

## wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 08:55 pm GMT

DDB ID		ZARV
I DD ID	•	IANI
EMDB ID	:	EMD-11378
Title	:	Twist-Tower_twist-corrected-variant
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		Dietz, H.
Deposited on	:	2020-10-26
Resolution	:	8.50 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 8.50 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	8064	19% 62%	32%	5%			
2	AB	47	57%	38%	•			
3	AC	53	<b>6</b> 2%	36%	•			
4	AD	48	56%	38%	6%			
5	AE	48	71%	27%	•			
6	AF	55	56%	35%	9%			
7	AG	48	75%	23%	•			
8	AH	31	68%	26%	6%			
9	AI	28	71%	25%	•			
10	AJ	48	81%	15%	•			
11	AK	32	66%	34%				
12	AL	52	71%	25%	•			
13	AM	38	84%	1	6%			
14	AN	46	74%	24%	•			
15	AO	46	72%	26%	•			
16	AP	48	71%	27%	•			
17	AQ	48	67%	25%				



Mol	Chain	Length	Quality of chain					
18	AR	46	9%	20%	•			
19	AS	50	24%	28%	<b>.</b>			
20		47	15%					
20	AI	47	20%	23%	•			
21	AU	40	62% 53%	32%	5%			
22	AV	45	69%	29%	•			
23	AW	48	75%	21%	·			
24	AX	37	54%	43%	•			
25	AY	47	6%	32%	<del>.</del>			
26	AZ	40	<b>6</b> 5%	32%	•			
27	Aa	53	8%	26%	•			
28	Ab	39	67%	31%	•			
29	Ac	31	29%	139	<b>%</b> •			
30	Ad	45	62%	31%	7%			
31	Ae	52	37%	27%	<u> </u>			
20	Λf	46	• •					
32	AI	40	63% 7%	33%	•			
33	Ag	30	63% <u>8%</u>	33%	•			
34	Ah	39	82% 65%	15%	•			
35	Ai	48	60%	31%	8%			
36	Aj	40	72%	22%	5%			
37	Ak	38	79%	18%	•			
38	Al	56	27%	29%				
39	Am	38	24%	16%				
40	An	45	67%	29%	·			
41	Ao	46	13%	22%	•			
42	Ар	48	69%	29%	•			

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Conti	nued fron	n previous	page					
Mol	Chain	Length	Quality of chain					
43	Aq	32	59%	34% 6%				
44	Ar	48	19% 67%	31% •				
45	As	48	58%	42%				
46	At	54	19% 67%	30% •				
47	Au	46	78%	22%				
48	Av	48	38%	29% 6%				
49	Aw	48	83%	8% •				
50	Ax	45	<b>6</b> 7%	31%				
51	Av	31	19%	19% •				
52	Az	30	30%	40%				
53	AO	32	66%	34%				
54	A1	48	29%	20%				
55	A2	46	67%	2004				
56	A3	30	10%	30%				
57	A4	45	13%	20%				
58	Δ5	45	47%	160/				
50	10	40	19%	10%				
60	AO	40	67%	31% •				
00	A	40	67% 58%	25% 8%				
61	A8	60	73%	23% •				
62	A9	38	63%	34% •				
63	BA	48	60% 48%	40%				
64	BB	31	68% 57%	29% •				
65	BC	60	75%	25%				
66	BD	53		15% 6%				
67	BE	32	75%	25%				



Continue	nued from	n previous	page						
Mol	Chain	Length	Quality of chain						
68	BF	38	63%	32%	5%				
69	BG	47	9% 57%	34%	9%				
70	BH	57	68%	28%	•				
71	BI	45	76%	20%	•				
72	BJ	45	69%	31%					
73	BK	48	63%	33%	•				
74	BL	45	<b>6</b> 4%	36%					
75	BM	48	69%	29%	•				
76	BN	30	73%	17%	10%				
77	ВО	45	62%	31%	7%				
78	BP	45	67%	31%	•				
79	BQ	45	64%	36%					
80	BR	38	66%	29%	5%				
81	BS	48	77%	21%	•				
82	BT	52	71%	25%	•				
83	BU	39	59%	31%	10%				
84	BV	32	56%	38%	6%				
85	BW	31	<b>6</b> 5%	35%					
86	BX	45	84%	1	16%				
87	BY	52	77%	21%	•				
88	ΒZ	46	80%	20	%				
89	Ba	46	<b>6</b> 3%	33%	•				
90	Bb	38	53%	32%	16%				
91	Bc	45	64%	29%	7%				
92	Bd	48	71%	25%	•				



Conti	nued fron	n previous	page					
Mol	Chain	Length	Quality of chain					
93	Be	45	62%	33%	•			
94	Bf	38	66%	29%	5%			
95	Bg	38	26% 47%	45%	8%			
96	Bh	40	<b>6</b> 5%	28%	8%			
97	Bi	49	63%	33%	•			
98	Bj	48	<b>6</b> 5%	29%	6%			
99	Bk	30	63%	30%	7%			
100	Bl	40	68%	32%				
101	Bm	38	66%	32%	·			
102	Bn	43	7% 70%	28%	•			
103	Bo	45	60%	38%	•			
104	Вр	47	53%	34%	13%			
105	Bq	48	81%	179	% •			
106	Br	38	71%	26%	•			
107	Bs	30	40%	37%	17%			
108	Bt	45	64%	33%	•			
109	Bu	49	69%	24%	6%			
110	Bv	40	70%	22%	8%			
111	Bw	37	73%	19%	8%			
112	Bx	52	63%	29%	8%			
113	By	30	63%	33%	•			
114	Bz	40	78%	229	6			
115	B0	30	70%	30%				
116	B1	52	62%	37%	•			
117	B2	30	53% 67%	33%				



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Mol	Chain	Length	Quality of chain						
			11%						
118	B3	56	68%	29% •					
110	D4	4.9	19%						
119	B4	48	77% 21% •						
120	R5	31	2370	2004					
120	D0	- 51	29%						
121	B6	45	47%	53%					
	-		16%						
122	B7	37	76%	22% •					
			27%						
123	B8	52	65%	35%					
194	DO	20	21%						
124	D9	- 30	50%	45% 5%					
125	$\mathbf{C}\mathbf{A}$	32	59%	41%					
120			6%	T1/0					
126	CB	32	53%	34% 12%					
			40%						
127	CC	30	63%	37%					
100	CD	50	59%						
128	CD	59	66%	25% 8%					
120	CE	52	750/	210/					
125		02	15%	2170 ·					
130	$\operatorname{CF}$	40	65%	35%					
			<b>_</b>						
131	CG	31	61%	35% •					
100	OII	50	9%						
132	CH	53	58%	36% 6%					
133	CI	30	700/	200/ 100/					
100			10%	20% 10%					
134	CJ	49	63%	35% •					
			71%						
135	CK	56	62%	30% 7%					
100	at	01	<u> </u>						
136	CL	31	71%	29%					
137	$\mathbf{C}\mathbf{M}$	30	• • •	470/					
101	OW	02	25%	4770					
138	CN	40	60%	38% •					
			23%						
139	CO	30	70%	20% 10%					
1.40		F 1	22%						
140	CP	54	69%	24% 7%					
1/1	CO	18	750/	210/					
1.1.1	्र	10	38%	2170 ·					
142	CR	45	67%	31% •					



Mol	Chain	Length	Quality of chain				
143	CS	48	58%	40%	<b>.</b>		
144	СТ	38	<b>-</b>	42%	5%		
145	CU	30	13%	270	270		
140	00		28%	37%			
146	CV	32	75%		25%		
147	CW	47	70%	26%	6 •		
148	CX	48	71%	259	% •		
149	CY	48	63%	33%	•		
150	CZ	46	65%	30%	•		
151	Ca	39	69%	26%	5%		
152	Cb	45	80%		16% •		
153	Cc	30	47%	43%	10%		
154	Cd	38	79%		16% 5%		
155	Ce	30	63%	33%	•		
156	Cf	40	62%	35%	•		
157	Cg	38	68%	21%	11%		
158	Ch	45	60%	40%			
159	Ci	48	52%	35%	6%		
160	Ci	54	50%	270/	70/		
161	Ck	46	26%	27 /2	7 70		
101		40	9%	20	70 ·		
102	U	40	60%	31%	9%		
163	Cm	38	58%	42%			
164	Cn	45	73%		27%		
165	Со	37	54%	41%	5%		
166	Ср	37	51%	41%	8%		
167	Cq	36	78%		17% 6%		

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Mol	Chain	Length	Quality of cha	in
168	$\operatorname{Cr}$	38	5%	37% 8%
169	$\mathbf{Cs}$	39	67%	26% 8%
170	$\operatorname{Ct}$	38	55%	42% ·
171	Cu	36	69%	31%
172	Cv	37	57%	32% 11%
173	Cw	31	61%	39%
174	Cx	37	73%	16% 11%
175	Су	45	42 % 56%	42%
176	Cz	52	67%	25% 8%
177	C0	60	72%	23% 5%
178	C1	47	60%	36% •
179	C2	32	69%	28% ·
180	C3	37	78%	22%
181	C4	57	72%	28%
182	C5	44	59%	41%
183	C6	47	68%	28% •
184	C7	47	72%	26% •
185	C8	38	71%	26% ·
186	C9	37	68%	32%
187	DA	60	48%	47% 5%
188	DB	43	74%	23% •
189	DC	46	67%	33%
190	DD	38	58%	39% •
191	DE	46	61%	37% •
192	DF	31	68%	29% •





## 2 Entry composition (i)

There are 192 unique types of molecules in this entry. The entry contains 331913 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		1	AltConf	Trace			
1	AA	8064	Total 164972	C 78873	N 29001	O 49035	Р 8063	0	0

• Molecule 2 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	47	Total 972	C 463	N 191	0 272	Р 46	0	0

• Molecule 3 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
3	AC	53	Total 1091	C 520	N 212	O 307	Р 52	0	0

• Molecule 4 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
4	AD	48	Total 989	C 472	N 188	0 282	Р 47	0	0

• Molecule 5 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
5	AE	48	Total 971	C 465	N 171	0 288	Р 47	0	0

• Molecule 6 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
6	AF	55	Total 1131	C 540	N 216	0 321	Р 54	0	0

• Molecule 7 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
7	AG	48	Total 970	С 471	N 150	O 302	Р 47	0	0

• Molecule 8 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
8	AH	31	Total 636	C 307	N 116	0 183	Р 30	0	0

• Molecule 9 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	AI	28	Total 570	C 277	N 92	0 174	Р 27	0	0

• Molecule 10 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
10	AJ	48	Total 977	C 468	N 177	0 285	Р 47	0	0

• Molecule 11 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
11	AK	32	Total 657	C 312	N 123	0 191	Р 31	0	0

• Molecule 12 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
12	AL	52	Total 1065	C 511	N 188	0 315	Р 51	0	0

• Molecule 13 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$		AltConf	Trace		
13	AM	38	Total 766	С 374	N 121	0 234	Р 37	0	0

• Molecule 14 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
14	AN	46	Total 946	C 453	N 174	O 274	Р 45	0	0

• Molecule 15 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
15	AO	46	Total 947	C 450	N 192	O 260	Р 45	0	0

• Molecule 16 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
16	AP	48	Total 982	C 470	N 175	O 290	Р 47	0	0

• Molecule 17 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
17	AQ	48	Total 972	C 473	N 157	O 295	Р 47	0	0

• Molecule 18 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
18	AR	46	Total 942	C 451	N 170	0 276	Р 45	0	0

• Molecule 19 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
19	AS	50	Total 1012	C 488	N 184	0 291	Р 49	0	0

• Molecule 20 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
20	AT	47	Total 959	C 458	N 184	0 271	Р 46	0	0

• Molecule 21 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
21	AU	40	Total 823	C 391	N 164	O 229	Р 39	0	0

• Molecule 22 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
22	AV	45	Total 918	С 445	N 149	O 280	Р 44	0	0

• Molecule 23 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
23	AW	48	Total 982	C 467	N 187	0 281	Р 47	0	0

• Molecule 24 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
24	AX	37	Total 763	C 360	N 156	0 211	Р 36	0	0

• Molecule 25 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
25	AY	47	Total 966	C 466	N 176	0 278	Р 46	0	0

• Molecule 26 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
26	AZ	40	Total 813	C 388	N 152	0 234	Р 39	0	0

• Molecule 27 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
27	Aa	53	Total 1086	C 519	N 204	0 311	Р 52	0	0

• Molecule 28 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms		AltConf	Trace	
28	Ab	39	Total 798	C 383	N 145	0 232	P 38	0	0

• Molecule 29 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
29	Ac	31	Total 624	C 300	N 108	0 186	Р 30	0	0

• Molecule 30 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
30	Ad	45	Total 927	C 443	N 187	O 253	Р 44	0	0

• Molecule 31 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
31	Ae	52	Total 1056	C 509	N 175	0 321	Р 51	0	0

• Molecule 32 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
32	Af	46	Total 936	C 449	N 169	0 273	Р 45	0	0

• Molecule 33 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
33	Ag	30	Total 616	C 296	N 109	0 182	Р 29	0	0

• Molecule 34 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
34	Ah	39	Total 801	C 380	N 157	O 226	Р 38	0	0

