  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3










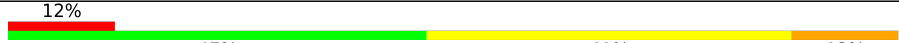


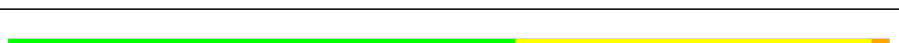

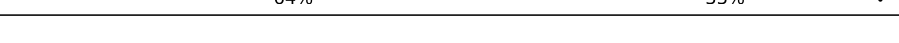

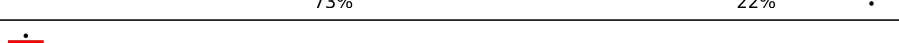
# 1 Overall quality at a glance

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

The reported resolution of this entry is 10.38 Å.














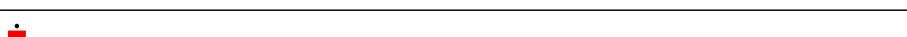
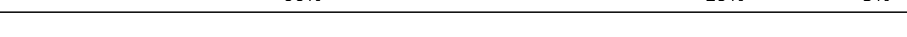
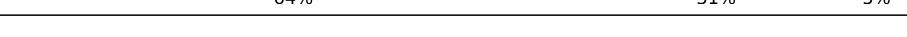



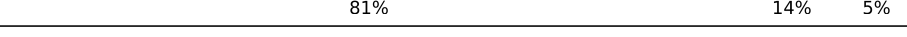





There are no overall percentile quality scores available for this entry.

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  $\geq 3$ , 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	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%

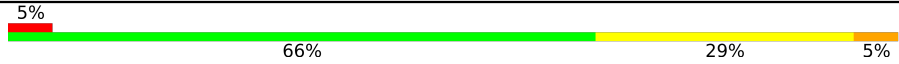


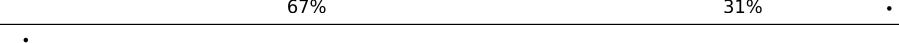
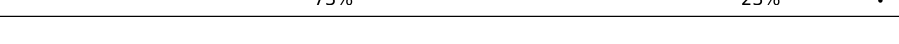
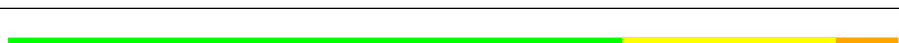
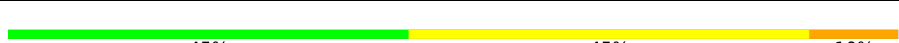




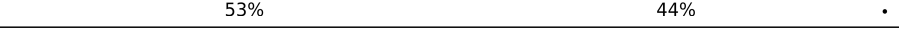
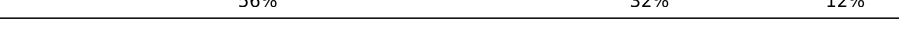

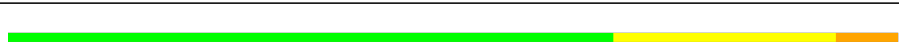





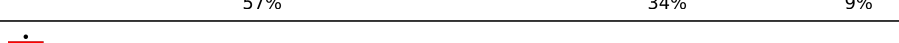
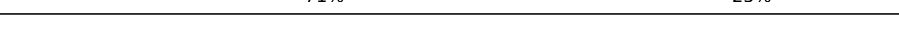



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Mol	Chain	Length	Quality of chain
18	AR	28	
19	AS	42	
20	AT	52	
21	AU	49	
22	AV	52	
23	AW	42	
24	AX	38	
25	AY	31	
26	AZ	49	
27	Aa	41	
28	Ab	42	
29	Ac	42	
30	Ad	34	
31	Ae	41	
32	Af	42	
33	Ag	28	
34	Ah	34	
35	Ai	49	
36	Aj	42	
37	Ak	59	
38	Al	42	
39	Am	42	
40	An	42	
41	Ao	28	
42	Ap	28	

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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% 2%
46	At	52	 67% 31% 2%
47	Au	52	 73% 23% 4%
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% 2%
54	A1	45	 7% 62% 31% 7%
55	A2	34	 53% 44% 3%
56	A3	41	 56% 32% 12%
57	A4	42	 74% 24% 2%
58	A5	31	 61% 35% 4%
59	A6	28	 68% 25% 7%
60	A7	34	 62% 38% 2%
61	A8	34	 68% 32% 2%
62	A9	42	 64% 33% 3%
63	BA	35	 63% 26% 11%
64	BB	45	 58% 38% 4%
65	BC	35	 57% 34% 9%
66	BD	28	 71% 25% 4%
67	BE	28	 64% 36% 2%

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Mol	Chain	Length	Quality of chain
68	BF	41	
69	BG	35	
70	BH	42	
71	BI	42	
72	BJ	45	
73	BK	31	
74	BL	42	
75	BM	49	
76	BN	41	
77	BO	42	
78	BP	34	
79	BQ	37	

## 2 Entry composition

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
7	AG	34	Total	C	N	O	P	0	0
			688	331	119	205	33		

- Molecule 8 is a DNA chain called STAPLE STRAND.

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

- Molecule 9 is a DNA chain called STAPLE STRAND.

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

- Molecule 10 is a DNA chain called STAPLE STRAND.

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

- Molecule 11 is a DNA chain called STAPLE STRAND.

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

- Molecule 12 is a DNA chain called STAPLE STRAND.

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

- Molecule 13 is a DNA chain called STAPLE STRAND.

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

- Molecule 14 is a DNA chain called STAPLE STRAND.

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

- Molecule 15 is a DNA chain called STAPLE STRAND.

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

- Molecule 16 is a DNA chain called STAPLE STRAND.

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

- Molecule 17 is a DNA chain called STAPLE STRAND.

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

- Molecule 18 is a DNA chain called STAPLE STRAND.

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

- Molecule 19 is a DNA chain called STAPLE STRAND.

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

- Molecule 20 is a DNA chain called STAPLE STRAND.

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

- Molecule 21 is a DNA chain called STAPLE STRAND.



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

- Molecule 22 is a DNA chain called STAPLE STRAND.

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

- Molecule 23 is a DNA chain called STAPLE STRAND.

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

- Molecule 24 is a DNA chain called STAPLE STRAND.

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

- Molecule 25 is a DNA chain called STAPLE STRAND.

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

- Molecule 26 is a DNA chain called STAPLE STRAND.

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

- Molecule 27 is a DNA chain called STAPLE STRAND.

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

- Molecule 28 is a DNA chain called STAPLE STRAND.

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

- Molecule 29 is a DNA chain called STAPLE STRAND.

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

- Molecule 30 is a DNA chain called STAPLE STRAND.

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

- Molecule 31 is a DNA chain called STAPLE STRAND.

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

- Molecule 32 is a DNA chain called STAPLE STRAND.

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

- Molecule 33 is a DNA chain called STAPLE STRAND.

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

- Molecule 34 is a DNA chain called STAPLE STRAND.

