

wwPDB EM Validation Summary Report (i)

Dec 19, 2022 – 11:21 am GMT

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 (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.31.3
	: : : : :

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 $\geq=3, 2, 1$ 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 c	hain	
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	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%	



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	6 6%	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%	149	% 5%					
37	Ak	59	6 9%	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	Ар	28	46%	54%						

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Mol	Chain	Length	Quality of ch	nain
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	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	6 2%	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%



Mol	Chain	Length	Quality of chain			
68	BF	41	5%	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	ВО	42	71%	24%	5%	
78	BP	34	59%	38%	•	
79	BQ	37	62%	35%	•	

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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			AltConf	Trace			
1	AA	2873	Total 58849	C 28004	N 10702	O 17271	Р 2872	0	0

• Molecule 2 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
2	AB	34	Total 691	C 331	N 125	O 202	Р 33	0	0

• Molecule 3 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
3	AC	48	Total 967	C 464	N 160	O 296	Р 47	0	0

• Molecule 4 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
4	AD	34	Total 702	C 337	N 134	0 198	Р 33	0	0

• Molecule 5 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
5	AE	41	Total 838	C 400	N 155	0 243	Р 40	0	0

• Molecule 6 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
6	AF	41	Total 831	C 398	N 145	0 248	Р 40	0	0

• Molecule 7 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
7	AG	34	Total 688	C 331	N 119	O 205	Р 33	0	0

• Molecule 8 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
8	AH	42	Total 857	C 409	N 149	O 258	Р 41	0	0

• Molecule 9 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
9	AI	28	Total 575	C 275	N 109	0 164	Р 27	0	0

• Molecule 10 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
10	AJ	34	Total 674	C 329	N 94	0 218	Р 33	0	0

• Molecule 11 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
11	AK	42	Total 859	C 413	N 151	0 254	Р 41	0	0

• Molecule 12 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
12	AL	42	Total 865	C 411	N 162	0 251	Р 41	0	0

• Molecule 13 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
13	AM	42	Total 864	C 412	N 161	O 250	Р 41	0	0

• Molecule 14 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
14	AN	42	Total 877	C 410	N 184	O 242	Р 41	0	0

• Molecule 15 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
15	AO	49	Total 1007	C 478	N 194	0 287	Р 48	0	0

• Molecule 16 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
16	AP	49	Total 999	C 479	N 178	O 294	Р 48	0	0

• Molecule 17 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace	
17	AQ	28	Total 561	C 271	N 86	0 177	Р 27	0	0

• Molecule 18 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}		AltConf	Trace	
18	AR	28	Total 564	C 273	N 90	0 174	Р 27	0	0

• Molecule 19 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
19	AS	42	Total 857	C 412	N 143	0 261	Р 41	0	0

• Molecule 20 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}		AltConf	Trace		
20	AT	52	Total 1049	C 503	N 181	0 314	Р 51	0	0

• Molecule 21 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
21	AU	49	Total 1011	$\begin{array}{c} \mathrm{C} \\ 479 \end{array}$	N 187	O 297	Р 48	0	0

• Molecule 22 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
22	AV	52	Total 1064	C 507	N 195	0 311	Р 51	0	0

• Molecule 23 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
23	AW	42	Total 860	C 408	N 165	0 246	Р 41	0	0

• Molecule 24 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
24	AX	38	Total 762	C 369	N 117	O 239	Р 37	0	0

• Molecule 25 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
25	AY	31	Total 628	C 304	N 107	0 187	Р 30	0	0

• Molecule 26 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
26	AZ	49	Total 1000	C 478	N 185	O 289	Р 48	0	0

• Molecule 27 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
27	Aa	41	Total 832	C 398	N 163	0 231	Р 40	0	0

• Molecule 28 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
28	Ab	42	Total 856	C 407	N 163	O 245	Р 41	0	0

• Molecule 29 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
29	Ac	42	Total 860	C 410	N 154	0 255	Р 41	0	0