• Molecule 35 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
35	Ai	48	Total 981	$\begin{array}{c} \mathrm{C} \\ 475 \end{array}$	N 158	O 301	Р 47	0	0

• Molecule 36 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
36	Aj	40	Total 820	C 392	N 163	O 226	Р 39	0	0

• Molecule 37 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
37	Ak	38	Total 775	C 371	N 145	0 222	Р 37	0	0

• Molecule 38 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
38	Al	56	Total 1136	C 546	N 207	0 328	Р 55	0	0

• Molecule 39 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
39	Am	38	Total 772	C 375	N 126	0 234	Р 37	0	0

• Molecule 40 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
40	An	45	Total 912	C 435	N 168	O 265	Р 44	0	0

• Molecule 41 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
41	Ao	46	Total 942	C 450	N 180	O 267	Р 45	0	0

• Molecule 42 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
42	Ap	48	Total 974	$\begin{array}{c} \mathrm{C} \\ 470 \end{array}$	N 166	0 291	Р 47	0	0

• Molecule 43 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
43	Aq	32	Total 662	C 317	N 130	0 184	Р 31	0	0

• Molecule 44 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
44	Ar	48	Total 988	C 475	N 179	0 287	Р 47	0	0

• Molecule 45 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
45	As	48	Total 991	C 471	N 204	O 269	Р 47	0	0

• Molecule 46 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
46	At	54	Total 1105	C 528	N 210	0 314	Р 53	0	0

• Molecule 47 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
47	Au	46	Total 934	C 452	N 166	0 271	Р 45	0	0

• Molecule 48 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
48	Av	48	Total 985	С 473	N 187	0 278	Р 47	0	0

• Molecule 49 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
49	Aw	48	Total 964	C 466	N 155	O 296	Р 47	0	0

• Molecule 50 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
50	Ax	45	Total 917	C 439	N 179	O 255	Р 44	0	0

• Molecule 51 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
51	Ау	31	Total 643	C 304	N 131	0 178	Р 30	0	0

• Molecule 52 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
52	Az	30	Total 613	C 293	N 118	0 173	Р 29	0	0

• Molecule 53 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
53	A0	32	Total 647	C 308	N 124	0 184	Р 31	0	0

• Molecule 54 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
54	A1	48	Total 984	C 471	N 186	O 280	Р 47	0	0

• Molecule 55 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$		AltConf	Trace		
55	A2	46	Total 941	C 452	N 181	O 263	Р 45	0	0

• Molecule 56 is a DNA chain called STAPLE STRAND.



	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
56	A3	30	Total 615	C 204	N 117	0	P 20	0	0

• Molecule 57 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A		AltConf	Trace		
57	A4	45	Total 914	C 440	N 166	0 264	Р 44	0	0

• Molecule 58 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
58	A5	45	Total 923	С 447	N 165	O 267	Р 44	0	0

• Molecule 59 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
59	A6	48	Total 994	C 474	N 198	0 275	Р 47	0	0

• Molecule 60 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$		AltConf	Trace		
60	A7	48	Total 977	С 474	N 168	0 288	Р 47	0	0

• Molecule 61 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
61	A8	60	Total 1206	C 582	N 192	0 373	Р 59	0	0

• Molecule 62 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
62	A9	38	Total 778	C 371	N 151	O 219	Р 37	0	0

• Molecule 63 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
63	BA	48	Total 980	C 469	N 188	O 276	Р 47	0	0

• Molecule 64 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
64	BB	31	Total 637	C 303	N 129	0 175	Р 30	0	0

• Molecule 65 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
65	BC	60	Total 1223	C 583	N 224	O 357	Р 59	0	0

• Molecule 66 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
66	BD	53	Total 1088	C 521	N 211	0 304	Р 52	0	0

• Molecule 67 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
67	BE	32	Total 648	C 312	N 120	0 185	Р 31	0	0

• Molecule 68 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
68	BF	38	Total 779	C 373	N 155	0 214	Р 37	0	0

• Molecule 69 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
69	BG	47	Total 959	C 462	N 162	O 289	Р 46	0	0

• Molecule 70 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms		AltConf	Trace	
70	BH	57	Total 1159	$\begin{array}{c} \mathrm{C} \\ 563 \end{array}$	N 178	O 362	Р 56	0	0

• Molecule 71 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
71	BI	45	Total 917	C 437	N 172	0 264	Р 44	0	0

• Molecule 72 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
72	BJ	45	Total 927	C 442	N 179	O 262	Р 44	0	0

• Molecule 73 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
73	BK	48	Total 981	C 470	N 178	0 286	Р 47	0	0

• Molecule 74 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
74	BL	45	Total 918	C 441	N 165	0 268	Р 44	0	0

• Molecule 75 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
75	BM	48	Total 990	C 475	N 188	O 280	Р 47	0	0

• Molecule 76 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$		AltConf	Trace		
76	BN	30	Total 618	C 296	N 118	0 175	Р 29	0	0

• Molecule 77 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
77	BO	45	Total 914	C 438	N 165	O 267	Р 44	0	0

• Molecule 78 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
78	BP	45	Total 920	C 440	N 178	O 258	Р 44	0	0

• Molecule 79 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
79	BQ	45	Total 929	C 443	N 181	0 261	Р 44	0	0

• Molecule 80 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
80	BR	38	Total 770	C 370	N 134	0 229	Р 37	0	0

• Molecule 81 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
81	BS	48	Total 972	C 471	N 168	0 286	Р 47	0	0

• Molecule 82 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
82	BT	52	Total 1070	C 507	N 213	O 299	Р 51	0	0

• Molecule 83 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$		AltConf	Trace		
83	BU	39	Total 784	C 375	N 138	0 233	Р 38	0	0

• Molecule 84 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
84	BV	32	Total 646	C 311	N 109	0 195	Р 31	0	0

• Molecule 85 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
85	BW	31	Total 624	C 297	N 117	0 180	Р 30	0	0

• Molecule 86 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
86	BX	45	Total 913	C 438	N 168	O 263	Р 44	0	0

• Molecule 87 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
87	BY	52	Total 1065	C 512	N 196	O 306	Р 51	0	0

• Molecule 88 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
88	BZ	46	Total 957	C 453	N 189	0 270	Р 45	0	0

• Molecule 89 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
89	Ba	46	Total 952	C 452	N 190	O 265	Р 45	0	0

• Molecule 90 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$		AltConf	Trace		
90	Bb	38	Total 791	C 376	N 161	0 217	Р 37	0	0

• Molecule 91 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
91	Bc	45	Total 923	C 444	N 165	O 270	Р 44	0	0

• Molecule 92 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
92	Bd	48	Total 985	C 473	N 190	0 275	Р 47	0	0

• Molecule 93 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
93	Be	45	Total 908	C 432	N 174	0 258	Р 44	0	0

• Molecule 94 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
94	Bf	38	Total 776	C 375	N 138	0 226	Р 37	0	0

• Molecule 95 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
95	Bg	38	Total 783	C 373	N 149	0 224	Р 37	0	0

• Molecule 96 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
96	Bh	40	Total 814	C 388	N 161	O 226	Р 39	0	0

• Molecule 97 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$		AltConf	Trace		
97	Bi	49	Total 993	C 483	N 159	O 303	Р 48	0	0

• Molecule 98 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
98	Bj	48	Total 991	$\begin{array}{c} \mathrm{C} \\ 475 \end{array}$	N 194	O 275	Р 47	0	0

• Molecule 99 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
99	Bk	30	Total 620	C 296	N 124	0 171	Р 29	0	0

• Molecule 100 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
100	Bl	40	Total 829	C 394	N 167	O 229	Р 39	0	0

• Molecule 101 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
101	Bm	38	Total 773	C 370	N 149	0 217	Р 37	0	0

• Molecule 102 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
102	Bn	43	Total 878	C 425	N 154	0 257	Р 42	0	0

• Molecule 103 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
103	Во	45	Total 914	С 445	N 149	0 276	Р 44	0	0

• Molecule 104 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
104	Вр	47	Total 974	C 463	N 194	0 271	Р 46	0	0

• Molecule 105 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
105	Bq	48	Total 984	С 474	N 165	O 298	Р 47	0	0

• Molecule 106 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
106	Br	38	Total 778	C 375	N 138	0 228	Р 37	0	0

• Molecule 107 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
107	Bs	30	Total 609	C 296	N 100	0 184	Р 29	0	0

• Molecule 108 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
108	Bt	45	Total 919	C 445	N 155	0 275	Р 44	0	0

• Molecule 109 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
109	Bu	49	Total 1004	C 487	N 167	O 302	Р 48	0	0

• Molecule 110 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
110	Bv	40	Total 815	C 387	N 159	O 230	Р 39	0	0

• Molecule 111 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
111	Bw	37	Total 752	C 365	N 136	0 215	Р 36	0	0

• Molecule 112 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
112	Bx	52	Total 1059	C 516	N 168	O 324	Р 51	0	0

• Molecule 113 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
113	Ву	30	Total 625	C 297	N 126	0 173	Р 29	0	0

• Molecule 114 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
114	Bz	40	Total 821	C 393	N 162	0 227	Р 39	0	0

• Molecule 115 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
115	B0	30	Total 613	C 296	N 112	0 176	Р 29	0	0

• Molecule 116 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
116	B1	52	Total 1065	C 520	N 170	0 324	Р 51	0	0

• Molecule 117 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
117	B2	30	Total 614	C 295	N 116	0 174	Р 29	0	0

• Molecule 118 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
118	B3	56	Total 1143	C 545	N 214	O 329	Р 55	0	0

• Molecule 119 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms		AltConf	Trace	
119	B4	48	Total 988	C 468	N 195	O 278	Р 47	0	0

• Molecule 120 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
120	B5	31	Total 632	C 308	N 106	0 188	Р 30	0	0

• Molecule 121 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
121	B6	45	Total 929	C 444	N 171	0 270	Р 44	0	0

• Molecule 122 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
122	Β7	37	Total 761	C 362	N 145	0 218	Р 36	0	0

• Molecule 123 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
123	B8	52	Total 1066	C 510	N 183	0 322	Р 51	0	0

• Molecule 124 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
124	B9	38	Total 768	C 370	N 128	O 233	Р 37	0	0

• Molecule 125 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
125	CA	32	Total 644	C 307	N 119	0 187	Р 31	0	0

• Molecule 126 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
126	СВ	32	Total 656	C 313	N 122	O 190	Р 31	0	0

• Molecule 127 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
127	CC	30	Total 624	C 295	N 125	0 175	Р 29	0	0

• Molecule 128 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
128	CD	59	Total 1200	C 576	N 204	O 362	Р 58	0	0

• Molecule 129 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
129	CE	52	Total 1062	C 511	N 194	O 306	Р 51	0	0

• Molecule 130 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
130	CF	40	Total 816	C 387	N 162	0 228	Р 39	0	0

• Molecule 131 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
131	CG	31	Total 626	C 296	N 115	0 185	Р 30	0	0

• Molecule 132 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
132	CH	53	Total 1098	C 522	N 204	O 320	Р 52	0	0

• Molecule 133 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
133	CI	30	Total 614	C 293	N 115	O 177	Р 29	0	0

• Molecule 134 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
134	CJ	49	Total 988	C 483	N 144	0 313	Р 48	0	0

• Molecule 135 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
135	CK	56	Total 1138	C 548	N 181	0 354	Р 55	0	0

• Molecule 136 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
136	CL	31	Total 640	C 304	N 122	0 184	Р 30	0	0

• Molecule 137 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
137	CM	32	Total 653	C 311	N 127	0 184	Р 31	0	0

• Molecule 138 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
138	CN	40	Total 827	C 394	N 164	O 230	Р 39	0	0

• Molecule 139 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
139	СО	30	Total 607	C 291	N 108	0 179	Р 29	0	0

• Molecule 140 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
140	СР	54	Total 1106	C 527	N 196	O 330	Р 53	0	0

• Molecule 141 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
141	CQ	48	Total 976	C 465	N 180	0 284	Р 47	0	0

• Molecule 142 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
142	CR	45	Total 923	C 442	N 167	O 270	Р 44	0	0

• Molecule 143 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
143	$\mathbf{CS}$	48	Total 983	C 466	N 185	O 285	Р 47	0	0

• Molecule 144 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
144	CT	38	Total 769	C 366	N 144	0 222	Р 37	0	0

• Molecule 145 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
145	CU	30	Total 619	C 294	N 123	0 173	Р 29	0	0

• Molecule 146 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
146	CV	32	Total 652	C 309	N 126	0 186	Р 31	0	0

• Molecule 147 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
147	CW	47	Total 970	C 462	N 183	O 279	Р 46	0	0

• Molecule 148 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
148	CX	48	Total 974	C 472	N 158	0 297	Р 47	0	0

• Molecule 149 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
149	CY	48	Total 995	C 468	N 201	O 279	Р 47	0	0

• Molecule 150 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
150	CZ	46	Total 948	C 456	N 162	0 285	Р 45	0	0

• Molecule 151 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
151	Ca	39	Total 798	C 380	N 157	0 223	Р 38	0	0