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

- Molecule 35 is a DNA chain called STAPLE STRAND.

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

- Molecule 36 is a DNA chain called STAPLE STRAND.

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

- Molecule 37 is a DNA chain called STAPLE STRAND.

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

- Molecule 38 is a DNA chain called STAPLE STRAND.

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

- Molecule 39 is a DNA chain called STAPLE STRAND.

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

- Molecule 40 is a DNA chain called STAPLE STRAND.

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

- Molecule 41 is a DNA chain called STAPLE STRAND.

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

- Molecule 42 is a DNA chain called STAPLE STRAND.

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

- Molecule 43 is a DNA chain called STAPLE STRAND.

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

- Molecule 44 is a DNA chain called STAPLE STRAND.

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

- Molecule 45 is a DNA chain called STAPLE STRAND.

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

- Molecule 46 is a DNA chain called STAPLE STRAND.

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

- Molecule 47 is a DNA chain called STAPLE STRAND.

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

- Molecule 48 is a DNA chain called STAPLE STRAND.

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

- Molecule 49 is a DNA chain called STAPLE STRAND.

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

- Molecule 50 is a DNA chain called STAPLE STRAND.

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

- Molecule 51 is a DNA chain called STAPLE STRAND.

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

- Molecule 52 is a DNA chain called STAPLE STRAND.

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

- Molecule 53 is a DNA chain called STAPLE STRAND.

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

- Molecule 54 is a DNA chain called STAPLE STRAND.

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

- Molecule 55 is a DNA chain called STAPLE STRAND.

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

- Molecule 56 is a DNA chain called STAPLE STRAND.

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

- Molecule 57 is a DNA chain called STAPLE STRAND.

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

- Molecule 58 is a DNA chain called STAPLE STRAND.

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

- Molecule 59 is a DNA chain called STAPLE STRAND.

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

- Molecule 60 is a DNA chain called STAPLE STRAND.

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

- Molecule 61 is a DNA chain called STAPLE STRAND.

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

- Molecule 62 is a DNA chain called STAPLE STRAND.

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

- 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
70	BH	42	Total	C	N	O	P	0	0
			863	413	160	249	41		

- Molecule 71 is a DNA chain called STAPLE STRAND.

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

- Molecule 72 is a DNA chain called STAPLE STRAND.

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

- Molecule 73 is a DNA chain called STAPLE STRAND.

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

- Molecule 74 is a DNA chain called STAPLE STRAND.

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

- Molecule 75 is a DNA chain called STAPLE STRAND.

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

- Molecule 76 is a DNA chain called STAPLE STRAND.

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

- 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

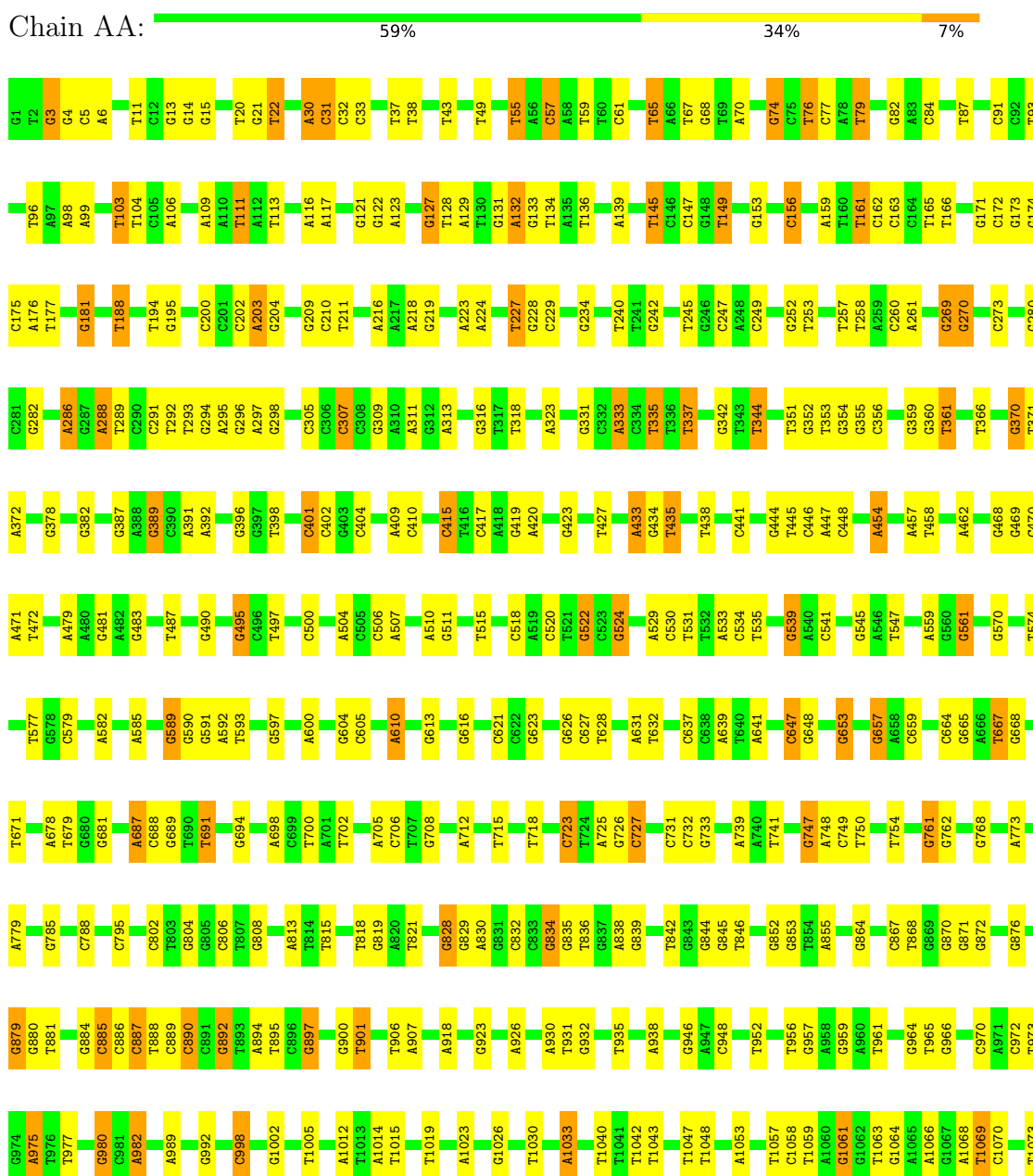
- Molecule 79 is a DNA chain called STAPLE STRAND.

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.