• Molecule 30 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
30	Ad	34	Total 697	C 337	N 116	0 211	Р 33	0	0

• Molecule 31 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
31	Ae	41	Total 826	C 401	N 130	O 255	Р 40	0	0

• Molecule 32 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
32	Af	42	Total 865	C 415	N 155	0 254	Р 41	0	0

• Molecule 33 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
33	Ag	28	Total 569	C 275	N 94	0 173	Р 27	0	0

• Molecule 34 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
34	Ah	34	Total 688	C 336	N 105	0 214	Р 33	0	0

• Molecule 35 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
35	Ai	49	Total 1007	C 481	N 194	0 284	Р 48	0	0

• Molecule 36 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
36	Aj	42	Total 851	C 407	N 154	0 249	Р 41	0	0

• Molecule 37 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
37	Ak	59	Total 1199	C 574	N 203	0 364	Р 58	0	0

• Molecule 38 is a DNA chain called STAPLE STRAND.

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

• Molecule 39 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
39	Am	42	Total 862	C 410	N 163	0 248	Р 41	0	0

• Molecule 40 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
40	An	42	Total 862	C 411	N 159	0 251	Р 41	0	0

• Molecule 41 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
41	Ao	28	Total 573	С 274	N 104	0 168	Р 27	0	0

• Molecule 42 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
42	Ap	28	Total 569	С 276	N 90	0 176	Р 27	0	0

• Molecule 43 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
43	Aq	41	Total 832	C 400	N 140	O 252	Р 40	0	0

• Molecule 44 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
44	Ar	52	Total 1052	C 510	N 165	O 326	Р 51	0	0

• Molecule 45 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
45	As	49	Total 985	C 470	N 169	O 298	Р 48	0	0

• Molecule 46 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
46	At	52	Total 1067	C 507	N 192	0 317	Р 51	0	0

• Molecule 47 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
47	Au	52	Total 1063	C 507	N 198	O 307	Р 51	0	0

• Molecule 48 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
48	Av	42	Total 849	C 404	N 160	0 244	Р 41	0	0

• Molecule 49 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
49	Aw	42	Total 872	C 409	N 179	0 243	Р 41	0	0

• Molecule 50 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
50	Ax	42	Total	C 407	N 162	0	P 41	0	0
			859	407	103	248	41		

• Molecule 51 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
51	Ау	41	Total 841	C 402	N 150	0 249	Р 40	0	0

• Molecule 52 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
52	Az	35	Total 717	C 339	N 141	O 203	Р 34	0	0

• Molecule 53 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
53	A0	41	Total 840	C 401	N 151	0 248	Р 40	0	0

• Molecule 54 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
54	A1	45	Total 923	C 439	N 167	0 273	Р 44	0	0

• Molecule 55 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
55	A2	34	Total 697	C 338	N 115	0 211	Р 33	0	0

• Molecule 56 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms	AltConf	Trace		
56	A3	41	Total 835	C 404	N 136	O 255	Р 40	0	0

• Molecule 57 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
57	A4	42	Total 852	C 409	N 158	0 244	Р 41	0	0

• Molecule 58 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
58	A5	31	Total 627	C 302	N 115	O 180	Р 30	0	0

• Molecule 59 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
59	A6	28	Total 573	C 277	N 95	0 174	Р 27	0	0

• Molecule 60 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
60	A7	34	Total 682	C 331	N 104	0 214	Р 33	0	0

• Molecule 61 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
61	A8	34	Total 697	C 335	N 127	O 202	Р 33	0	0

• Molecule 62 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
62	A9	42	Total 867	C 413	N 166	0 247	Р 41	0	0

• Molecule 63 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
63	BA	35	Total 708	C 337	N 137	O 200	Р 34	0	0

• Molecule 64 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
64	BB	45	Total 909	C 441	N 153	0 271	Р 44	0	0

• Molecule 65 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
65	BC	35	Total 725	C 346	N 137	O 208	Р 34	0	0

