

wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 08:49 pm GMT

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EMDB ID	:	EMD-11379
Title	:	TwistTower_native-twist
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Deposited on	:	2020-10-26
Resolution	:	7.40 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 7.40 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	• 69%	28%	•
2	AB	29	86%		14%
3	AC	48	75%	23%	•
4	AD	53	62%	36%	•
5	AE	60	52%	20%	•
6	AF	48	6% 71%	19%	10%
7	AG	48	69%	25%	6%
8	AH	60	85%		13% ·
9	AI	42	76%	21%	·
10	AJ	60	82%	1	7% •
11	AK	32	75%	19%	6%
12	AL	40	58%	35%	8%
13	AM	48	71%	27%	•
14	AN	32	66%	34%	
15	AO	48	73%	27%	
16	AP	40	70%	30%	
17	AQ	45	73%	24%	•



Mol	Chain	Length	Quality of chain		
18	AR	48	19%	23%)
19	AS	48	69%	29%	•
20	AT	45	69%	27%	•
21	AU	48	67%	31%	<u>.</u>
21	AV	40	67.0	200/	
22		58		30%	70/
20		50	74%	19%	7%
24	AA	60	83%	139	%•
25	AY	32	72%	28%	
26	AZ	48	71%	27%	•
27	Aa	40	85%		15%
28	Ab	48	69%	25%	6%
29	Ac	40	60%	38%	•
30	Ad	53	74%	23%	•
31	Ae	40	62%	28%	10%
32	Af	32	66%	31%	•
33	Ag	58	5%	22%	•
34	Ah	60	28%	22%	5%
35	Δi	48		2270	570
26		40	75%	21%	•
30	Al	40	69%	31%	
37	Ak	32	72%	19%	9%
38	Al	48	73%	25%	•
39	Am	58	74%	24%	•
40	An	60	82%	17	•
41	Ao	57	75%	23%	•
42	Ap	60	68%	27%	5%



Mol	Chain	Length	Quality of cha	in
43	Aq	48	69%	27% •
44	Ar	37	16%	16% 8%
45	As	40	82%	15% •
46	At	44	75%	25%
47	Au	40	68%	32%
18	Δν	40	600/	22%
40	Δ	56	08%	52%
49	AW		71%	29%
50	Ax	40	55%	45%
51	Ay	48	73%	23% •
52	Az	45	82%	18%
53	A0	32	66%	25% 9%
54	A1	48	• 65%	33% •
55	A2	48	6 9%	19% 12%
56	A3	56	62%	27% 11%
57	A4	45	73%	24% •
58	A5	48	71%	27%
59	A6	32	660/	210/
00	110	02	00%	31% ·
60	A7	32	75%	22% •
61	A8	32	78%	22%
62	A9	48	67%	33%
63	BA	45	80%	18% ·
64	BB	32	62%	25% 12%
65	BC	45	9%	27%
66	BD	57	5% 75%	23% •
67	BE	57	28%	19% 7%



Mol	Chain	Length	Quality of chain		
68	BF	45	67%	33%	
69	BG	40	65%	28%	8%
70	BH	57	7%	25%	•
71	BI	57	26%	26%	
72	BJ	45	71%	20%	
73	BK	32	72%	23%	
74	BL	56	710/	20%	
75	BM	20	/1%	29%	
75			84%	1	6%
70	BN	40	68%	32%	
77	BO	48	63%	35%	•
78	BP	58	69%	28%	•
79	BQ	57	72%	26%	•
80	BR	48	81%	19'	%
81	BS	48	77%	15%	8%
82	BT	48	71%	25%	•
83	BU	48	77%	21%	•
84	BV	58	9%81%	19'	%
85	BW	60	68%	28%	•
86	BX	32	72%	22%	6%
87	BY	40	62%	32%	5%
88	BZ	40	60%	38%	•
89	Ba	48	71%	21%	8%
90	Bb	48	52%	40%	8%
91	Be	32	75%		
92	Bd	48	75%	2270	