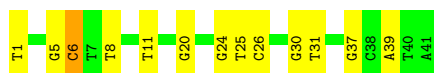
- Molecule 1: SCAFFOLD STRAND







Chain AF:  68% 29%



- Molecule 7: STAPLE STRAND

Chain AG:  56% 35% 9%



- Molecule 8: STAPLE STRAND

Chain AH:  50% 43% 7%



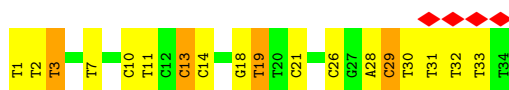
- Molecule 9: STAPLE STRAND

Chain AI:  54% 46%



- Molecule 10: STAPLE STRAND

Chain AJ:  12% 47% 41% 12%



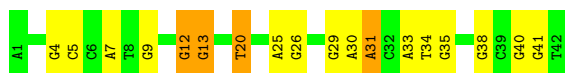
- Molecule 11: STAPLE STRAND

Chain AK:  57% 36% 7%



- Molecule 12: STAPLE STRAND

Chain AL:  57% 33% 10%



- Molecule 13: STAPLE STRAND

Chain AM:  57% 40%



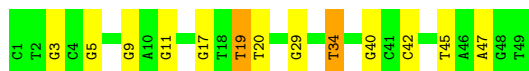
- Molecule 14: STAPLE STRAND



- Molecule 15: STAPLE STRAND



- Molecule 16: STAPLE STRAND



- Molecule 17: STAPLE STRAND



- Molecule 18: STAPLE STRAND



- Molecule 19: STAPLE STRAND



- Molecule 20: STAPLE STRAND

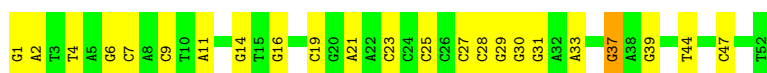




- Molecule 21: STAPLE STRAND



- Molecule 22: STAPLE STRAND



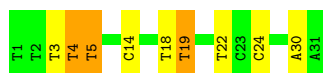
- Molecule 23: STAPLE STRAND



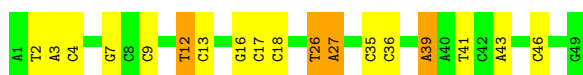
- Molecule 24: STAPLE STRAND



- Molecule 25: STAPLE STRAND



- Molecule 26: STAPLE STRAND



- Molecule 27: STAPLE STRAND





- Molecule 28: STAPLE STRAND



- Molecule 29: STAPLE STRAND



- Molecule 30: STAPLE STRAND



- Molecule 31: STAPLE STRAND



- Molecule 32: STAPLE STRAND



- Molecule 33: STAPLE STRAND



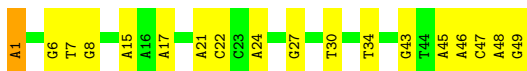
- Molecule 34: STAPLE STRAND



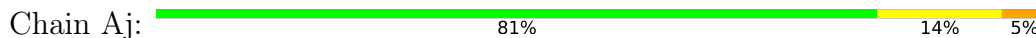




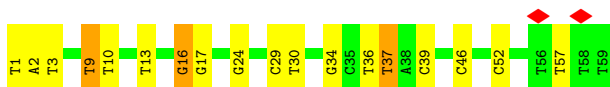
- Molecule 35: STAPLE STRAND



- Molecule 36: STAPLE STRAND



- Molecule 37: STAPLE STRAND



- Molecule 38: STAPLE STRAND



- Molecule 39: STAPLE STRAND



- Molecule 40: STAPLE STRAND



- Molecule 41: STAPLE STRAND





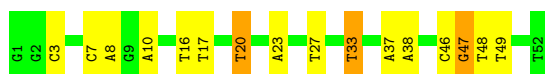
- Molecule 42: STAPLE STRAND



- Molecule 43: STAPLE STRAND



- Molecule 44: STAPLE STRAND



- Molecule 45: STAPLE STRAND



- Molecule 46: STAPLE STRAND



- Molecule 47: STAPLE STRAND

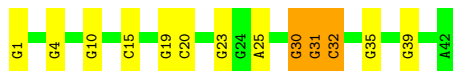


- Molecule 48: STAPLE STRAND





- Molecule 49: STAPLE STRAND



- Molecule 50: STAPLE STRAND



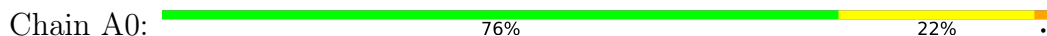
- Molecule 51: STAPLE STRAND



- Molecule 52: STAPLE STRAND



- Molecule 53: STAPLE STRAND

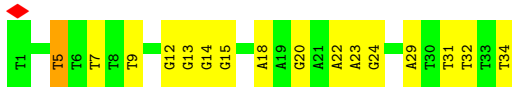


- Molecule 54: STAPLE STRAND

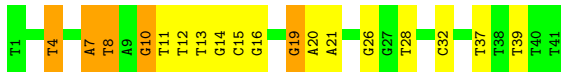


- Molecule 55: STAPLE STRAND

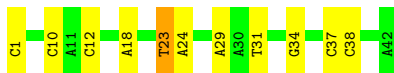
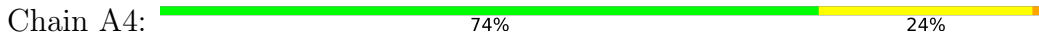




• Molecule 56: STAPLE STRAND



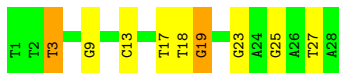
• Molecule 57: STAPLE STRAND



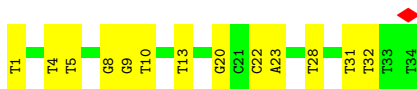
• Molecule 58: STAPLE STRAND



• Molecule 59: STAPLE STRAND



• Molecule 60: STAPLE STRAND

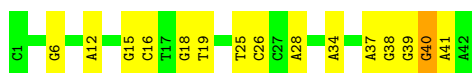


• Molecule 61: STAPLE STRAND

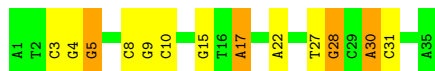


• Molecule 62: STAPLE STRAND





- Molecule 63: STAPLE STRAND



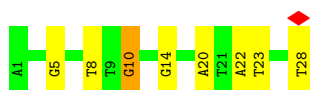
- Molecule 64: STAPLE STRAND



- Molecule 65: STAPLE STRAND



- Molecule 66: STAPLE STRAND



- Molecule 67: STAPLE STRAND

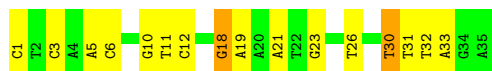


- Molecule 68: STAPLE STRAND

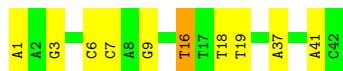
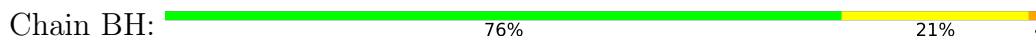


- Molecule 69: STAPLE STRAND





- Molecule 70: STAPLE STRAND



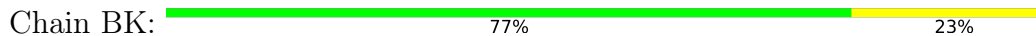
- Molecule 71: STAPLE STRAND



- Molecule 72: STAPLE STRAND



- Molecule 73: STAPLE STRAND



- Molecule 74: STAPLE STRAND



- Molecule 75: STAPLE STRAND



- Molecule 76: STAPLE STRAND

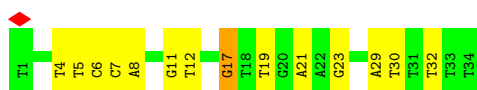




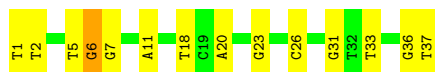
- Molecule 77: STAPLE STRAND



- Molecule 78: STAPLE STRAND



- Molecule 79: STAPLE STRAND



## 4 Experimental information

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 ( $e^-/\text{\AA}^2$ )	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 ( $\text{\AA}$ )	695.7, 695.7, 695.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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(°)	Ideal(°)
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.