• Molecule 66 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
66	BD	28	Total 570	C 277	N 92	0 174	Р 27	0	0

• Molecule 67 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
67	BE	28	Total 573	C 280	N 86	0 180	Р 27	0	0

• Molecule 68 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
68	BF	41	Total 827	C 401	N 124	O 262	Р 40	0	0

• Molecule 69 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
69	BG	35	Total 712	C 344	N 124	0 210	Р 34	0	0

• Molecule 70 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
70	BH	42	Total 863	C 413	N 160	O 249	Р 41	0	0

• Molecule 71 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
71	BI	42	Total 873	C 415	N 182	O 235	Р 41	0	0

• Molecule 72 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
72	BJ	45	Total 924	С 445	N 161	0 274	Р 44	0	0

• Molecule 73 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
73	BK	31	Total 633	C 305	N 112	0 186	Р 30	0	0

• Molecule 74 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
74	BL	42	Total 852	C 405	N 153	O 253	Р 41	0	0

• Molecule 75 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
75	BM	49	Total 1002	С 477	N 195	0 282	Р 48	0	0

• Molecule 76 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
76	BN	41	Total 840	C 401	N 151	0 248	Р 40	0	0

• Molecule 77 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
77	BO	42	Total 852	C 412	N 143	O 256	Р 41	0	0

• Molecule 78 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
78	BP	34	Total 687	C 335	N 103	O 216	Р 33	0	0

• Molecule 79 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
79	BQ	37	Total 755	C 362	N 133	0 224	Р 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