• Molecule 152 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
152	Cb	45	Total 933	C 441	N 189	O 259	Р 44	0	0

• Molecule 153 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
153	Cc	30	Total 616	C 293	N 112	0 182	Р 29	0	0

• Molecule 154 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
154	Cd	38	Total 779	C 368	N 151	O 223	Р 37	0	0

• Molecule 155 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
155	Ce	30	Total 603	C 288	N 105	0 181	Р 29	0	0

• Molecule 156 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
156	Cf	40	Total 803	C 385	N 149	O 230	Р 39	0	0

• Molecule 157 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
157	Cg	38	Total 779	C 371	N 145	O 226	Р 37	0	0

• Molecule 158 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
158	Ch	45	Total 928	C 441	N 177	O 266	Р 44	0	0

• Molecule 159 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
159	Ci	48	Total 977	C 469	N 158	O 303	Р 47	0	0

• Molecule 160 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
160	Сј	54	Total 1107	C 525	N 207	0 322	Р 53	0	0

• Molecule 161 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	AltConf	Trace			
161	Ck	46	Total 948	C 451	N 185	O 267	Р 45	0	0

• Molecule 162 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
162	Cl	45	Total 913	C 435	N 162	0 272	Р 44	0	0

• Molecule 163 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
163	Cm	38	Total 765	C 369	N 123	O 236	Р 37	0	0

• Molecule 164 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
164	Cn	45	Total 916	C 437	N 178	0 257	Р 44	0	0

• Molecule 165 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
165	Со	37	Total 752	C 364	N 125	0 227	Р 36	0	0

• Molecule 166 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			AltConf	Trace
166	Ср	37	Total 752	C 358	N 134	0 224	Р 36	0	0

• Molecule 167 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
167	Cq	36	Total 731	C 350	N 127	0 219	Р 35	0	0

• Molecule 168 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
168	Cr	38	Total 778	C 371	N 142	O 228	Р 37	0	0

• Molecule 169 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
169	Cs	39	Total 804	C 381	N 147	0 238	Р 38	0	0

• Molecule 170 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
170	Ct	38	Total 781	C 371	N 157	0 216	Р 37	0	0

• Molecule 171 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
171	Cu	36	Total 736	C 355	N 125	0 221	Р 35	0	0

• Molecule 172 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
172	Cv	37	Total 748	C 360	N 123	0 229	Р 36	0	0

• Molecule 173 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
173	Cw	31	Total 629	C 300	N 123	0 176	Р 30	0	0

• Molecule 174 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
174	Cx	37	Total 761	C 364	N 152	O 209	Р 36	0	0

• Molecule 175 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
175	Су	45	Total 917	C 436	N 167	O 270	Р 44	0	0

• Molecule 176 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A		AltConf	Trace		
176	Cz	52	Total 1061	C 510	N 180	O 320	Р 51	0	0

• Molecule 177 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms	AltConf	Trace		
177	C0	60	Total 1215	C 590	N 190	O 376	Р 59	0	0

• Molecule 178 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
178	C1	47	Total 964	C 461	N 178	0 279	Р 46	0	0

• Molecule 179 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
179	C2	32	Total 660	C 316	N 125	0 188	Р 31	0	0

• Molecule 180 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms		AltConf	Trace	
180	C3	37	Total 757	C 360	N 141	0 220	Р 36	0	0

• Molecule 181 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms		AltConf	Trace	
181	C4	57	Total 1159	C 561	N 189	O 353	Р 56	0	0

• Molecule 182 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		$\mathbf{A}$	toms	AltConf	Trace		
182	C5	44	Total 910	$\begin{array}{c} \mathrm{C} \\ 435 \end{array}$	N 177	O 255	Р 43	0	0

• Molecule 183 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
183	C6	47	Total 959	C 458	N 181	0 274	Р 46	0	0

• Molecule 184 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
184	C7	47	Total 957	C 456	N 186	O 269	Р 46	0	0

• Molecule 185 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
185	C8	38	Total 771	C 368	N 139	0 227	Р 37	0	0

• Molecule 186 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
186	C9	37	Total 766	C 366	N 150	0 214	Р 36	0	0

• Molecule 187 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
187	DA	60	Total 1225	C 589	N 221	O 356	Р 59	0	0

• Molecule 188 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	AltConf	Trace			
188	DB	43	Total 876	C 418	N 155	0 261	Р 42	0	0

• Molecule 189 is a DNA chain called STAPLE STRAND.


Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
189	DC	46	Total 952	$\begin{array}{c} \mathrm{C} \\ 453 \end{array}$	N 195	O 259	Р 45	0	0

 $\bullet\,$  Molecule 190 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
190	DD	38	Total 775	C 369	N 144	0 225	Р 37	0	0

• Molecule 191 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		$\mathbf{A}$	toms			AltConf	Trace
191	DE	46	Total 940	C 446	N 181	O 268	Р 45	0	0

• Molecule 192 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
192	DF	31	Total 638	C 304	N 125	0 179	Р 30	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













C2869	T2870 A2871	C2874	T2877 T2878	A2880	C2881	A2883 T2884	T2885 A2886	C2890	T2892	C2893 T2894	G2895 G2896	A2900	A2901 C2902	T2903 T2904	C2905 T2906	T2907	T2909		91629		C2922	C2924	T2925 A2926	T2927	T2928 T2929	T2930	62931	T2934	A2938	G2941 T2942	C2943	•
G2949	G2955 A2956	G2959 T2960	T2961 A2962	T2963	62970	A2979	C2986	T2993	G3001	<mark>63009</mark>	T3010 A3011	T3012	C3013 T3014	<mark>G3015</mark> C3016	A3017	<mark>G3021</mark>	A3025	T3035	T3038	A3046	C3048	<mark>G3053</mark>	T3056	C3065	A3069	A3070		13076	T3084	A3086		
G3087	T3088	T3092 T3092		A3096	13098 13098 A3099	<b>A</b> 3100	A3104 G3105	A3106	T3111 C3112	T3113	C3120 G3121	T3122 C3123	G3126	A3127	A3135 A3136	T3137	G3140	A3143	G3144	13149 A3150 A3151		G3163	13104 A3165	T3167	A3170	C3171 A3172	<mark>A3173</mark> T3174	G3175 A3176	T3177	<mark>G3182</mark>		
T3183	1310 <del>4</del> G3185	T3190 A3191	A3192 A3193 C3194	T3199	63203 63203	C3205	C3206	T3209 T3210	T3211	C3213	T3214 A3215	C3216	T3217 C3218	G3219	T3220 T3221	C3222	13223 G3224	G3225 T3226	T3230	<mark>C3233</mark>	A3237	G3239	G3240	G3244	C3245 C3246	T3247	T3250	G3 <mark>260</mark> A3261	G3262	G3265	C3200 T3267	
G3270	T3271	63279 A3279 T3280	T3281 T3282	G3283 G3284 G3265	T3286	T3289	A3292	T3295 C3296	C3297 G3298	G3299 T3300	T3301	T3306	A3311 T3312	T3313	T3318 T3319	<b>G3320</b>	A3324	63326 63326	4332/ T3328	C3329	(3331 (3331	<b>C3333</b>	<mark>C3337</mark>	63343	C3344	13349	T3353	C3357	T3360	T3361		
C3362	T3364	C3367	T3371	C3372 T3373	<mark>A3377 A3378</mark>	<mark>(3383</mark>	C3386	A3387 G3388	T3389 T3390	C3391	T3394	13396 C3396 C3396	C3398	T3399 T3400	A3401	T3402 G3403	A3404 T3405	C3409	C3410 G3411	T3412 C3413	T3414	G3417 C3418	C3421	G3422 T3423	T3424	C3426	G3427 G3428	C3429	A3432 G3433	A3436		
<b>G3443</b>	G3446	C3449	A3454 T3455	T3456	63476	A3477 T3478	<mark>G3479</mark> A3480	T3481	A3485	C3488 T3489	G3492	G3495	T3496 A3497	C3498 T3499	T3500 T3501	G3502	C3506	G3508 C3508	G3510 C3510 T3514	T3512	G3514 Tage 16	A3516 Total	1351/ A3518	<mark>G3522</mark>	G3525	G3526 G3527	<mark>G3528</mark> G3529	A3532	A3533			
A3534 63535	A3536 T3537	63538 A3539 G3540	T3543	A3547	13553	T3557	<b>G3560</b>	<b>T3566</b>	T3567 C3568	G3569	135/0	(3576 (3576	13577 13578	G3579 G3580	T3581 G3582	C3583 C3584	T3585 T3586	C3587	T3592 G3593	G3594 C3595	A3596 T3597	C3600	<mark>G3601</mark> T3602	A3603	T3607 A3608	C3609	C3611 C3611	G3612 T3613	A3616			
63619	G3620 A3621	T3625	<mark>C3628</mark> T3629	C3630 A3631 T3630	A3635	<mark>(3639</mark>	T3640	T3643 T3644	A3645 G3646	T3647 C3648	C3649 T3650	C3651			63664 63664	C3665	T3668	C3671 T3672	A3673	C3678	T3681	G3684 A3685	T3686 G3687	C3688 T3689	<b>G3690</b>	T3693	13694 T3695	C3696 G3697	<b>G</b> 3700			
C3701 T3702	G3706	G3709 G3709 G3709	A3713	T3714 C3715 C3716	C3717 C3718 G3718	C3719	G3724	T3730	A3733 A3734	C3737	C3742	C37 AF	C3746		C3752	G3753 A3754	C3755	G3757	A3759 A3759 T3760	A3761	G3766	T3768	A3770	G3772	G3774 03774 00777	13775	<b>G</b> 3780	G3783 G3784	T3785 T3786			
G3787	G3790 T3791	C3/92 G3796	<b>G</b> 3799	63800 63800	C2000 T3807 A3808	T3809	G3819 C3820	T3821	G3828 A3829	A3830 A3831	T3832 T3833	C3834 A3835	<mark>C3836</mark>	G3844 C3845	A3846 A3847	<b>G3848</b>	(3851	A3852	63859 A3860 T3861			A3003 A3870 A3671	G3872 G3872		G3882 A3883	G3884 C3885	C3886 T3887	G3896	A3897			
G3898 A3899	T3900 T3901	13902	T3909 G3910	A3913	A3916 T3917	T3918 A3919	T3920 T3921	A3922 T3923	T3924	C3927 A3928	A3929	T3931	C3933	T3936	63938	T3942	C3945	T3946 T3947	T3948 C3949	T3953	T3964	A3967	A3968 C3969	T3970 G3971	T3972	A3975	A3975 A3977	<b>G</b> 3978	G3981 T3982			
T3983 T3984	A3985 G3986	C3994	<mark>C3999</mark> A4000	G4001 A4002 A4003	A4005	T4006 T4007	T4012	T4015	A4016 A4017	C4018 G4019	T4020 C4021	T4022 G4023	G4028	G4031		A4037 C4038	T4039	T4040 T4041	A4042	G4043 A4044	T4045 C4046	G4047	T4049	A4050	G4052	C4053	14054 A4055	A4056	C4057 T4058	A4059	T4060 G4061	A4062 G4063