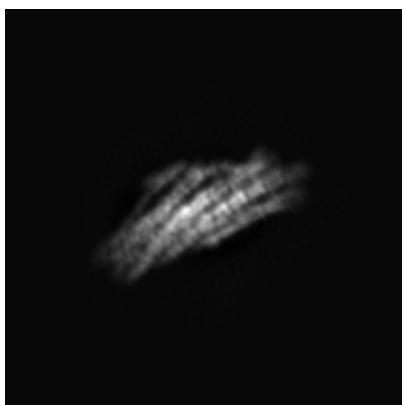
## 6 Map visualisation [i](#)

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.

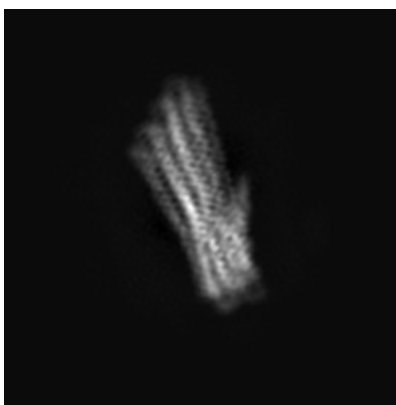
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

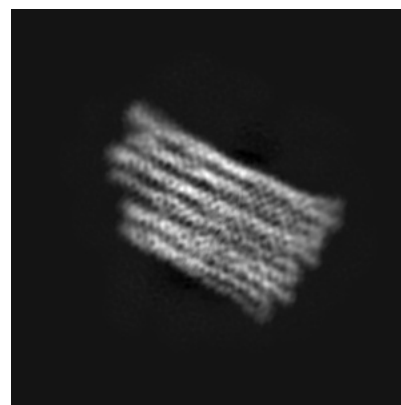
#### 6.1.1 Primary map



X



Y



Z

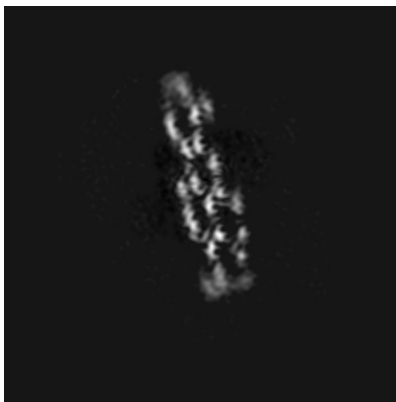
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

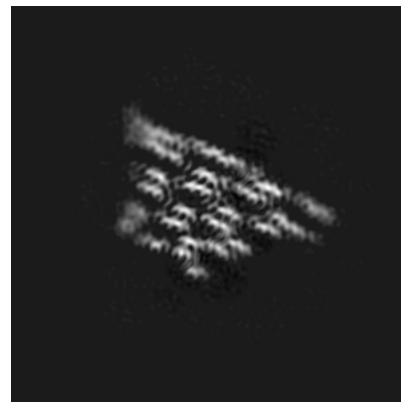
#### 6.2.1 Primary map



X Index: 150



Y Index: 150

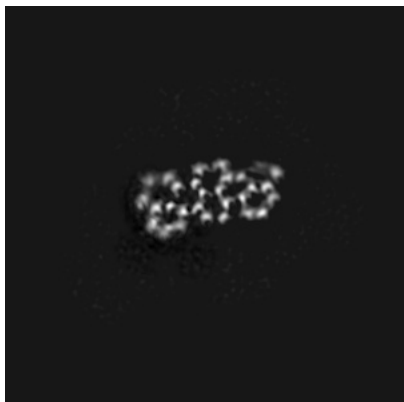


Z Index: 150

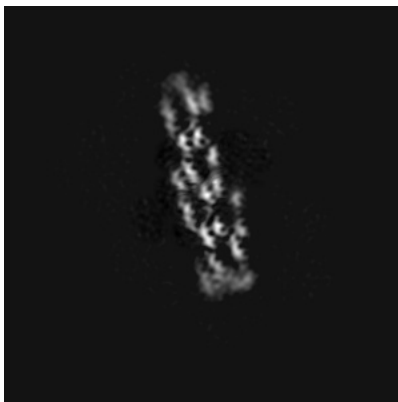
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

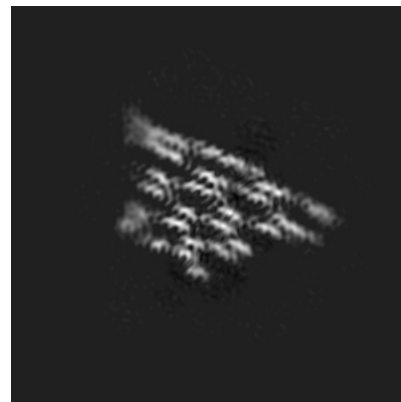
### 6.3.1 Primary map



X Index: 133



Y Index: 147

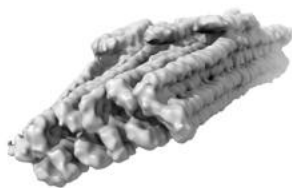


Z Index: 149

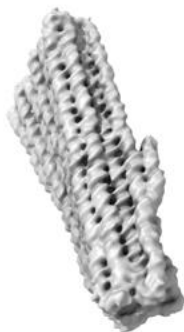
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

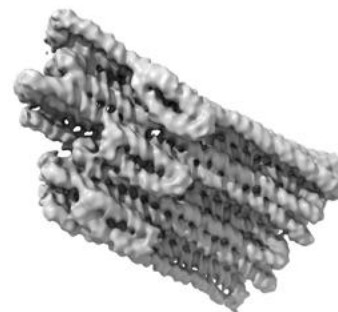
### 6.4.1 Primary map



X



Y



Z

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.