	A1078 T1079	T1082	C1083 T1084	C1085	T1087	C1097	H4 101	TOILI	C1104	T1106	G1107	T1110	T1111 T1111	T1112 T1113	10,10	C1171	A1124	61127		A1130	C1133	C1134 C1135	C1136 C1137	T1138	A1142	C1116	A1146	T1147 C1148	A1149 A1150	A1151	29119	T1158	T1161 G1162	A1163	T1166	10110
T1171	T1172 T1173	T1175	C1179	G1180	A1185	11186 C1187	T1188	G1189 C1190	T1191	76119	T1 195	C1201	A1202	A1203 A1204	A1205	A1205 A1207	A1208	01203	C1213	G1214 C1215	T1216 A1217	177H	A1220 61221	C1222	G1223 G1224	T1225	G1227	T1228 T1229	T1234	G1235	C1236 C1237	G1238 G1239	A1240	A1244	61245 A1246	G1248
T1249	A1250	11250 T1259	G1265	A1266	G1268	G1269 T1270	A1271	A1272 C1273	T1274	G1276 G1276	C1277	11278 T1279	4100C	61287	C1288	G1289 C1290	H 17007	A1295		A1298 A1299	A1300 T1201	11301 A1302	C130F	T1306	T1307 C1308	T1309 T1310		A1313	G1316	T1323	A1324 G1325	T1326 T1327	A1328	G1330	A1333	T1338
T1339	G1343	C1346	G1350	<u>61362</u>		C1356 C1357	H T T	11361 A1362	T1 3 GE	41366	C1367	C1370	G1371	T1373	C1374	61376 G1376	C1377	A1380	T1381	C1382 C1383	T1384	C00719	A1388	A1391	G1392	T1397		G1401 C1402	C1403 A1404	G1405	C1409	G1410 A1411	T1412		C1427 C1427	G1429
G1430	G1441	C1 443	G1444 A1445	T1446 A1AA7	G1448	.1.1 4 49	C1452	61454 61454	A1 / FO	AC4-LA	C1462	C1467	G1468 C1460	T1470	C1471	G1472 G1473	G1474	C14/3 T1476	201	C1480 G1481	G1482	G1483 G1484	G1485	T1487	G1490	A1 /06		C1501	G1504 C1505		60915	C1516 G1517	A1518	T1521	A1524	A1529
C1530	G1534	T1536	A1537 C1538	C1539 T1540	A1541	C1542 A1543	17 U 71	1154/ G1548	A1549	ACCT 5	A1553	11554 G1555		G1561		C1565 A1566	C1567	C1569	T1570	C1573	C1574	C/CT5	G1579	A1585	G1586 G1587	C1588	G1601	A1605	G1606 C1607		G1612 G1613	G1614	G1617	C1621	G1623	41625
G1626	A1627 G1628 G1628	67010	G1634 A1635	G1636 C1637	G1638	A1639 G1640	C1641	C1644	C1 617	61648		19919	G1656	C1658	T1659	000	T1668	A1671	G1672	T1673 C1674	C1675 T1676	G1677	T1678	G1681	G1682 T1683	T1684 T1684		C1688 C1689	A1690 C1691	1 00	C1694 T1695	C1698	T1699 T1700	G1701	G1703	
G1708	A1709 T1710	T1714	G1715 T1716	T1710	G1720	C1721 T1722	C1723	G1728	G1729	61731 G1731	G1732	61/33	A1737	C1739	14740	A1/40	A1749	C1751	G1752	C1753 C1754	A1755	A1758	C1 761	C1762	G1763 G1764	C1765	T1768	T1771	C1778	C1779	G1782	C1783 C1784	T1785		T1791	61793
C1794	C1795 T1796	T1799	G1800 C1801	A 1804	C1805	A1806 T1807	G1808	11809 T1810	C1811	11812 T1813	T1814	G1818	C1819	07015	T1824	C1825 C1826	C1827	C1020 T1829	G1830	A1831 T1832	T1025	11035 G1836	T1837	A1840	G1846	A 1861	C1852	C1853 G1854	C1855	T1858	T1863	G1864 A1865	G1866		A1872	
C1876	C1878		G1882 C1883	A1884	C1886	C1887 C1888	00 00 00	61892 A1893	C1894	CR2 TA	G1898	G1900		G1905	A1906	61907	A1910	C1916	G1917	A1918 G1919	G1920	A1921 A1922	G1923 C1924	G1925	G1926 A1927	C1021		C1934	A1 <mark>9</mark> 37	C1941	61942	A1945 A1946	C1947	G1949		T1954
	G1959 C1960	G1963	T1964 T1965	G1966 C1967	C1968	C1969 G1970	A1971	7./ AT I	T1 <mark>976</mark> T1077		G1987	G1989 C1989	1007	C1334 A1995	G1996	e Taal	T2000	C2002	C2003	G2004 A2005	C2006	1 2001	A2010	G2013	G2016	G2017		G2022 A2023	G2024 C2025	G2026	0.20.27	C2030 G2031	04000		G2044 G2044	C4-07 1
C2051	A2052 C2053	1 2054 C2055	A2056	G2060	C2062	A2063	C2066	02067 A2068	G2069	42010	T2074	A2075 C2076	A2077	T2081	A 2082	1 2083	T2086	C2089	G2090	G2091 C2092	T2093	62095 G2095	00000	00075	G2102 T2103	00100	T2110	T2111 G2112	T2113 G2114	A2115 66116	G2116 C2117	A2120	T2121	A2123	47 170	17171
A2133	G2136	G2143	C2144 T2145	101E0	T2153	67154	A2164	T2172	T 0476	0/171	G2179	62180	A2186	T2189	C2190		C2196	1219/ G2198	G2199	C2200 C2201	G2202	12203 C2204	G2205 T2206	00771	T2209 A2210	C2211	C2213	T2216	G2217 A2218	T2219	077.71	G2223 C2224	08002	C2231	62232 10001	00771
T2238	G2242	C2244	T2245	T2251	G2254	0.7.7.99	T2260	62261 G2262	C2263	0220 6		0.2211	C2280	T2282		C2285 T2286	G2287	G2289	A2290	A2291	C2294	C2296 C2296	T2297	G2299	C2300 G2301	C030F	C2306	C2307 A2308	T2311	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	C2316 G2317	C2318	62322	G2325		1 233U C2331
C2332	C2333 C2334 C2334	12336 12336	G2340	C2341	G2344	G2347	G2348	T2354	A2355	62357 C2357		62303	C2 <mark>367</mark>	000250	C2372	62373 A2374	T2375	G2377		C2380 T2381	T2382	A2387	C2388	T2391	T2392 G2393		A2397	C2400	T2401 G2402	A2403	A2404 T2405	G2406 G2407	C2408	A2411	12412 G2413	A2416