G4064	G4065	T4067	T4069 C4070	T4071	T4078 G4079	C4080	14081 A4082 C4083	A4084 G4085	G4086 C4087	G4088 T4089	14090 14090	T4092 A4093	<mark>G4094</mark> T4095	<mark>T4096</mark> T4097	G4104	A4111	A4112 C4113	T4114	C4115	64117 T4118	<b>G4119</b> ◆ T4120 ◆	T4121	64123	G4124	T4130 G4131	44132	C4136 C4136 C4137	T4138 A4139	G4142 C4143	64144		
C4145	C4149 T4150	A4151 T4152	C4153	C4155	T4156 G4157	A4158	A4159 A4160	A4161 T4162	G4163	A4164 G4165	G4166	G416/ T4168	G4169 G4170	T4171	G4172 G4173	C4174	T4175	T4177	64178 A4179	G4180 G4181	G4182	14183 G4184	G4185 C4186	G4187 G4188	T4189	64193	64196 44000	64202 64203 T4204	T4205	G4208 G4211	64212 T4213 G4214	G4215
C4216	A4220 C4221	T4222 A4223	A4224 A4225	C4226 C4227	T4228 C4229	c4230	G4 <mark>234</mark> T4 <u>2</u> 35	G4238	G4239 T4240	64241 A4242	T4243	C4245	A4246 C4247	C4248	A4250	C4253	G4256		74268 74268 74269	A4272	C4273 C4274	C4275 T4276	C4277 T4278	64279 64280 44201	C4282 C4282 C4283	C4287	T4288	T4291	C4296 T4297			
G4298	64299 T4300 A4301	<mark>C4302</mark> T4303	C4307	A4308 A4309	A4310 A4311	C4312	G4316	A4319	A4320 T4321	C4322	C4323 T4324	T4327	T4331	C4332	C4334	G4337 44338	64339 64339	64340 A4341 C4340	<b>T4343</b> <b>C4344</b>	44347	T4357	A4358 C4359	T4360	T4361	G4365	14368 T4369	C4370	G4372	T4375 A4376 M377	T4378		
A4379	G4380 G4381	T4382	64386	A4389 T4390	A4391 G4392	C4401	A4402 T4403 T4403	A4405	DOTE V	<b>T4410</b> <b>T4410</b>	T4412 T4412 AAA13	T4415	G4418	G4419 C4420	A4421 C4422	T4423 G4424	T4425 T4426	A4427 C4428	G4433	G4434 C4435	A4436 C4437	C4443	C4444	T4446	T4447 A4448	C4452	T4453	A4455	14456 C4460	A4461		
G4462	T4463 A4464	C4465	C4467	T4468 C4469	C4470 T4471	G4472 T4473	A4474	A4483	G4484 C4485	C4486	A448/ T4488	G4489 T4490	A4491	T4492 G4493	A4494	C4495 G4496	C4497	T4499 A4500	C4501 T4502	G4503	A4506 C4507	G4508 G4509	T4510	14514 T4515	G4518 A4519	G4520	C4525	T4528 T4529	C4531	G4538 G4539 C4540	T4541	
T4542	T4546	G4549 G4550	44551 74657	14556	T4557	G4563 T4564	G4565 A4566	A4567 T4568	A4569 T4570	C4571 A4572	A4573 G4574	C4577	A4578 A4579	A4587	C4588	G4591	T4594	C4598	C4601	C4602 T4603	G4604 T4605	C4606	A4607 A4608	T4609 G4610	C4611	14012 G4613	G4614 <b>C</b> 4615	G4616	C4618	G4620 04621	T4622	
C4623	T4624 G4625	G4626 TA627	1402/ G4628	G4629	G4631	C4635	T4636 G4637	G4638 T4639	G4640	G4641 C4642	G4643	G4644 C4645	T4646	T4648	G4653	G4656	C4660	T4661 C4662	T4663 G4664	64666 64666 64667	G4668 T4669	G4671 G4671	G4682	G4685	G4686 C4687	G4689	C4690	14693	G4701 C4702	G4703 G4704 T4705	14/06	
C4707	G4715 G4716 G4716	G4721	<mark>G4722</mark> T4723	G4727	G4728	G4730	A4731 T4732	T4733	14/34 T4735	G4736	T4738	T4741	G4 742 A4743	A4744	G4747	G4750	G4751 C4752	A4753	A4755	C4756 • G4757 •	C4758	A4750	A4761	G4767 G4768	G4769	T4771	A4772 T4773	G4774	C4776	G4778 A4779	G4784 C4785	C4786 G4787
	A4792 A4793	G4798	A4801	T4805	G4808 A4809	C4810	A4814	G4818 G4818	C4819 A4820	C4823	14824 T4825	4620 A4827 T4828	14020 T4829 C4830	C4834	G4835 C4836	T4837	T4840	G4848 T4849	G4850 C4851	C4854	T4855 A4856	G4859	A4860 T4861	G4862 G4863 T1964	14004 T4865 T4866	C4867 A4868	T4869 T4870	G4871 G4872				
T4873	C4876 G4877	T4878	G4883	C4886	G4889 C4890	G4895	G4896 T4897	G4901	T4903	G4904 C4905	14900	64910 64911 TA 010	14912 64913 A4914	T4915	T4918 64919	C4920	64922	C4924	14925 C4926	T4927 A4928	T4931	C4932	A4935 A4936 A4037	T4938 T4938 (44939	T4942	C4943 A4944	A4945 G4946	T4947 C4948	•			
G4955	64956 T4957 G4958	A4961	A4962 T4963	T4964	C4967 C4968	A4972	G4 <mark>975</mark>	T4978	A4979 A4980 m4004	14982 14982	C4985	0067-000	C4998	T4999	C5009 A5010	A5011	T5012	T5021 (	T5023 C5024	G5025	T5030 T5031	T5032 G5033	15034 C5035 TEA26	T5037	C5041 G5042	C5043 T5044	G5045 G5046	C5051	70000			
A5053	15054 A5055 T5056	G5057 A5058	A5059	T5062 T5063	C5064	G5069 A5070	T5071		T5082	A5085			T5103	T5104	T5110	45118	T5119	T5121	C5124	45126 C5127	C5128	G5134	G5138	T5141 T5142	T5143 T5144 Ce14E	G5149	T5150	<mark>G5153</mark>				

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C5158 A5159 T5163	T5167 A5172 G5173	G5176 T5177 C5178 C5178 T5179 T5180	A5181 A5182 T5183 C5184 A5185	T5186 G5187 A5190	T5193 C5194 T5195 <b>T5196</b> T5196	15199 (5199 A5203	T5204 T5205 G5208 T5209	T5212 T5213 A5214 T5215	G5219 C5224	<b>G5227</b> G5228 T5229 T5230	1521 C5232 C5233 T5233 T5235	15237	
G5238 <mark>G5239</mark> T5240 A5241 A5241	T5246 G5247 G5251	G2252 C5253 T5254 A5255 T5256	C5257 T5258 G5258 C5269 C5260 T5261	T5262 A5263 C5264	T5268 A5275 G5278	G5279 C5280 T5281 T5282	C5283 C5284 A5287	A5292 T5295 G5299	C5300 T5301 A5307 T5308	T5309 G5310 T5315	15316 65317 65320 15321 T5321	A5323	
A5326 T5327 G5331 C5332	C5339 C5339 C5339	T5342 T5343 G5347 T5348	(5349 (5350 (5351 15353 15353	A5354 T5357	C5360 T5361 G5362 A5363 T5364	45365 T5366 G5369	A5375 A5376 A5379 A5379	C5380 C5381 C5382 C5383 C5384 C5384	15385 15390 15391 (5392	G5397 G5406 TEA06	T5408 T5412 C5413 T5414	C5415 C5416	
C5420 T5421 A5422 A5423	T5424 G5425 C5426 G5427	C5433 T5437 T5438 T5438 T5438	T5440 A5441 G5443 G5443	T5447 T5448 C5453	T5454 G5455 T5456 A5457	65460 65461 C5462 T5463	G5464 C5465 T5466 T5474	T5475 T5476 T5477 T5478	634/9 A5480 C5481 C5482 T5483	T5484 A5485 A5486 A5487 A5487	Cortoo A5489 A5490 A5491 A5492	45493 65497 T5498 ♦	
T5499 T5500 C5501 T5502	T5503 A5504 T5505 T5506 T5506	(1000000000000000000000000000000000000	A5518 A5519 A5520 T5521	A5522 A5523 T5524 A5525 T5525	15529 65528 65528 75529 T5530	T5533 T5534 A5535	T5536 G5540 T5541 A5542	A5543 C5544 T5545 G5546 G5547	C5548 A5554 G5555	G5556 C5557 T5558 A5565	G5566 A5567 C5568 C5568	A5576 G5577 C5578	
65579 15580 15581 65582 65583	T5584 A5585 A5586 G5587 A5588	G5603 T5604 A5605 G5606	G5609 <b>T5612</b> G5613	45618 65621	C5623 A5623 A5624 C5625	A5634 G5640 G5641 C5642	C5645 A5646	A50459 C5650 C5651 T5652 C5653			G5665 A5666 G5667 G5668	G5672 A5678	
C5682 C5683 C5684	C5686 C5687 C5687 T5688	C5690 T5691 A5693	A5698 C5699 C5701	G5702	C5709 T5710 T5711 C5712		65720 65721 85721 15722 15723	T5724 G5725 C5726 T5727 T5728	G5729 C5730 T5731 A5732	G5735 G5736 G5737	C5/38 G5739 C5740 G5741 G5742 T5743	A5744 A5745 A5746 G5747 A5748	cs755 ♦
G5756 A5757 T5758 G5759	A5763 T5764 A5765	A5766	T5775 G5776 C5777	15/78 15779 15780 15781	G5786 A5787 T5788 G5789	A5790 G5791 T5792 G5793	Co/94 G5795 G5796 G5796 T5797 A5798	C5799 T5809 C5812	T5816 G5820 G5821	A5822 A5823 T5824 G5825	A5828 A5833 A5834	C5841 G5842 A5843 T5844	<b>T5845</b>
A5846 G5849 A5850 T5851	T5852 G5853 G5854	45860 T5863 C5864 C5865 T5865	C5867 C5868 C5868 T5869 A5870	A5871 G5876 G5877 G5877	AJ 0.0 15879 (5881 (5881 (5882	A5883 T5884 A5885	43500 15889 15890 15895	T5896 G5897 T5898 T5899	C5900 ↔ A5901 G5902 G5903	Ab 904 C5905 T5906 T5907	T5909           C5910           T5911	T5917 G5918 A5919 T5920	A5921
A5925 G5926 G5926 G5927	(5929 (5929 (5931 (5931 T5932	T5933 C5934 T5935 T5939	T5940 A5941 G5942 C5943 T5044		<b>G5951</b> T5952 <b>T5953</b> <b>G5954</b>	T5955 T5956 T5957 A5958 T5958	15960 (5961	T5970 65971 65972	45973 G5976 A5977 A5978	T5979 T5980 A5981 C5982	15983 T5984 A5986 T5990	T591 T592 G593 T5994 C5995	
65996 65997 66000	T6003 T6007 T6008 C6009	T6010 T6016 G6025	T6030 G6031 C6032	C6038 C6039 T6040	T6045 A6046 C6047 A6048	T6049 G6050 T6051 T6052	60093 6054 66055 76056 76056	T6058 G6059 T6060 T6061 A6062	T6065 A6066 T6067 G6068	Ge069 C6070 G6071	A6078 A6079 T6080 G6084	C6085 C6086 C6087 T6088	
A6089 C6090 <b>T6091</b> G6092	16094 16094 16100 ♦	T6101 C6104 T6105	T6109	<b>T6115</b> A6116 A6117 G6118	A6119 A6120 T6121 T6122	T6123 G6124 T6125 A6126	A6129 C6130 G6131	G6137 C6141 T6142	G6149 T6152	Coll50 T6160 A6161	A6165 T6166 C6172 C6173	66174 16175 66176 16177	
T6184 T6185 A6186 T6187	T6188 A6191 C6192 G6193	C6194 C6195 T6196 T6196	T6200 T6203 C6204 ◆	A6205 C6208 G6209	G6213 G6214 G6215 ♦	A6216 T6217 T6218	T6219 C6220 A6221 A6222	A6223 C6224 A6230 A6231	T6232 T6233 T6234	46235 G6236 G6237 T6238 T6238	A6240 G6241 A6242 A6242	G6244 A6245 A6248 A6249 A6250	T6251