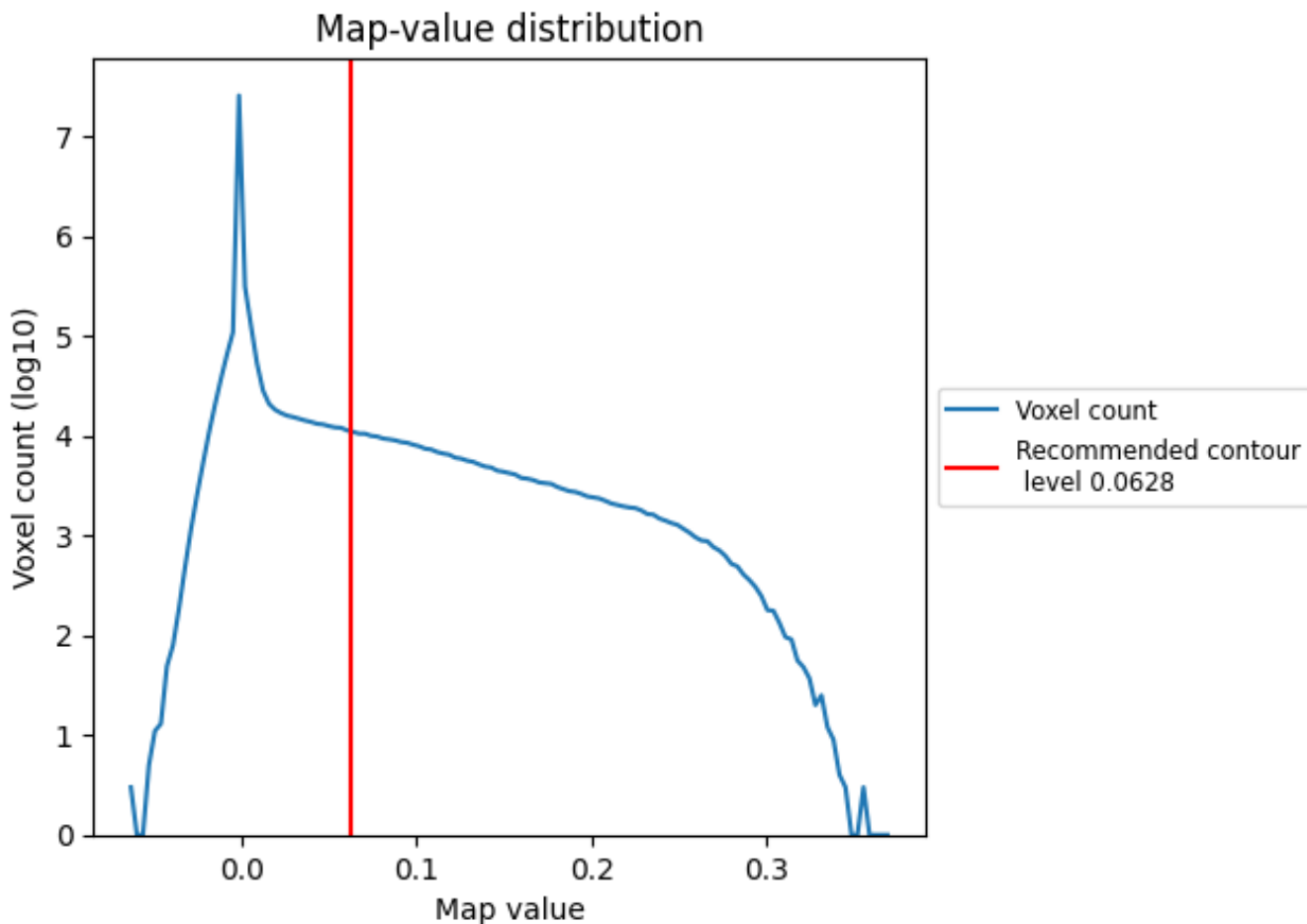
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

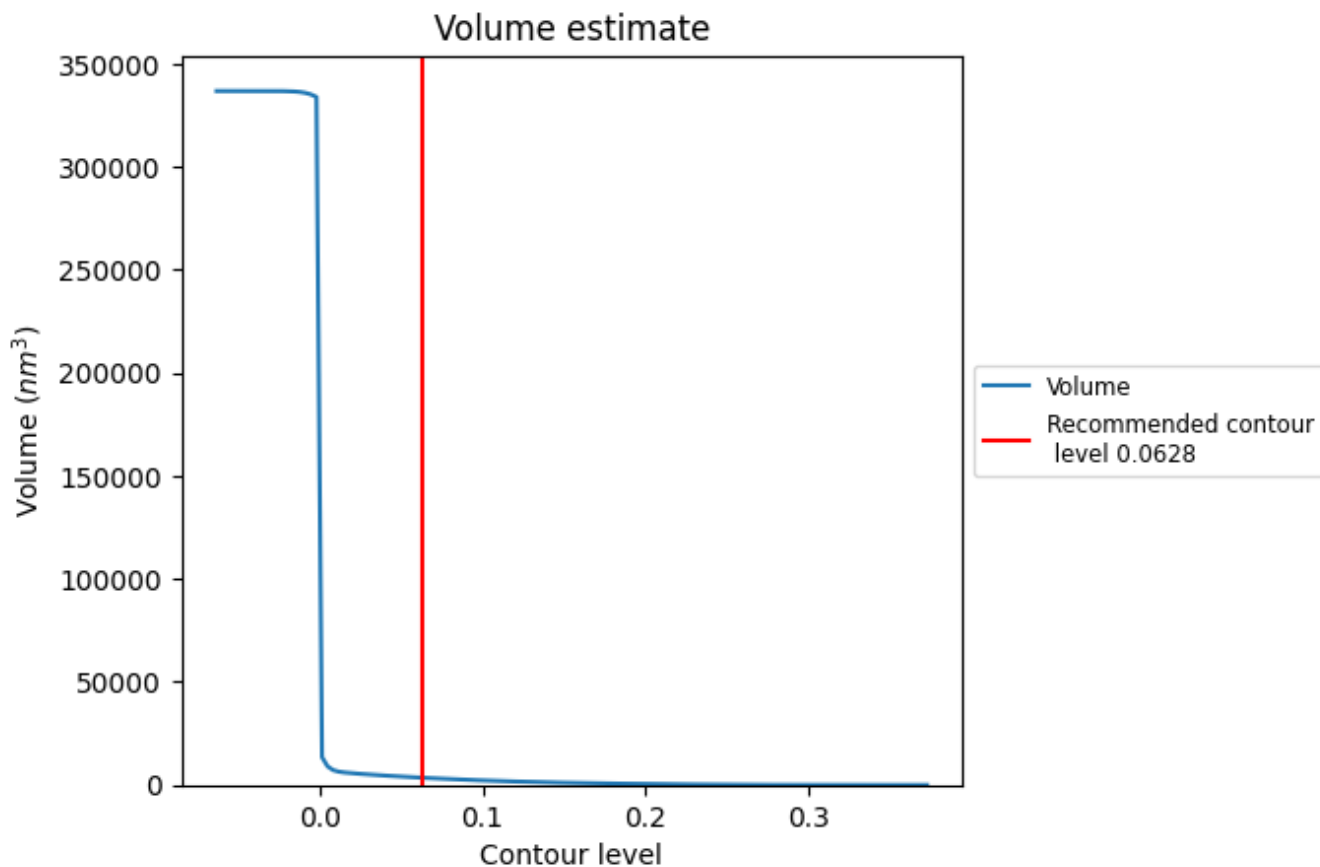
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