Chain AF:	68%	29%	6 ·
T1 65 17 11 11 11 11 11 125 125	C26 131 131 131 131 131 131 131 131 131 13		
• Molecule 7: STA	APLE STRAND		
Chain AG:	56%	35%	9%
11 66 66 66 67 61 61 61 719 81 81 819	722 124 125 125 125 123 134 134		
• Molecule 8: STA	APLE STRAND		
Chain AH:	50%	43%	7%
A1 62 65 65 67 67 61 61 112 112 115 616 616 616	0.17 1123 1123 1123 1123 1123 1123 1123 11		
• Molecule 9: STA	APLE STRAND		
Chain AI:	54%	46%	
• Molecule 10: ST	APLE STRAND		
Chain A I:			120/
Ollam A5.	47%	41%	12%
11 12 13 13 13 17 11 11 111 111 111 111 111 1	1219 1210 121 121 121 122 122 122 123 123 133 133		
• Molecule 11: ST	CAPLE STRAND		
Chain AK:	57%	36%	7%
C1 A2 G3 G1 G11 G11 G12 G12 G12 G12	A23 G24 T30 G31 T36 G32 G32 C37 C37 C37 C37 C37 C37 C37 C37 C37 C37		
• Molecule 12: ST	APLE STRAND		
Chain AL:	57%	33%	10%
A1 6 G4 7 8 6 12 6 13 7 12 6 12 6 12 7 12 6 12 7 12 6 12 7 12 6 12 7 12 6 12 7 12 7 12 7 12 7 12 7 12 7 12 7 12 7	425 425 433 433 433 433 433 433 433 433 434 649 649 649 649 649 641 641		
• Molecule 13: ST	APLE STRAND		
Chain AM.	570/		
	5776		·
	PROT	EIN DATA BANK	