C6255	A6257	A6260 T6261	A6262 T6263	T6265 T6266 T6266	G6268	A6270 ← A6271 ← A6272	A6273 G6274 ◆ T6275 ◆	T6276 T6277	T6278	C6281 G6282 C6283	C6 287	T6288 T6289	16290 66291	C6293	10235 66296 66297	A6299 T6300	A6304 T6305	T6306 T6307	G6308 C6309 A6310	T6311 G6314	C6315 A6316 T6317	T6318 T6319 A6320
C6321	T6323 A6324	T6325	T6328 T6328 T6329	T6333	A 6335 C 6336 C 6337	C6338 A6339 A6340	C6341 C6342 T6343	G6350 A6351 ♦	G6352 G6353 T6354	T6355 A6356 A6357	A6358	G6362 T6363 A 6364	76366	C6367 T6368 C6369	T6370	66380 66380 66381	T6382	A6391 T6392	T6393 C6394	A 6395 C 6396	T6400 G6401 A6402	C6403
T6404	A6411	C6413 C6414 C6414	10415 C6416 T6417	T6418 A6419	<b>A6420</b> T6421 C6422 T6423	G6426 C6427	T6428 A6429	T6430 C6433	T6436 G6437 TeA35	10430 T6439 T6440 T6441	G6445	66447 T6448	T6451 A6452	A6453 G6454	G6456 G6456 A6457	T6461 T6462	A6463 A6464	T6465 T6466	G6471 C6472 C6473	4041 3 46474 C6475	G6476 A6477 A6477 T6478	-
C6482	G6484	A6486	16496	16497 C6498 A6499	C6500 T6501 C6502	46505 76506 76506	T6510	G6512 A6513 Tec14	10014 A6521	16523 G6524	T6525 T6526	T6527	A6534	A6537	A6538 G6539 G6540	T6541	T6545 C6546 A6547	A6548	A6554	TG556	A6562	
A6567	T6569 A6570	A6571 T6572 T6572	T6575	G6576 T6580	C6581	G6584	T6588 T6589 T6590	G6591 T6592 T6593	T6594	46596 T6597 C6598	A6599 T6600	C6601	00012 A6613 G6614	G6615 T6616	◆ A661/ A6618 T6619	T6620 G6621	A6623	T6625 G6626	A6630	A0031 T6632 T6633	C6634	C6637
G6641 C6642	G6643 C6644	G6645 A6646	T6649	G6651 T6652	A0033 A6654 C6655	T6656 T6657	T6662 T6663	G6669 C6669	A6670 A6671 A6672	• • • • • • • • • • • • • •	T6681	0000000000000000000000000000000000000	T6689	T6692 T6692	T6693	G6699	T6701 G6702	T6703 A6704	G6709 G6709	A6711	T6713 G6714	A6717 C6718 T6719
33 G6720 94 T6721	16 + T6723	97 46724 98 47725 16725	99 C6727 00 A6728	02 T6729 03 C6730 04 T6731	06 ♦ G6732 07 ♦ A6733	09 C6/34 16736 16736	16737 16738 22	.0 4 ♦ 46745 46746	. T6751 .8 T6751		24 T6758 24 T6759 T6760	27 28 28 29 29 29 20 20 20 20 20 20 20 20 20 20 20 20 20	80 15/64 81 ♦ A6765 82 ♦ T6766	16767 16768 16768 16768 04	87 16770 16773 16773	to T6774	4	C C C C C C C C C C C C C C C C C C C	A6782 A6783 A6783 A6784	54 T6785	57 A6787 16788 16789 16789	-
861 862 7679	863 A679 T679	866 867 868	869 T675 870 A680 871 G680	6680 874 T680 T680	880 C680 881 T680 882 $\blacklozenge$ A680	883 <b>•</b> A680 884 • C680	885 886 887 887 8887 7681 7681 7683 7683	889 890 891			897	900 901 902 A682 A682	903 904 068 068 068 068 068 068 068 068		909 909 910	911 A684 912 1684	914 6684 917 6684 6684	918 A684	922	924 • T685 925 • G685 A685	926 928 928 A686	
(6931 + T6 reas	6933	6935 6935 76 76 76 76	6940 C6	6943		6955 • A6 6956 • A6			6966 <b>A</b> 6 6966 <b>A</b> 6 6967 <b>A</b>	6968	6976 ♦ T6	6978	6980 C6 6981 C6	6985	(6989 (6990 (6991 (6991	6992 6993 6994 ● 66	110 110 110 110 110 110 110 110 110	7000 7600 7601	7002 7003		7010 A6	7012
T7016	T7019 T7020	T7023	T7026	C7028	C7030 ♦ T7036 ♦	A7037	T7039 A7040 T7041	C7042 T7043	G7047 A7048 C7049 ◆	G7050	C7054	A7057 T7058	17060	T7063 A7064 G7065	T7066	C7075	CT077	A7082 G7083	A7084 T7085	A7091 G7092 A7093	T7094 A7095 A7096	C7097
C7098	C7101 ← C7102 ←	T7107	T7111 T7112 T7113	C7114 C7117 C7117	T7118 G7119 T7120	T7 121 G7 122 A7 123	T7124 T7125 T7126 G7127	C7128	A7130	G7 139 🔶 A7 140	T7141	T7143 T7144 G7145	A7146 G7149	A7150 G7151 G7152	G7153 T7154 T7155	T7156 T7159	A7160 T7161	T7162 T7163	G/ 104 A7 165 G7 166	G/16/ T7168 T7169	C7170 A7171 ♥ G7172 ♥	
C7 173	G7176 G7177	T7178 G7179 A7180	T7181 G7182 C7183	T7 184 T7 185	A7189	T7193 T7194	T7197 T7198 T7199	G7206	C7212 A7213 G7214	C7215 C7216 T7217	<mark>G7218</mark> G7219 C7220	A7221	G7231	C7243	G7245 A7246 C7247	C7 248 G7 249 C7 250	C7251 T7252 C7253	A7254 C7255 C7256	T7257 C7258 T7759	17261 T7261		







11 12 12 12 13 13 14 14 15 15 34 15 38 13 33 13 34 14 15 38 13 38 13 34 15 38 13 38 13 38 13 38 13 38 13 38 13 38 13 38 13 38 13 38 13 38 13 38 13 15 15 17 17 17 17 17 17 17 17 17 17 17 17 17		
• Molecule 4: STAPLE STRAND		
Chain AD: 56%	38%	6%
T1           T2           G3           A4           A5           A13           C21           C23           C33           A31           A31           A33           A34           A34           C33           C33           C33           C33           C34           C35           C36           C37 <td< td=""><td></td><td></td></td<>		
• Molecule 5: STAPLE STRAND		
Chain AE: 71%	27%	•
C1 12 12 12 12 12 12 12 12 12 1		
• Molecule 6: STAPLE STRAND		
Chain AF: 56%	35%	9%
61 12 12 12 13 14 14 14 14 14 14 14 14 14 14 14 14 14	8 <mark>8 98 198 198 198 198 198 198 198 198 198</mark>	
• Molecule 7: STAPLE STRAND		
Chain AG: 75%	23%	- -
11 13 13 14 14 14 15 15 15 15 15 15 15 15 15 15 15 15 15	134 136 A37 A37 A37 A37 A41 C42 C43 C42 C43 C42 C43	A40 A47 C48
• Molecule 8: STAPLE STRAND		
Chain AH: 68%	26%	6%
41 62 62 68 48 417 417 713 69 09 09 123 09 123		
• Molecule 9: STAPLE STRAND		
• Molecule 9: STAPLE STRAND Chain AI: 71%	25%	
• Molecule 9: STAPLE STRAND       Chain AI:       71%	25%	
Image: Solution of the second state	25%	·





• Molecule 11: STAPLE STRAND





















• Molecule 59: STA	APLE STRAND	
Chain A6:	67%	31% •
A1 C4 C4 C4 C4 C1 C1 C1 C1 C2 C2 A2 C2 A2 C2 A2 C2 A2 C2 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4 C4	A23 122 128 A30 A30 A32 A33 A34 A34 A32 A32 A32 A32 A32 A32 A32 A32 A32 A32	
• Molecule 60: STA	APLE STRAND	
Chain A7:	67%	25% 8%
11 14 65 65 65 66 68 89 80 810 111 111 111	A14 115 A20 A20 A24 C27 A24 T23 T33 T33 T33 T33 T33 T33 C38 C38 C38 C38 C38 C38 C38 C38 C38 C	A39 A41 A42 A43 T44 T48 T48
• Molecule 61: STA	APLE STRAND	
Chain A8:	58% 73%	23% •
C1 C2 A3 A5 A5 C4 A5 C4 C4 C1 C1 C1 C1	412 ↓ 113 ↓ 113 ↓ 115 ↓ 115 ↓ 115 ↓ 115 ↓ 115 ↓ 126 ↓ 120 ↓ 122 ↓ 226 ↓ 226 ↓ 228 ↓ 228 ↓ 233 ↓ 133 \end{split}	T34 T35 T35 T35 T37 T38 T40 T41 A41 A42 C44 C44 C48 C44 C48 C48 C48 C48 C48 C48
• Molecule 62: STA	APLE STRAND	
Chain A9:	50% 63%	34% ·
11       12       12       12       15       15       15       15       15       15       15       15       16       17       18       17       17       18       17       17       18       19       19       19       19       19       19       19       19       19       19 <td>C17 C17 C18 C18 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20</td> <td></td>	C17 C17 C18 C18 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	
• Molecule 63: STA	APLE STRAND	
Chain BA:	60%	40%
C1 C5 C5 C5 A7 A14 A14 C15 A14 A17 A17 A17	118 628 628 635 133 133 133 133 133 133 133 133 133 1	
• Molecule 64: STA	APLE STRAND	
Chain BB:	48% 68%	29% ·
C1 C2 A8 A10 C11 C11 C13 C13 C13 C13 C13 C13 C13 C13	121 (22 <b>A33</b> <b>A25</b> A26 A26 A26 A26 A29 T30 T31	
• Molecule 65: STA	APLE STRAND	
Chain BC:	57%	25%





























• Molecule 119: STAPLE STRAND







• Molecule	126: STAPLE STRAND		
Chain CB:	53%	34%	12%
A1 A6 17 17 18 610 611	T15 C16 A17 A17 A18 A23 A23 A23 A23 A23 A23 A25 C24 A25 C26 C24 A25 C26 C26 C27 A25 C26 C26 C26 C27 A18 A18 A17 A18 A17 A18 A17 A18 A17 A17 A17 A17 A17 A17 A17 A17 A17 A17		
• Molecule	127: STAPLE STRAND		
Chain CC:	63%		37%
G1 G2 G3 G3 G3 G3 G3 G3 G3 G3 G3 G3 G3 G3 G3	G10 C11 712 A15 A15 A16 A16 A16 A16 A18 A18 A18 A18 A18 A18 A18 A18 A18 A18	2	
• Molecule	128: STAPLE STRAND		
Chain CD:	59% 66%	25	% 8%
C1 C7 C7 C7 C9 G10 C9 G10	A15 G16 C17 C17 C17 C18 C19 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	T30     A31       A31     A31       T32     A34       A33     A34       A38     A38       A39     A39       A40     A41       A50     A50	152 153 C54 A55 C56 G57 C56 G57 C56
• Molecule	129: STAPLE STRAND		
Chain CE:	12%		21% ·
G1 A5 A9 A10 A15	118           119           120           135           135           137           137           137           137           137           137           137           137           137           137           137           137           137           137           137           137           138           137           138           137           138           138           139           137           138           138           139           139           138           139           139           139           139           139           139           139           139           139           139           139           139           139           139           139           139           139	<b>T52</b>	
• Molecule	130: STAPLE STRAND		
Chain CF:	65%		35%
G1 T2 A3 A7 C8 A9 A10	A11 C12 C12 A14 A14 A14 A18 A18 A18 A18 A18 A28 C26 C28 C28 C28 C28 C28 C28 C28 C28	140 C32	
• Molecule	131: STAPLE STRAND		
Chain CG:	• 61%	35	% •
G1 G2 G5 G5 C5 A8 A8	610 411 112 113 113 113 113 113 113 1		
• Molecule	132: STAPLE STRAND		
Chain CH:	9% 58%	36%	6%





• Molecule 139: STAPLE STRAND







• Molecule 146: STA	PLE STRAND	
Chain CV:	75%	25%
C1 64 A5 A6 C15 C15 C15 C15 C15 C15 C15 C15 C15 C15	(223 (224 130 (331 132	
• Molecule 147: STA	PLE STRAND	
Chain CW:	70%	26% ·
TI A4 A8 C11 C11 C11 C11 C11 C11 C11 C11 C11 C1	22 26 430 431 633 633 635 636 636 636 636 636 636 746 746 746	
• Molecule 148: STA	PLE STRAND	
Chain CX:	71%	25% •
11 46 47 47 48 48 48 48 48 48 69 62 62 622 622 622 622 622 622	126 127 127 128 129 129 133 133 133 133 133 133 133 133 133 13	- 99 - 97 - 11
• Molecule 149: STA	PLE STRAND	
Chain CY:	63%	33% •
5 5 5 8 6 3 8 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	A27 A27 C28 C40 C40 C41 C41 C42 C42 C42 C42 C42 C42 C42 C42 C42 C42	
• Molecule 150: STA	PLE STRAND	
Chain CZ:	65%	30% •
A1 17 17 17 18 18 19 119 119 119 119 119 119 119 11	123         123         125         126         126         137         135         137         137         141         145         146	
• Molecule 151: STA	PLE STRAND	
Chain Ca:	69%	26% 5%
G1 C2 C2 C3 C3 T14 A17 A17 A18 A24 A30 A24 A30 A31 A31 A31 A31 A31 A31 A31 A31 A31 A31	G32 134 135 135 133 133 133 133 133 133 133 133	
• Molecule 152: STA	PLE STRAND	
Chain Cb:	80%	16% ·
A1 G2 G3 A13 A13 C3 C3 A31 C34 A31 T32	A33 A34 A40 C45 C45	
	PROTEIN DA	

• Molecule 153: S'	TAPLE STRAND		
Chain Cc:	47%	43%	10%
11 02 03 04 05 06 06 06 06 06 06 06 06 06 06 06 06 06	015 021 022 022 022 025 025 026 029 029 029		
• Molecule 154: S'	TAPLE STRAND		
Chain Cd:	% 79%	1	6% 5%
C1 C1 C16 C16 C16 C21 C21 C22 C22 C22 C22 C22 C22 C22 C22	023 633 0 73 6 73 6 73 7 73 8 73 8 73 8 73 8 73 8 73 8 73 8		
• Molecule 155: S'	TAPLE STRAND		
Chain Ce:	63%	33%	•
01 17 17 17 17 17 17 17 17 17 17 17 17 17	C27 628 630 630		
• Molecule 156: S'	TAPLE STRAND		
Chain Cf:	62%	35%	•
C1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	122 122 123 128 128 128 128 128 128 128 128 128 128		
• Molecule 157: S'	TAPLE STRAND		
Chain Cg:	68%	21%	11%
11 14 01 118 019 118 019 122 023	C28 C28 C29 C29 C31 C33 C33 C33 C33 C33 C33 C33 C33 C33		
• Molecule 158: S'	TAPLE STRAND		
Chain Ch:	60%	40%	
61 62 710 611 613 613 615 615 615 615 615 615 615 615	C 18 C 19 C 19 C 22 C 22 C 22 C 22 C 22 C 22 C 22 C 23 C 23 C 33 C 33	G41 C42 T43 T44 T45	
• Molecule 159: S'	TAPLE STRAND		
Chain Ci:	52% 58%	35%	6%
C1 23 24 25 26 26 26 27 26 26 27 26 26 26 26 26 26 26 26 26 26	613 114 115 115 115 117 118 119 120 123 123 123 123 123 123 123 123	C32 C32 C34 C35 C35 C35 C35 C42 C42 C42 C42 C42 C42 C42 C42 C42 C43 C42 C43 C42 C43 C42 C42 C42 C42 C42 C42 C42 C42 C42 C42	