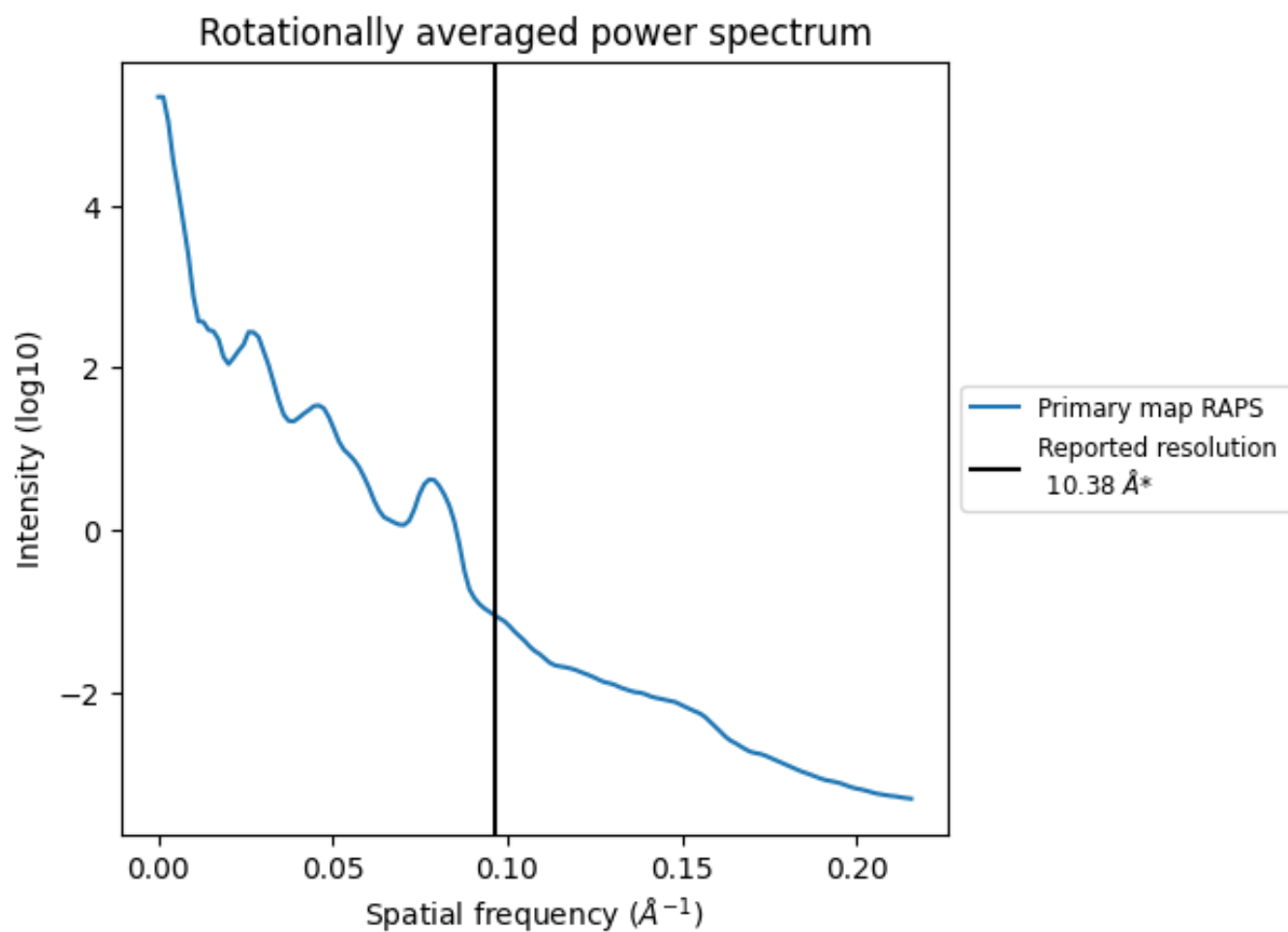
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3511  $\text{nm}^3$ ; 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](#)