 Molecule 21: STAPLE STRAND Chain AU: <u>65%</u> 22% 12% Molecule 22: STAPLE STRAND Chain AV: <u>56%</u> 42% . Molecule 23: STAPLE STRAND Chain AW: <u>64%</u> 33% . StapLe STAPLE STRAND Chain AW: <u>64%</u> 33% . StapLe STAPLE STRAND Chain AX: <u>55%</u> 45% 35% 36% 36% 36% 36% 36% 36% 36% 36% 36% 36	11 22 25 45 45 41 411 411 411 411 411 411 411 4	C17 C28 C28 C28 C33 C33 C33 C33 C33 C33 C33 C33 C33 C3		
Chain AU: 65% 22% 12% I 8 4 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	• Molecule 21: STA	PLE STRAND		
* **** *** **** ****** • Molecule 22: STAPLE STRAND Chain AV: 56% 42% * Molecule 23: STAPLE STRAND Chain AW: 64% 33% • Molecule 23: STAPLE STRAND Chain AW: 64% 33% • Molecule 24: STAPLE STRAND Chain AX: 55% 45% • Molecule 24: STAPLE STRAND Chain AX: 55% 45% • Molecule 25: STAPLE STRAND Chain AY: 7% 1% • Molecule 26: STAPLE STRAND Chain AY: 7% 1% • Molecule 26: STAPLE STRAND Chain AY: 7% 1% • Molecule 26: STAPLE STRAND Chain AY: 6% 2% • Molecule 26: STAPLE STRAND Chain AZ: 6% 8% 8% • Molecule 26: STAPLE STRAND Chain AZ: 6% 8% 8% • Molecule 27: STAPLE STRAND Chain AZ: 6% 8% 8% • Molecule 27: STAPLE STRAND Chain Aa: 10% 10%	Chain AU:	65%	22%	12%
 Molecule 22: STAPLE STRAND Chain AV: 56% 42% . Staple 23: STAPLE STRAND Chain AW: 64% 33% . Chain AW: 64% 33% . Molecule 24: STAPLE STRAND Chain AX: 55% 45% 55% 56% 56% 56% 56% 56% 56% 56% 56% 5	11 16 17 19 110 110 117 117 117 117 117 123 123	628 629 631 134 135 135 135 631 135 631 644 649 649		
Chain AV: 56% 42% \$	• Molecule 22: STA	PLE STRAND		
0 2 0 2 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Chain AV:	56%	42%	•
 Molecule 23: STAPLE STRAND Chain AW: 64% 33% Chain AW: 64% 33% Chain AX: 55% 45% Molecule 24: STAPLE STRAND Chain AX: 55% 45% Chain AX: 55% 45% A solution of the stress of the stress	G1 42 73 73 73 73 73 73 71 71 110 715 714 7110 715 715 715 715 715 715 715 715 715 715	C 19 C 19 C 19 C 19 C 19 C 19 C 19 C 19	144 152	
Chain AW: 64% 33% • Molecule 24: STAPLE STRAND Chain AX: 55% 45% • • • • • • • • • • • • • • • • • • •	• Molecule 23: STA	PLE STRAND		
• • • • • • • • • • • • • • • • • • •	Chain AW:	64%	33%	·
 Molecule 24: STAPLE STRAND Chain AX: 55% 45% 8 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9	61 62 62 62 63 64 64 64 65 65 65 65 65 62 62 62 62 62 62 62 62 62 62 62 62 62	C 31 C 32 C 32 C 33 C 33 C 33 C 33 C 33 C 33		
Chain AX: 55% 45% 8 2	• Molecule 24: STA	PLE STRAND		
• •	Chain AX:	55%	45%	
 Molecule 25: STAPLE STRAND Chain AY: 71% 19% 10% I I I I I I I I I I I I I I I I I I I	11 0 11 11 11 11 11 12 12 12 12 12 12 12	623 624 625 625 624 633 633 633 633 633 633 633 638 638 638		
Chain AY: 71% 19% 10% H H H H H H H H H H H H H H H H H H H	• Molecule 25: STA	PLE STRAND		
I I I I I I I I I I I I I I I I I I I	Chain AY:	71%	19%	10%
 Molecule 26: STAPLE STRAND Chain AZ: 63% 29% 8% Chain AZ: 29% 8% Chain Az: 29% 202 202 202 202 202 202 202 202 202 20	11 12 13 14 15 16 119 119 119 119 119 123 123 123 123 122 123 122 123 122	A 30 B 31 B 12 B 12 B 12 B 12 B 12 B 12 B 12 B 1		
Chain AZ: 63% 29% 8% • 8 * • • • • • • • • • • • • •	• Molecule 26: STA	PLE STRAND		
• •	Chain AZ:	63%	29%	8%
Molecule 27: STAPLE STRAND Chain Aa: 71% 27% .	A 43 43 43 44 44 44 44 44 44 44 44 44 44 4	126 127 126 126 123 141 141 141 141 141 141 141 141 141 14		
Chain Aa: 71% 27% ·	• Molecule 27: STA	PLE STRAND		
	Chain Aa:	71%	27%	•