• Molecule 160: S	STAPLE STRAND			
Chain Cj:	56%	37%	7%	
A1 64 65 69 69 61 61 61 61 616 616	617 220 221 221 221 222 228 628 628 628 633 633 633 633 633 640 440 440	28 11 11 12 1		
• Molecule 161: S	TAPLE STRAND			
Chain Ck:	26%	289	•	
61 42 43 49 611 712 611 712 611 712 611 712 61 712 712 712 712 712 712 712 71	C21 C21 A25 A25 A26 C21 A26 C37 C33 C33 C33 C33 C33 C33 C33 C33 C33	146 1		
• Molecule 162: S	TAPLE STRAND			
Chain Cl:	60%	31%	9%	
61 14 14 14 16 16 10 11 11 11 11 11 11 11 11 11 11 11 11	A22 A26 A26 A26 A32 C33 A32 C33 C33 C33 C33 C33 C33 C33 C33 C33 C			
• Molecule 163: S	TAPLE STRAND			
Chain Cm:	58%	42%		
61 13 13 14 14 15 05 011 013 013 014 014 014 115	C16 T20 A21 A24 C26 C30 C30 C30 C30 C32 C30 C32 C33 C33 C32 C32 C32 C32 C32 C32 C32			
• Molecule 164: S	TAPLE STRAND			
Chain Cn:	36% 73%	2	27%	
A1 76 612 613 612 613 612 613	C14 A17 C18 C18 C18 C21 C21 C22 C23 A24 A26 A26 A26 A26 A26 A26 A28 A28 A28 A28 A28 A28 A28 A28 A28 A28	A4 0		
• Molecule 165: S	TAPLE STRAND			
Chain Co:	30% 54%	41%	5%	
11 16 17 18 18 18 11 11 11 11 13 113 113 113	A19 420 121 022 022 022 126 424 126 126 126 131 131 133 133 133 133 133 133 133 13			
• Molecule 166: S	TAPLE STRAND			
Chain Cp:	51%	41%	8%	











• Molecule 18	80: STAPLE STRAND	
Chain C3:	78%	22%
1121 1121 1121 1121 1121	622 623 624 624 624 427 434 434 434 434 434 434 137	
• Molecule 18	81: STAPLE STRAND	
Chain C4:	72%	28%
12 13 13 13	C15 C15 C15 C15 C20 C20 C20 C20 C20 C20 C20 C20	C57 C57
• Molecule 18	82: STAPLE STRAND	
Chain C5:	95% 59%	41%
11 12 13 14 15 15 15 15 15 15	A8 A10 A10 G12 G12 C13 C13 C13 C13 C13 G16 G17 G18 G17 G18 G17 G18 G18 G20 G20 G20 G20 G20 G20 G21 A25 A26 A28 A28 A28 A28 A28 A28 A28 A28 A28 A28	A31 632 633 633 633 634 A35 A35 638 638 638 638 638 638 638 638 638 638
• Molecule 18	83: STAPLE STRAND	
Chain C6:	68%	28% •
A1 A5 A5 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A7 A5 A5 A5 A5 A5 A5 A5 A5 A5 A5 A5 A5 A5	111 113 114 114 114 114 114 114 1135 133 133 133 133 133 133 133 133 13	× 50
• Molecule 18	84: STAPLE STRAND	
Chain C7:	13% 72%	26% ·
C1 A6 A7 A8 A8 A10 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	A15 A15 A18 A23 A23 C24 C26 C38 C38 C38 C38 C38 C38 C38 C38 C38 C38	
• Molecule 18	85: STAPLE STRAND	
Chain C8:	29% 71%	26% ·
C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C	A12 (13) (15) (15) (15) (15) (15) (15) (15) (12) (12) (12) (12) (12) (12) (12) (12	
• Molecule 18	86: STAPLE STRAND	
Chain C9:	41% 68%	32%






# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	51	Depositor
Minimum defocus (nm)	328.5	Depositor
Maximum defocus (nm)	2444.2	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON III $(4k \ge 4k)$	Depositor
Maximum map value	0.793	Depositor
Minimum map value	-0.309	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	639.39996, 639.39996, 639.39996	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.7799997, 2.7799997, 2.7799997	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).

Mal	Chain	B	ond lengths	be Bond angles	
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	AA	1.21	12/184801~(0.0%)	1.40	2511/285260~(0.9%)
2	AB	1.22	0/1095	1.44	18/1690~(1.1%)
3	AC	1.21	1/1228~(0.1%)	1.36	12/1894~(0.6%)
4	AD	1.20	0/1112	1.35	15/1716~(0.9%)
5	AE	1.24	0/1086	1.37	13/1672~(0.8%)
6	AF	1.20	0/1272	1.36	17/1962~(0.9%)
7	AG	1.17	0/1080	1.33	13/1665~(0.8%)
8	AH	1.19	0/714	1.39	11/1101~(1.0%)
9	AI	1.18	0/636	1.30	4/981~(0.4%)
10	AJ	1.19	0/1095	1.31	5/1687~(0.3%)
11	AK	1.26	0/737	1.45	10/1137~(0.9%)
12	AL	1.18	0/1193	1.38	18/1841~(1.0%)
13	AM	1.12	0/854	1.22	7/1315~(0.5%)
14	AN	1.17	0/1062	1.27	7/1639~(0.4%)
15	AO	1.20	0/1068	1.33	9/1646~(0.5%)
16	AP	1.20	0/1100	1.34	9/1697~(0.5%)
17	AQ	1.16	0/1085	1.26	8/1672~(0.5%)
18	AR	1.19	0/1056	1.24	3/1629~(0.2%)
19	AS	1.17	0/1135	1.22	7/1746~(0.4%)
20	AT	1.21	1/1078~(0.1%)	1.34	11/1660~(0.7%)
21	AU	1.22	0/927	1.28	6/1429~(0.4%)
22	AV	1.24	0/1025	1.44	15/1582~(0.9%)
23	AW	1.19	0/1103	1.24	4/1700~(0.2%)
24	AX	1.20	0/860	1.44	13/1326~(1.0%)
25	AY	1.20	0/1085	1.40	12/1674~(0.7%)
26	AZ	1.24	0/912	1.47	14/1404~(1.0%)
27	Aa	1.20	1/1220~(0.1%)	1.29	12/1881~(0.6%)
28	Ab	1.19	0/895	1.35	12/1380~(0.9%)
29	Ac	1.18	0/697	1.30	5/1072~(0.5%)
30	Ad	1.19	0/1046	1.44	19/1612~(1.2%)
31	Ae	1.18	0/1179	1.30	13/1818~(0.7%)
32	Af	1.23	0/1049	1.41	15/1616~(0.9%)
33	Ag	1.23	0/690	1.34	9/1065~(0.8%)
34	Ah	1.19	0/901	1.38	8/1389~(0.6%)



Mal	Chain	B	ond lengths	Bond angles	
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
35	Ai	1.19	0/1095	1.28	12/1691~(0.7%)
36	Aj	1.20	0/924	1.43	12/1423~(0.8%)
37	Ak	1.18	0/870	1.45	11/1340~(0.8%)
38	Al	1.22	0/1274	1.38	10/1961~(0.5%)
39	Am	1.17	0/862	1.26	4/1329~(0.3%)
40	An	1.18	0/1022	1.34	7/1573~(0.4%)
41	Ao	1.19	0/1059	1.27	7/1632~(0.4%)
42	Ap	1.18	0/1089	1.42	15/1678~(0.9%)
43	Aq	1.24	0/746	1.40	8/1151~(0.7%)
44	Ar	1.23	0/1109	1.30	7/1712~(0.4%)
45	As	1.20	0/1119	1.46	24/1725~(1.4%)
46	At	1.19	0/1242	1.35	14/1914~(0.7%)
47	Au	1.11	0/1047	1.23	5/1612~(0.3%)
48	Av	1.16	0/1108	1.38	14/1708~(0.8%)
49	Aw	1.21	0/1074	1.21	6/1653~(0.4%)
50	Ax	1.18	0/1032	1.40	9/1588~(0.6%)
51	Ay	1.28	0/725	1.29	2/1119~(0.2%)
52	Az	1.20	0/689	1.36	9/1061~(0.8%)
53	A0	1.22	0/726	1.38	6/1116~(0.5%)
54	A1	1.22	0/1106	1.38	11/1705~(0.6%)
55	A2	1.15	0/1059	1.33	13/1631~(0.8%)
56	A3	1.23	0/691	1.32	8/1065~(0.8%)
57	A4	1.16	0/1025	1.32	8/1578~(0.5%)
58	A5	1.14	0/1036	1.26	6/1598~(0.4%)
59	A6	1.24	0/1121	1.47	16/1730~(0.9%)
60	A7	1.16	0/1094	1.32	14/1686~(0.8%)
61	A8	1.21	0/1343	1.47	15/2068~(0.7%)
62	A9	1.28	5/875~(0.6%)	1.32	8/1348~(0.6%)
63	BA	1.19	0/1102	1.41	15/1697~(0.9%)
64	BB	1.29	1/718~(0.1%)	1.38	10/1106~(0.9%)
65	BC	1.19	0/1371	1.30	16/2113~(0.8%)
66	BD	1.22	0/1225	1.33	7/1888~(0.4%)
67	BE	1.17	0/727	1.33	5/1118 (0.4%)
68	BF	1.21	0/878	1.37	8/1352~(0.6%)
69	BG	1.22	0/1072	1.40	15/1654~(0.9%)
70	BH	1.15	0/1291	1.26	14/1993~(0.7%)
71	BI	1.24	0/1029	1.26	4/1585~(0.3%)
72	BJ	1.20	0/1043	1.35	7/1609~(0.4%)
73	BK	1.20	0/1100	1.34	$13/1696 \ (0.8\%)$
74	BL	1.20	0/1029	1.39	13/1586 (0.8%)
75	BM	1.23	0/1114	1.36	12/1719 (0.7%)
76	BN	1.20	0/695	1.38	8/1072 (0.7%)
77	BO	1.26	1/1024~(0.1%)	1.38	13/1577~(0.8%)



Mal	Bond lengths Bond		Bond angles		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
78	BP	1.25	0/1035	1.42	9/1594~(0.6%)
79	BQ	1.18	0/1046	1.31	6/1614 (0.4%)
80	BR	1.21	0/861	1.33	6/1326 (0.5%)
81	BS	1.11	0/1088	1.21	7/1675~(0.4%)
82	BT	1.24	0/1205	1.35	10/1858 (0.5%)
83	BU	1.23	0/876	1.51	18/1347 (1.3%)
84	BV	1.20	0/721	1.39	10/1110 (0.9%)
85	BW	1.16	0/699	1.38	8/1074 (0.7%)
86	BX	1.21	0/1024	1.31	5/1576~(0.3%)
87	BY	1.17	0/1196	1.37	10/1844 (0.5%)
88	BZ	1.20	0/1078	1.26	7/1666 (0.4%)
89	Ba	1.21	0/1073	1.35	12/1656~(0.7%)
90	Bb	1.27	0/893	1.38	13/1379~(0.9%)
91	Bc	1.23	0/1035	1.37	16/1597~(1.0%)
92	Bd	1.20	0/1109	1.31	9/1709~(0.5%)
93	Be	1.18	0/1019	1.38	15/1566~(1.0%)
94	Bf	1.20	0/870	1.34	8/1341~(0.6%)
95	Bg	1.23	0/880	1.49	18/1358~(1.3%)
96	Bh	1.20	0/916	1.35	12/1409~(0.9%)
97	Bi	1.16	0/1108	1.44	17/1708~(1.0%)
98	Bj	1.22	0/1117	1.48	16/1723~(0.9%)
99	Bk	1.21	0/699	1.43	13/1078~(1.2%)
100	Bl	1.21	0/935	1.39	11/1443~(0.8%)
101	Bm	1.18	0/869	1.37	9/1337~(0.7%)
102	Bn	1.18	0/984	1.27	10/1517~(0.7%)
103	Bo	1.21	1/1021~(0.1%)	1.36	11/1574~(0.7%)
104	Bp	1.32	3/1098~(0.3%)	1.67	28/1695~(1.7%)
105	Bq	1.19	0/1100	1.26	4/1699~(0.2%)
106	Br	1.19	0/872	1.31	8/1345~(0.6%)
107	Bs	1.18	0/680	1.46	14/1048~(1.3%)
108	Bt	1.19	0/1028	1.41	12/1586~(0.8%)
109	Bu	1.18	0/1123	1.33	11/1734~(0.6%)
110	Bv	1.22	0/916	1.39	10/1410~(0.7%)
111	Bw	1.14	0/844	1.32	10/1299~(0.8%)
112	Bx	1.14	0/1182	1.26	8/1824~(0.4%)
113	By	1.19	0/705	1.47	13/1089~(1.2%)
114	Bz	1.18	0/925	1.36	9/1425~(0.6%)
115	B0	1.18	0/688	1.23	3/1060~(0.3%)
116	B1	1.13	0/1190	1.31	13/1838~(0.7%)
117	B2	1.20	0/690	1.29	7/1063~(0.7%)
118	B3	1.19	0/1283	1.26	9/1977~(0.5%)
119	B4	1.20	0/1112	1.34	8/1715~(0.5%)
120	B5	1.17	0/707	1.30	3/1090~(0.3%)