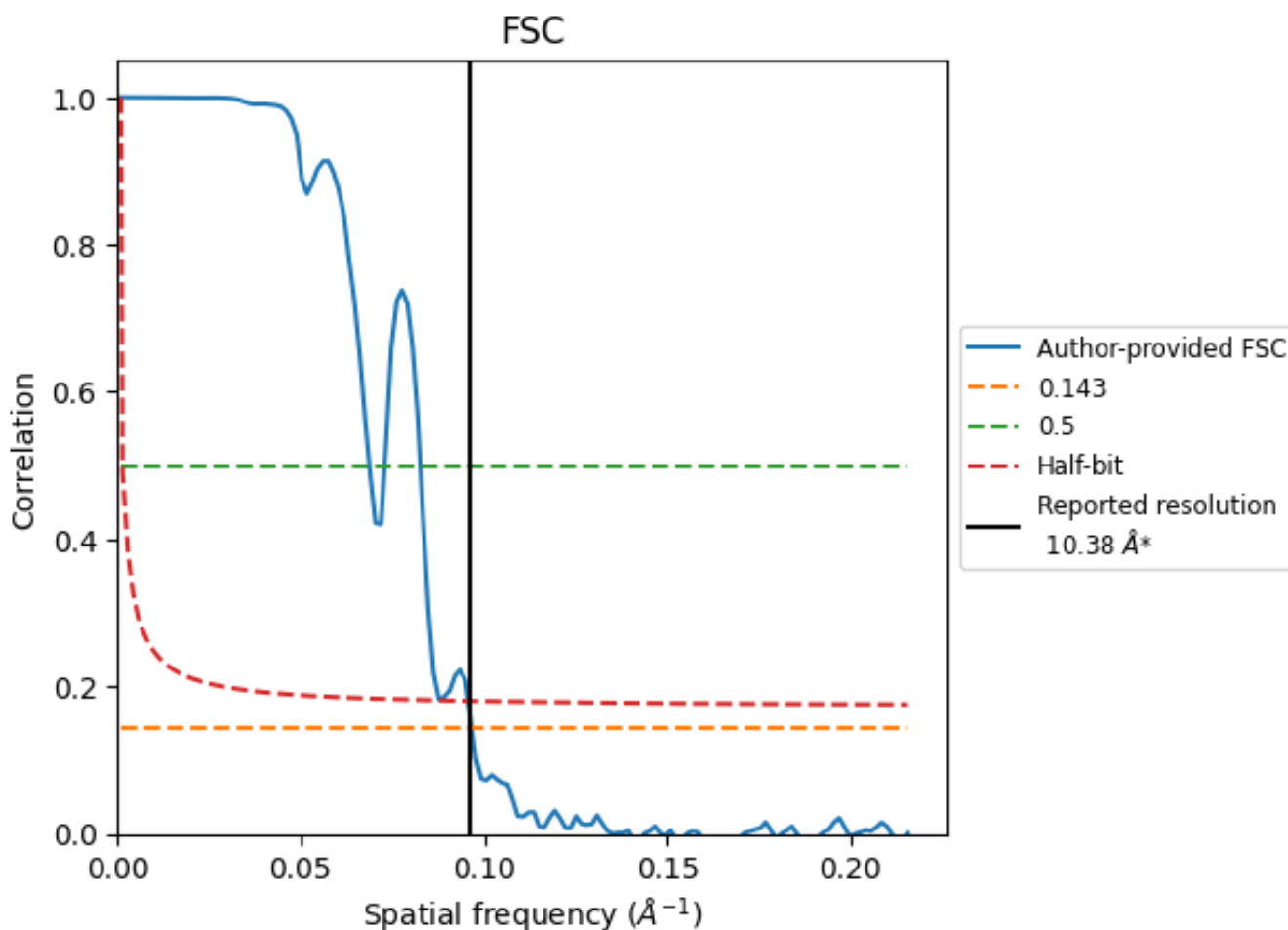


\*Reported resolution corresponds to spatial frequency of  $0.096 \text{\AA}^{-1}$

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

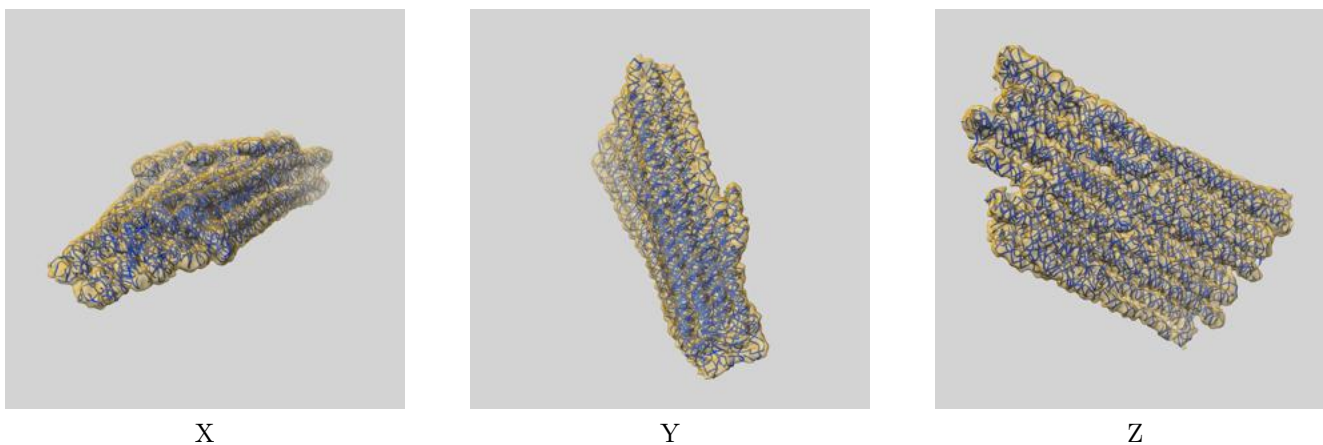
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.38	-	-
Author-provided FSC curve	10.34	14.56	10.45
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

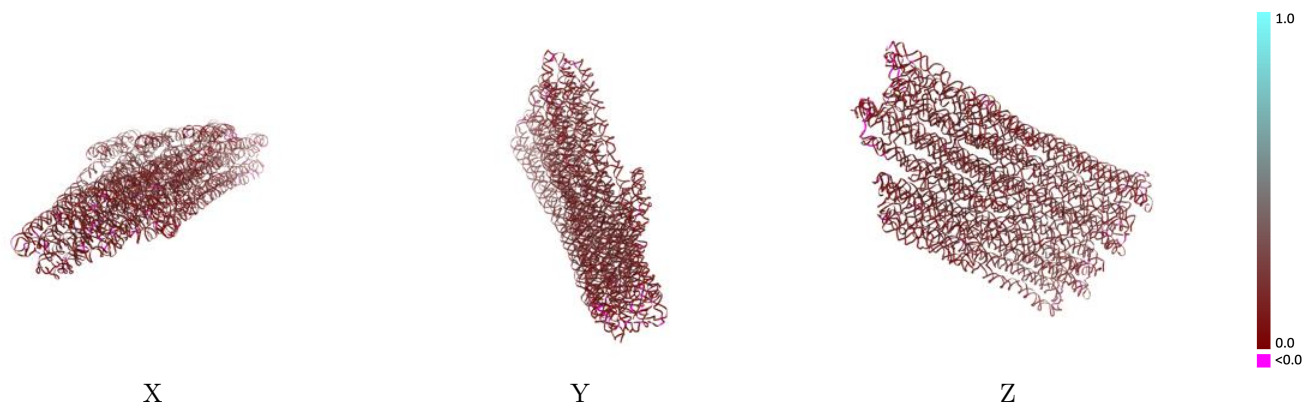
This section contains information regarding the fit between EMDB map EMD-12516 and PDB model 7NPN. Per-residue inclusion information can be found in section 3 on page 18.

### 9.1 Map-model overlay [i](#)



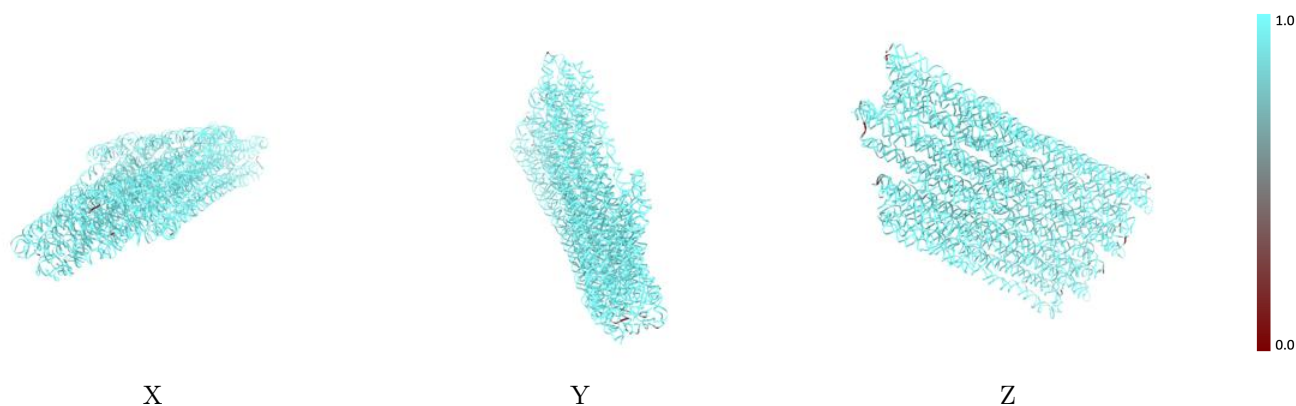
The images above show the 3D surface view of the map at the recommended contour level 0.0628 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