• Molecule 28: STAPLE STRAND

Chain Ab:	52%	43%	5%
A1 A9 G10 A13 A13 A14 A13 C16 C17 C15 C15 C19	C20 C21 C22 C23 C23 C23 C23 C23 C23 C23 C23 C23		
• Molecule 29: S	TAPLE STRAND		
Chain Ac:	64%	29%	7%
C1 12 63 64 64 64 64 64 64 64 64 64 64 64 64 64	027 128 429 630 634 135 135 135 135 135 142		
• Molecule 30: S	TAPLE STRAND		
Chain Ad:	68%	29%	·
11 12 13 14 14 115 115 116 116 116 118	419 420 424 132 133 133 133		
• Molecule 31: S	TAPLE STRAND		
Chain Ae:	66%	29%	5%
11 13 15 15 15 15 15 15 12 12 12 12	A20 133 A33 A33 A33 141 141		
• Molecule 32: S	TAPLE STRAND		
Chain Af:	64%	31%	5%
11 62 85 86 86 86 89 610 610 114 114	G16 118 122 122 133 134 133 133 133 133 133 133 133 133		
• Molecule 33: S	TAPLE STRAND		
Chain Ag:	61%	36%	·
11 14 14 14 14 11 11 12 120 520	621 123 123 124 124 124 123 123		
• Molecule 34: S	TAPLE STRAND		
Chain Ah:	50%	41%	9%













• Molecule 49: STAPLE STRAND





11 15 17 17 17 17 17 17 17 17 17 17 17 17 17	ALO ALO (220 (220 (22) A.22 (23) (23) (23) (23) (23) (23) (23) (2		
• Molecule 56: STA	APLE STRAND		
Chain A3:	56%	32%	12%
T1 T4 A7 A9 G10 G14 T111 T111 T112 T113 C16 G16 G16 G16	619 A20 A21 A21 A21 A21 C26 C26 C26 C27 C27 C28 C27 C28 C27 C28 T28 T28 T38 T39 T41		
• Molecule 57: STA	APLE STRAND		
Chain A4:	74%		24% •
C1 C10 C10 A11 A12 A12 A29 A29 A29 A29 A29 A29 A29 A29 A29 A2	63 4 5 3 4 4 5 3 3 4 4 5 3 3 4 4 5 5 3 8 5 5 3 8 5 5 5 5 5 5 5 5 5 5 5 5		
• Molecule 58: STA	APLE STRAND		
Chain A5:	61%	35%	•
A1 C2 A3 A4 A6 G7 A6 A6 C10 C10 C113 A15 A15 A15 A15 A15 A15 A15 A15 A15 A15	C 18 A 25 A 25 A 25 T 29 T 29 T 30 T 30 T 30		
• Molecule 59: STA	APLE STRAND		
Chain A6:	68%	25%	7%
11 13 13 13 11 11 11 13 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14	G25 126 127 128 128		
• Molecule 60: STA	APLE STRAND		
Chain A7:	62%	38%	
11 15 15 11 11 11 11 12 12 12 12 12 12 12 12 12	A23 173 133 133 133 133		
• Molecule 61: STA	APLE STRAND		
Chain A8:	68%	32	2%
C1 17 18 110 110 113 113 113 113 113 113 113 113	A 23 G 30 T 34 T 34 T 34		
• Molecule 62: STA	APLE STRAND		
Chain A9:	64%	33%	















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 $(e^-/\text{\AA}^2)$	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 (Å)	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 (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		B	ond lengths	Bond angles			
	Chain	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	$0/\overline{766}$	1.62	$17/1181 \ (1.4\%)$		



Mal	Chain	B	ond lengths	-	Bond angles
	Chain	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%)



Mal	Chain	B	ond 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



Continued from previous page...

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



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

Continued from previous page...

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	Ζ	$Observed(^{o})$	$Ideal(^{o})$
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



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.

Largest variance slices (i) 6.3

6.3.1Primary 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.

Orthogonal surface views (i) 6.4

6.4.1**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.



6.5 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 $\rm nm^3;$ 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 ${\rm \AA^{-1}}$



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 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	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 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.



1.0

0.0 <0.0

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.

\mathbf{Chain}	Atom inclusion	$\mathbf{Q} extsf{-score}$
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
Ар	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