Mal	Chain	B	ond lengths	Bond angles	
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
121	B6	1.20	0/1043	1.36	14/1611~(0.9%)
122	B7	1.21	0/855	1.31	5/1319~(0.4%)
123	B8	1.23	0/1192	1.28	12/1841~(0.7%)
124	B9	1.24	0/857	1.38	11/1320~(0.8%)
125	CA	1.21	0/721	1.38	11/1108 (1.0%)
126	CB	1.20	0/736	1.47	10/1135~(0.9%)
127	CC	1.26	0/703	1.39	9/1086~(0.8%)
128	CD	1.26	5/1341~(0.4%)	1.45	21/2068~(1.0%)
129	CE	1.19	0/1192	1.32	8/1837~(0.4%)
130	CF	1.21	0/918	1.38	7/1413~(0.5%)
131	CG	1.30	0/700	1.42	10/1077~(0.9%)
132	СН	1.24	0/1233	1.49	19/1906~(1.0%)
133	CI	1.23	0/689	1.50	13/1062~(1.2%)
134	CJ	1.17	0/1098	1.33	11/1693~(0.6%)
135	CK	1.21	0/1268	1.37	21/1957~(1.1%)
136	CL	1.20	0/719	1.39	9/1110~(0.8%)
137	CM	1.24	0/734	1.46	10/1130~(0.9%)
138	CN	1.22	0/932	1.36	12/1438~(0.8%)
139	CO	1.19	0/679	1.37	9/1045~(0.9%)
140	CP	1.23	0/1238	1.39	15/1911~(0.8%)
141	CQ	1.21	0/1094	1.35	5/1685~(0.3%)
142	CR	1.21	0/1035	1.30	8/1597~(0.5%)
143	CS	1.22	0/1103	1.43	16/1701~(0.9%)
144	CT	1.21	0/862	1.55	16/1326~(1.2%)
145	CU	1.23	0/697	1.34	6/1075~(0.6%)
146	CV	1.17	0/732	1.25	1/1127~(0.1%)
147	CW	1.19	0/1090	1.30	12/1683~(0.7%)
148	CX	1.19	0/1087	1.39	14/1676~(0.8%)
149	CY	1.25	0/1121	1.42	15/1731~(0.9%)
150	CZ	1.20	0/1061	1.35	14/1640~(0.9%)
151	Ca	1.19	0/898	1.29	6/1383~(0.4%)
152	Cb	1.22	0/1052	1.28	6/1624~(0.4%)
153	Cc	1.19	0/690	1.38	7/1065~(0.7%)
154	Cd	1.22	0/875	1.44	13/1349 (1.0%)
155	Ce	1.21	0/673	1.29	3/1035~(0.3%)
156	Cf	1.20	0/900	1.47	$11/1382 \ (0.8\%)$
157	Cg	1.21	0/874	1.31	6/1348~(0.4%)
158	Ch	1.20	0/1043	1.36	9/1610 (0.6%)
159	Ci	1.24	0/1089	1.55	26/1681 (1.5%)
160	Cj	1.29	0/1242	1.47	17/1916 (0.9%)
161	Ck	1.22	0/1067	1.42	21/1646 (1.3%)
162	Cl	1.24	0/1021	1.43	15/1573 (1.0%)
163	Cm	1.21	0/852	1.45	13/1312~(1.0%)



Mal	Chain	Bond lengths		Bond angles	
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5
164	Cn	1.16	0/1030	1.28	6/1585~(0.4%)
165	Co	1.17	0/840	1.47	17/1295~(1.3%)
166	Ср	1.25	0/841	1.43	13/1296~(1.0%)
167	Cq	1.23	0/817	1.40	8/1259~(0.6%)
168	Cr	1.24	0/872	1.38	14/1345~(1.0%)
169	Cs	1.22	0/901	1.29	7/1392~(0.5%)
170	Ct	1.25	0/880	1.46	13/1356~(1.0%)
171	Cu	1.23	0/823	1.33	6/1270~(0.5%)
172	Cv	1.25	0/834	1.41	11/1285~(0.9%)
173	Cw	1.18	0/707	1.33	6/1087~(0.6%)
174	Cx	1.19	0/858	1.41	11/1322~(0.8%)
175	Су	1.23	0/1027	1.37	8/1583~(0.5%)
176	Cz	1.21	0/1186	1.37	11/1830~(0.6%)
177	C0	1.15	0/1354	1.36	17/2088~(0.8%)
178	C1	1.18	0/1082	1.30	10/1669~(0.6%)
179	C2	1.21	0/742	1.38	7/1145~(0.6%)
180	C3	1.24	0/849	1.39	7/1309~(0.5%)
181	C4	1.16	0/1294	1.33	13/1996~(0.7%)
182	C5	1.19	0/1025	1.46	19/1582~(1.2%)
183	C6	1.20	0/1077	1.37	11/1659~(0.7%)
184	C7	1.18	0/1076	1.37	10/1656~(0.6%)
185	C8	1.18	0/863	1.30	6/1329~(0.5%)
186	C9	1.19	0/863	1.32	7/1332~(0.5%)
187	DA	1.18	0/1374	1.40	22/2118~(1.0%)
188	DB	1.23	0/980	1.43	10/1511~(0.7%)
189	DC	1.17	0/1075	1.31	11/1658~(0.7%)
190	DD	1.17	0/869	1.39	12/1339~(0.9%)
191	DE	1.21	0/1056	1.35	13/1627~(0.8%)
192	DF	1.19	0/718	1.35	9/1107~(0.8%)
All	All	1.21	31/372075~(0.0%)	1.38	4574/573956~(0.8%)

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	26	1811
2	AB	0	10
3	AC	0	13
4	AD	0	12
5	AE	0	5



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Mol	Chain	#Chirality outliers	#Planarity outliers
6	AF	0	17
7	AG	0	5
8	AH	0	6
9	AI	0	6
10	AJ	0	7
11	AK	0	4
12	AL	0	5
13	AM	0	2
14	AN	0	8
15	AO	0	8
16	AP	0	10
17	AQ	0	7
18	AR	0	10
19	AS	0	12
20	AT	0	8
21	AU	0	12
22	AV	0	6
23	AW	0	10
24	AX	0	9
25	AY	0	9
26	AZ	0	7
27	Aa	0	12
28	Ab	0	7
29	Ac	0	4
30	Ad	0	8
31	Ae	0	10
32	Af	0	9
33	Ag	0	6
34	Ah	0	3
35	Ai	0	14
36	Aj	0	5
37	Ak	0	2
38	Al	0	9
39	Am	0	6
40	An	0	12
41	Ao	0	7
42	Ap	0	6
43	Aq	0	11
44	Ar	0	11
45	As	0	5
46	At	0	10
47	Au	0	7



Mol	Chain	#Chirality outliers	#Planarity outliers
48	Av	0	8
49	Aw	0	5
50	Ax	0	9
51	Ay	0	6
52	Az	0	7
53	A0	0	5
54	A1	0	9
55	A2	0	8
56	A3	0	6
57	A4	0	7
58	A5	0	5
59	A6	0	9
60	A7	0	10
61	A8	0	11
62	A9	0	7
63	BA	0	7
64	BB	0	7
65	BC	0	6
66	BD	0	7
67	BE	0	5
68	BF	0	10
69	BG	0	15
70	BH	0	10
71	BI	0	9
72	BJ	0	9
73	BK	0	13
74	BL	0	8
75	BM	0	9
76	BN	0	6
77	BO	0	11
78	BP	0	12
79	BQ	0	12
80	BR	0	10
81	BS	0	8
82	BT	0	12
83	BU	0	7
84	BV	0	9
85	BW	0	5
86	BX	0	2
87	BY	0	6
88	BZ	0	4
89	Ba	0	10



Mol	Chain	#Chirality outliers	<b>#Planarity outliers</b>
90	Bb	0	16
91	Bc	0	8
92	Bd	0	8
93	Be	0	9
94	Bf	0	9
95	Bg	0	11
96	Bh	0	9
97	Bi	0	11
98	Bj	0	9
99	Bk	0	5
100	Bl	0	5
101	Bm	0	9
102	Bn	0	6
103	Bo	0	11
104	Bp	0	12
105	Bq	0	7
106	Br	0	7
107	Bs	0	12
108	Bt	0	8
109	Bu	0	11
110	Bv	0	8
111	Bw	0	9
112	Bx	0	17
113	By	0	4
114	Bz	0	4
115	B0	0	6
116	B1	0	13
117	B2	0	4
118	B3	0	14
119	B4	0	5
120	B5	0	6
121	B6	0	17
122	B7	0	5
123	B8	0	12
124	B9	0	14
125	CA	0	5
126	CB	0	13
127		0	6
128	CD	0	12
129	CE	0	9
130	CF	0	·7
131	CG	0	7



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Mol	Chain	#Chirality outliers	#Planarity outliers
132	CH	0	14
133	CI	0	4
134	CJ	0	11
135	CK	0	11
136	CL	0	4
137	CM	0	9
138	CN	0	8
139	СО	0	7
140	CP	0	12
141	CQ	0	11
142	CR	0	9
143	CS	0	11
144	CT	0	11
145	CU	0	6
146	CV	0	7
147	CW	0	9
148	CX	0	8
149	CY	0	9
150	CZ	0	10
151	Ca	0	9
152	Cb	0	5
153	Cc	0	14
154	Cd	0	4
155	Ce	0	10
156	Cf	0	7
157	Cg	0	11
158	Ch	0	11
159	Ci	0	8
160	Cj	0	18
161	Ck	0	6
162	Cl	0	11
163	Cm	0	7
164	Cn	0	7
165	Co	0	8
166	Cp	0	11
167	Cq	0	4
168	Cr	0	11
169	Cs	0	12
170	Ct	0	9
171	Cu	0	5
172	Cv	0	11
173	Cw	0	7



Mol	Chain	#Chirality outliers	#Planarity outliers
174	Cx	0	8
175	Су	0	16
176	Cz	0	13
177	C0	0	11
178	C1	0	12
179	C2	0	6
180	C3	0	2
181	C4	0	8
182	C5	0	7
183	C6	0	11
184	C7	0	8
185	C8	0	9
186	C9	0	7
187	DA	0	16
188	DB	0	5
189	DC	0	6
190	DD	0	9
191	DE	0	10
192	DF	0	4
All	All	26	3449

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
128	CD	51	DG	C4'-C3'	7.13	1.60	1.53
62	A9	9	DA	C5'-C4'	6.85	1.58	1.51
128	CD	52	DT	C5'-C4'	6.70	1.58	1.51
128	CD	51	DG	C5'-C4'	6.17	1.58	1.51
104	Bp	22	DA	C5'-C4'	6.02	1.57	1.51

The worst 5 of 4574 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	AA	1068	DG	P-O3'-C3'	16.13	139.06	119.70
1	AA	1599	DT	P-O3'-C3'	16.01	138.92	119.70
160	Cj	27	DG	P-O3'-C3'	15.34	138.10	119.70
1	AA	645	DA	P-O3'-C3'	14.96	137.65	119.70
1	AA	5153	DG	P-O3'-C3'	14.88	137.55	119.70

5 of 26 chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
1	AA	1155	DG	C3'
1	AA	1417	DA	C4',C3'
1	AA	3394	DT	C3'
1	AA	3534	DA	C4',C3'
1	AA	3922	DA	C4',C3'

5 of 3449 planarity outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Group
1	AA	1	DT	Sidechain
1	AA	10	DG	Sidechain
1	AA	14	DT	Sidechain
1	AA	18	DC	Sidechain
1	AA	3	DA	Sidechain

### 5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	164972	0	91297	0	0
2	AB	972	0	529	0	0
3	AC	1091	0	596	0	0
4	AD	989	0	542	0	0
5	AE	971	0	543	0	0
6	AF	1131	0	620	0	0
7	AG	970	0	554	0	0
8	AH	636	0	354	0	0
9	AI	570	0	324	0	0
10	AJ	977	0	543	0	0
11	AK	657	0	361	0	0
12	AL	1065	0	592	0	0
13	AM	766	0	439	0	0
14	AN	946	0	522	0	0
15	AO	947	0	514	0	0
16	AP	982	0	545	0	0
17	AQ	972	0	553	0	0
18	AR	942	0	522	0	0
19	AS	1012	0	566	0	0