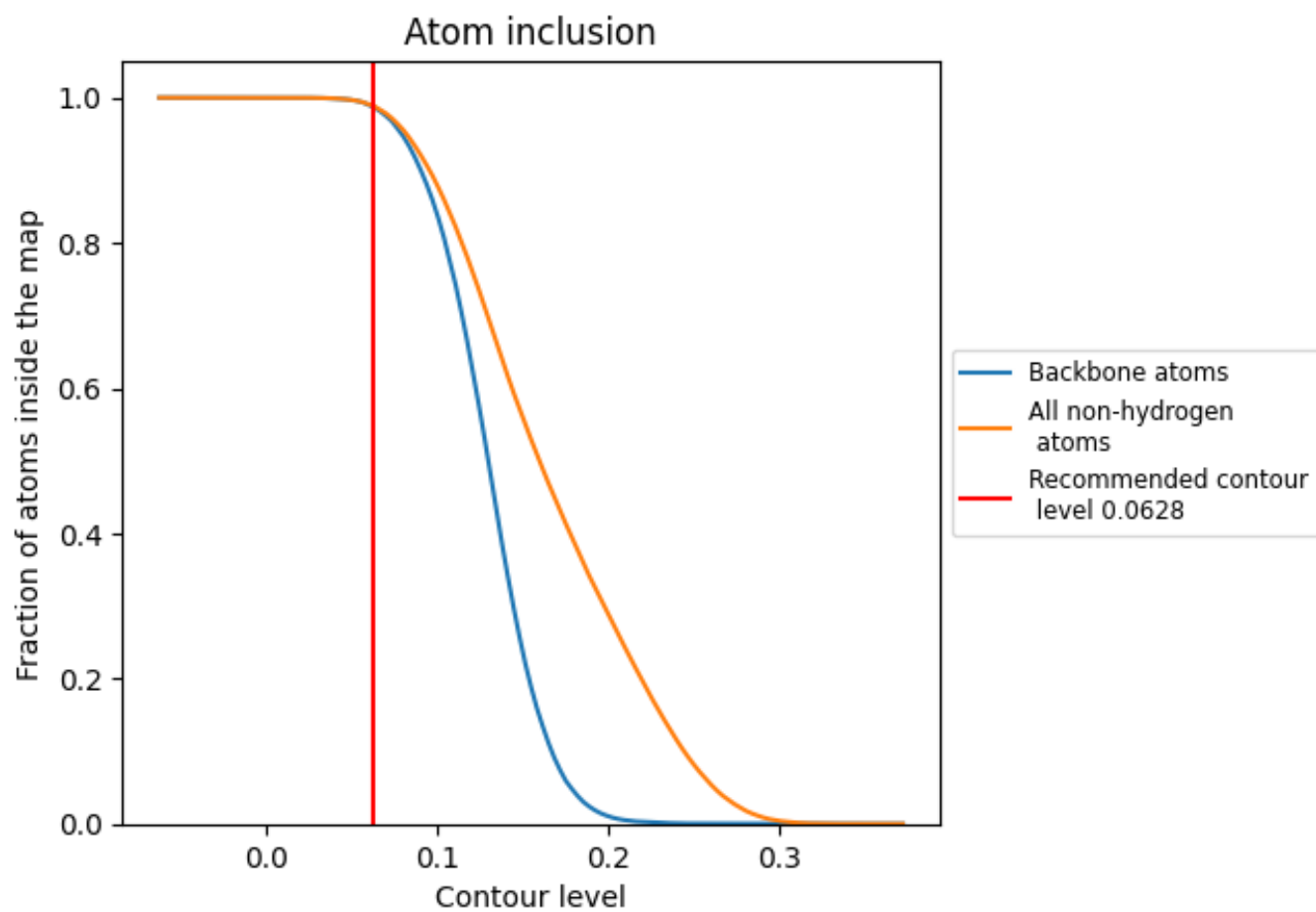
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.0628).



## 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





















































































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	0.9883	0.1650
A0	0.9976	0.1910
A1	0.9307	0.1530
A2	0.9598	0.1210
A3	0.9880	0.1620
A4	0.9977	0.1810
A5	0.9856	0.1520
A6	0.9843	0.1280
A7	0.9311	0.1230
A8	0.9986	0.1930
A9	1.0000	0.1800
AA	0.9945	0.1700
AB	0.9971	0.1520
AC	0.9866	0.1460
AD	0.9957	0.1910
AE	0.9905	0.1720
AF	0.9940	0.1810
AG	0.9898	0.1510
AH	1.0000	0.1630
AI	0.9791	0.1480
AJ	0.8724	0.1060
AK	1.0000	0.1910
AL	0.9988	0.1710
AM	1.0000	0.1920
AN	1.0000	0.1700
AO	1.0000	0.1700
AP	1.0000	0.1770
AQ	0.9216	0.1280
AR	0.9663	0.1080
AS	0.9475	0.0840
AT	0.9981	0.1780
AU	1.0000	0.1720
AV	0.9897	0.1510
AW	0.9977	0.1850
AX	0.9961	0.1330









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Chain	Atom inclusion	Q-score
AY	 0.9522	 0.1430
AZ	 1.0000	 0.1870
Aa	 0.9976	 0.1670
Ab	 0.9977	 0.1780
Ac	 0.9988	 0.1680
Ad	 0.9598	 0.1260
Ae	 0.9528	 0.1370
Af	 1.0000	 0.1840
Ag	 0.9736	 0.1330
Ah	 0.9346	 0.1090
Ai	 1.0000	 0.1750
Aj	 1.0000	 0.1670
Ak	 0.9541	 0.1480
Al	 0.9965	 0.1940
Am	 0.9977	 0.1710
An	 0.9988	 0.1740
Ao	 0.9808	 0.1430
Ap	 0.9262	 0.0890
Aq	 0.9279	 0.1090
Ar	 0.9981	 0.1790
As	 1.0000	 0.1880
At	 0.9841	 0.1500
Au	 0.9210	 0.1380
Av	 0.9976	 0.1940
Aw	 0.9954	 0.1890
Ax	 0.9977	 0.1800
Ay	 0.9976	 0.1610
Az	 1.0000	 0.1760
BA	 0.9986	 0.1670
BB	 0.9604	 0.1370
BC	 1.0000	 0.1650
BD	 0.9509	 0.1430
BE	 0.9599	 0.1340
BF	 0.9299	 0.1210
BG	 0.9888	 0.1660
BH	 0.9988	 0.1760
BI	 1.0000	 0.1960
BJ	 0.9913	 0.1620
BK	 0.9558	 0.1450
BL	 1.0000	 0.1710
BM	 0.9980	 0.1830
BN	 0.9988	 0.1710

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Chain	Atom inclusion	Q-score
BO	 0.9988	 0.1780
BP	 0.9563	 0.1420
BQ	 0.9921	 0.1530