Conti	Continuea from previous page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
20	AT	959	0	528	0	0		
21	AU	823	0	448	0	0		
22	AV	918	0	519	0	0		
23	AW	982	0	539	0	0		
24	AX	763	0	412	0	0		
25	AY	966	0	536	0	0		
26	AZ	813	0	450	0	0		
27	Aa	1086	0	598	0	0		
28	Ab	798	0	443	0	0		
29	Ac	624	0	352	0	0		
30	Ad	927	0	505	0	0		
31	Ae	1056	0	595	0	0		
32	Af	936	0	521	0	0		
33	Ag	616	0	343	0	0		
34	Ah	801	0	437	0	0		
35	Ai	981	0	554	0	0		
36	Aj	820	0	449	0	0		
37	Ak	775	0	429	0	0		
38	Al	1136	0	633	0	0		
39	Am	772	0	438	0	0		
40	An	912	0	506	0	0		
41	Ao	942	0	518	0	0		
42	Ap	974	0	548	0	0		
43	Aq	662	0	362	0	0		
44	Ar	988	0	547	0	0		
45	As	991	0	536	0	0		
46	At	1105	0	608	0	0		
47	Au	934	0	524	0	0		
48	Av	985	0	543	0	0		
49	Aw	964	0	549	0	0		
50	Ax	917	0	505	0	0		
51	Ay	643	0	347	0	0		
52	Az	613	0	338	0	0		
53	A0	647	0	358	0	0		
54	A1	984	0	542	0	0		
55	A2	941	0	519	0	0		
56	A3	615	0	339	0	0		
57	A4	914	0	510	0	0		
58	A5	923	0	515	0	0		
59	A6	994	0	540	0	0		
60	A7	977	0	550	0	0		
61	A8	1206	0	686	0	0		



Conti	nuea fron	<i>i previous</i>	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
62	A9	778	0	427	0	0
63	BA	980	0	540	0	0
64	BB	637	0	347	0	0
65	BC	1223	0	676	0	0
66	BD	1088	0	597	0	0
67	BE	648	0	362	0	0
68	BF	779	0	427	0	0
69	BG	959	0	538	0	0
70	BH	1159	0	660	0	0
71	BI	917	0	506	0	0
72	BJ	927	0	507	0	0
73	BK	981	0	544	0	0
74	BL	918	0	511	0	0
75	BM	990	0	544	0	0
76	BN	618	0	340	0	0
77	BO	914	0	509	0	0
78	BP	920	0	506	0	0
79	BQ	929	0	507	0	0
80	BR	770	0	432	0	0
81	BS	972	0	548	0	0
82	BT	1070	0	581	0	0
83	BU	784	0	440	0	0
84	BV	646	0	365	0	0
85	BW	624	0	347	0	0
86	BX	913	0	508	0	0
87	BY	1065	0	590	0	0
88	BZ	957	0	517	0	0
89	Ba	952	0	516	0	0
90	Bb	791	0	427	0	0
91	Bc	923	0	513	0	0
92	Bd	985	0	542	0	0
93	Be	908	0	502	0	0
94	Bf	776	0	434	0	0
95	Bg	783	0	429	0	0
96	Bh	814	0	447	0	0
97	Bi	993	0	565	0	0
98	Bj	991	0	542	0	0
99	Bk	620	0	338	0	0
100	Bl	829	0	449	0	0
101	Bm	773	0	427	0	0
102	Bn	878	0	492	0	0
103	Bo	914	0	519	0	0



Conti	Continuea from previous page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
104	Bp	974	0	528	0	0		
105	Bq	984	0	551	0	0		
106	Br	778	0	434	0	0		
107	Bs	609	0	346	0	0		
108	Bt	919	0	517	0	0		
109	Bu	1004	0	565	0	0		
110	Bv	815	0	447	0	0		
111	Bw	752	0	422	0	0		
112	Bx	1059	0	602	0	0		
113	By	625	0	338	0	0		
114	Bz	821	0	450	0	0		
115	B0	613	0	342	0	0		
116	B1	1065	0	604	0	0		
117	B2	614	0	340	0	0		
118	B3	1143	0	630	0	0		
119	B4	988	0	537	0	0		
120	B5	632	0	358	0	0		
121	B6	929	0	511	0	0		
122	B7	761	0	417	0	0		
123	B8	1066	0	593	0	0		
124	B9	768	0	434	0	0		
125	CA	644	0	359	0	0		
126	CB	656	0	362	0	0		
127	CC	624	0	337	0	0		
128	CD	1200	0	672	0	0		
129	CE	1062	0	590	0	0		
130	CF	816	0	446	0	0		
131	CG	626	0	347	0	0		
132	CH	1098	0	600	0	0		
133	CI	614	0	339	0	0		
134	CJ	988	0	570	0	0		
135	CK	1138	0	643	0	0		
136	CL	640	0	350	0	0		
137	CM	653	0	359	0	0		
138	CN	827	0	450	0	0		
139	CO	607	0	340	0	0		
140	CP	1106	0	612	0	0		
141	CQ	976	0	540	0	0		
142	CR	923	0	511	0	0		
143	CS	983	0	539	0	0		
144	CT	769	0	426	0	0		
145	CU	619	0	337	0	0		



Conti	nueu fron	<i>i previous</i>	page		1	
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
146	CV	652	0	358	0	0
147	CW	970	0	531	0	0
148	CX	974	0	552	0	0
149	CY	995	0	535	0	0
150	CZ	948	0	528	0	0
151	Ca	798	0	437	0	0
152	Cb	933	0	503	0	0
153	Cc	616	0	340	0	0
154	Cd	779	0	425	0	0
155	Се	603	0	339	0	0
156	Cf	803	0	449	0	0
157	Cg	779	0	429	0	0
158	Ch	928	0	507	0	0
159	Ci	977	0	550	0	0
160	Сј	1107	0	607	0	0
161	Ck	948	0	517	0	0
162	Cl	913	0	508	0	0
163	Cm	765	0	435	0	0
164	Cn	916	0	504	0	0
165	Co	752	0	425	0	0
166	Ср	752	0	418	0	0
167	Cq	731	0	409	0	0
168	Cr	778	0	430	0	0
169	Cs	804	0	441	0	0
170	Ct	781	0	425	0	0
171	Cu	736	0	413	0	0
172	Cv	748	0	423	0	0
173	Cw	629	0	347	0	0
174	Cx	761	0	416	0	0
175	Cy	917	0	507	0	0
176	Cz	1061	0	594	0	0
177	CO	1215	0	692	0	0
178	C1	964	0	532	0	0
179	C2	660	0	363	0	0
180	C3	757	0	417	0	0
181	C4	1159	0	655	0	0
182	C5	910	0	497	0	0
183	C6	959	0	529	0	0
184	C7	957	0	526	0	0
185	C8	771	0	429	0	0
186	C9	766	0	418	0	0
187	DA	1225	0	681	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
188	DB	876	0	487	0	0
189	DC	952	0	515	0	0
190	DD	775	0	428	0	0
191	DE	940	0	515	0	0
192	DF	638	0	349	0	0
All	All	331913	0	183783	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 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-11378. 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: 115



Z Index: 115

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: 130

Y Index: 97

Z Index: 119

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



The images above show the 3D surface view of the map at the recommended contour level 0.11. 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  $6439 \text{ nm}^3$ ; this corresponds to an approximate mass of 5817 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 0.118  ${\rm \AA^{-1}}$ 



## 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 0.118  $\text{\AA}^{-1}$ 



## 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	8.50	-	-
Author-provided FSC curve	8.45	10.32	8.61
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-11378 and PDB model 7ARY. Per-residue inclusion information can be found in section 3 on page 38.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.11 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 (0.11).



## 9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 68% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.6784	0.0580
A0	0.8547	0.1060
A1	0.5976	0.0140
A2	0.7396	0.0490
A3	0.7593	0.0710
A4	0.6685	0.0520
A5	0.4756	0.0360
A6	0.6167	-0.0000
A7	0.6121	0.0430
A8	0.3731	0.0690
A9	0.4447	0.0240
AA	0.6844	0.0600
AB	0.8704	0.1090
AC	0.8139	0.0630
AD	0.8059	0.1160
AE	0.8548	0.1230
AF	0.8895	0.1220
AG	0.2021	0.0360
AH	0.9009	0.1400
AI	0.9649	0.1160
AJ	0.8649	0.1110
AK	0.8219	0.1140
AL	0.6629	0.1040
AM	0.8185	0.1220
AN	0.6670	0.1010
AO	0.8395	0.1190
AP	0.7230	0.0610
AQ	0.2901	0.0590
AR	0.7686	0.1110
AS	0.6650	0.0970
AT	0.6809	0.0330
AU	0.6574	0.0050
AV	0.4063	0.0420
AW	0.8462	0.1020
AX	0.7654	0.0960



Chain	Atom inclusion	Q-score
AY	0.7919	0.0770
AZ	0.7724	0.0920
Aa	0.8573	0.1100
Ab	0.7469	0.0480
Ac	0.6442	0.0640
Ad	0.8447	0.1220
Ae	0.5218	0.0940
Af	0.8066	0.1280
Ag	0.8149	0.0990
Ah	0.7228	0.0650
Ai	0.3435	0.0860
Aj	0.8500	0.0930
Ak	0.7058	0.0570
Al	0.6083	0.0240
Am	0.6541	0.0500
An	0.8783	0.1200
Ao	0.7962	0.0750
Ap	0.7105	0.0560
Aq	0.7477	0.0800
Ar	0.6366	0.0290
As	0.6337	0.0240
At	0.6833	0.0410
Au	0.7259	0.0430
Av	0.6041	0.0430
Aw	0.1162	0.0240
Ax	0.8092	0.1020
Ay	0.6563	0.0470
Az	0.5661	0.0260
B0	0.6313	0.0080
B1	0.6582	0.0520
B2	0.5554	-0.0010
B3	0.6763	0.0380
B4	0.6680	0.0010
B5	0.5538	0.0290
B6	0.6437	0.0150
B7	0.6873	0.0860
B8	0.5610	0.0620
B9	0.5846	-0.0160
BA	0.6612	0.0170
BB	0.4647	0.0220
BC	0.3794	0.0820
BD	0.8557	0.1140



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Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
BE	0.7901	0.0670
BF	0.7754	0.0750
BG	0.6569	0.0320
BH	0.4029	0.0890
BI	0.7503	0.0860
BJ	0.7465	0.0600
BK	0.6901	0.0400
BL	0.8214	0.1110
BM	0.5828	0.0170
BN	0.5000	-0.0140
BO	0.7243	0.0630
BP	0.5728	0.0050
BQ	0.6017	0.0110
BR	0.7325	0.0380
BS	0.6749	0.0550
BT	0.7308	0.1090
BU	0.7245	0.0500
BV	0.5619	0.0100
BW	0.7548	0.0920
BX	0.6068	0.0120
BY	0.7174	0.1210
BZ	0.7806	0.0910
Ba	0.8435	0.0950
Bb	0.7143	0.0280
Bc	0.5623	0.0020
Bd	0.6416	0.0350
Be	0.8579	0.1080
Bf	0.6598	0.0200
Bg	0.6360	0.0320
Bh	0.7592	0.0940
Bi	0.7059	0.1080
Bj	0.7427	0.0600
Bk	0.8113	0.1160
Bl	0.6707	0.0280
Bm	0.7141	0.0460
Bn	0.7882	0.0590
Bo	0.7473	0.0690
Bp	0.7495	0.0380
Bq	0.6972	0.0910
Br	0.7352	0.0600
Bs	0.5156	-0.0120
Bt	0.7029	0.0520



Chain	Atom inclusion	Q-score
Bu	0.7739	0.0540
Bv	0.6172	0.0200
Bw	0.5066	-0.0270
Bx	0.6072	0.0450
By	0.4672	0.0030
Bz	0.5250	-0.0130
C0	0.6626	0.0450
C1	0.3828	0.0790
C2	0.4500	0.0660
C3	0.6301	-0.0260
C4	0.6764	0.0480
C5	0.0363	0.0450
C6	0.5933	-0.0190
C7	0.7189	0.0550
C8	0.6706	0.0330
C9	0.5470	0.0090
CA	0.5497	-0.0200
CB	0.8338	0.0750
CC	0.5417	-0.0490
CD	0.3683	0.0680
CE	0.7232	0.0340
CF	0.6765	0.0180
CG	0.8067	0.0820
CH	0.7796	0.0720
CI	0.6384	0.0110
CJ	0.8117	0.0470
CK	0.2557	0.0630
CL	0.7875	0.0990
CM	0.7152	0.0240
CN	0.5937	0.0070
CO	0.6853	0.0170
СР	0.6962	0.0910
CQ	0.8156	0.0860
CR	0.5298	-0.0430
CS	0.7650	0.0690
CT	0.7698	0.0710
CU	0.6688	-0.0130
CV	0.6166	-0.0110
CW	0.7567	0.0300
CX	0.6181	0.0940
CY	0.8874	0.1010
CZ	0.8154	0.0750



Chain	Atom inclusion	Q-score
Ca	0.7356	
Ch	0.6817	
	0.8084	
Cd	0.6983	0.0180
Ce	0.8226	
Cf	0.8966	
Ca	0.6277	
Ch	0.6983	
Ci	0.4545	
Ci	0.7986	
Ck	0.6741	
Cl	0.8215	
Cm	0.0219	
Cn	0.6059	
Co	0.5904	-0.0130
Co	0.8511	
	0.7989	
Cr	0.7931	
	0.7551	
Ct	0.7030	
Cu	0.0412	
Cy	0.85/13	
	0.6153	
	0.5296	00350
Cy	0.5250	
Cz	0.6027	
	0.6506	
DB		
	0.0434	0.0530
	0.000	
DE	0.3004	0.1270
DE	0.6630	0.0020
	0.0000	0.0040

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Chain Atom inclusion