Mol	Chain	Length	Quality of chain		
93	Be	48	73%	23%	•
94	Bf	48	73%	25%	·
95	Bg	40	50% 4	.2%	8%
96	Bh	56	68%	29%	•
97	Bi	40	70%	20%	10%
98	Bj	32	62%	34%	•
99	Bk	32	75%	25%	
100	Bl	48	73%	25%	•
101	Bm	56	77%	20%	•
102	Bn	48	77%	19%	•
103	Bo	48	73%	25%	•
104	Bp	40	75%	22%	•
105	Bq	48	67%	33%	
106	Br	48	69%	31%	
107	Bs	32	75%	25%	
108	Bt	40	68%	30%	•
109	Bu	40	72%	28%	
110	Bv	40	68%	28%	5%
111	Bw	60	• 77%	17%	7%
112	Bx	45	9%	24%	.
113	By	40	72%	28%	
114	Bz	32	75%	25%	
115	B0	60	5% 72%	28%	
116	B1	60	30%	17%	5%
117	B2	40	65%	30%	5%



Mol	Chain	Length	Quality of chain		
118	B3	32	75%	25%	
119	B4	32	69%	25%	6%
120	B5	60	7%	25%	•
121	B6	53	8%	32%	•
122	B7	48	75%	25%	
123	B8	32	81%	19%	
124	B9	48	63%	31%	6%
125	CA	48	67%	31%	•
126	CB	60	73%	25%	•
127	$\mathbf{C}\mathbf{C}$	37	76%	19%	5%
128	CD	57	72%	26%	
129	CE	32	66%	31%	•
130	CF	40	60%	38%	•
131	CG	32	• 69%	28%	•
132	CH	53	6% 60%	38%	•
133	CI	32	75%	25%	
134	CJ	57	67% 67%	28%	5%
135	CK	32	6% 69%	31%	
136	CL	40	68%	30%	•
137	CM	32	75%	22%	•
138	CN	56	80%	14%	5%
139	СО	48	• 69%	27%	•
140	CP	48	6 3%	31%	6%
141	CQ	57	9% 65%	33%	•
142	CR	60	52% 70%	30%	



Mol	Chain	Length	Quality of chain		
143	CS	48	• 69%	29%	·
144	CT	56	75%	21%	•
145	CU	37	78%	229	%
146	CV	32	75%	19%	6%
147	CW	32	62%	38%	
148	CX	57	74%	25%	•
149	CY	60	47%	180	% •
150	CZ	48	67%	31%	•
151	Ca	48	71%	27%	•
152	Cb	40	60%	38%	•
153	Cc	32	9%	41%	
154	Cd	40	62%	25%	12%
155	Ce	40	70%	25%	5%
156	Cf	32	69%	28%	•
157	Cg	40	70%	30%	
158	Ch	40	68%	25%	8%
159	Ci	48	69%	31%	
160	Сј	40	70%	30%	
161	Ck	48	71%	29%	
162	Cl	40	72%	25%	•
163	Cm	48	58%	40%	•
164	Cn	40	52%	48%	
165	Со	40	65%	30%	5%
166	Ср	37	8%70%	27%	•
167	Cq	37	19% 86%		11% •



Mol	Chain	Length	Quality of chain		
168	Cr	40	68%	25%	8%
169	\mathbf{Cs}	40	68%	32%	
170	Ct	45	69%	24%	7%
171	Cu	37	59%	41%	
172	Cv	40	65%	30%	5%
173	Cw	40	70%	30%	
174	Cx	32	66%	28%	6%
175	Су	32	69%	31%	
176	Cz	32	88%		12%
177	C0	57	68%	30%	•
178	C1	57	67%	30%	
179	C2	32	72%	22%	6%
180	C3	48	63%	35%	•
181	C4	48	71%	23%	6%
182	C5	48	73%	25%	•
183	C6	48	67%	31%	•
184	C7	40	68%	30%	•
185	C8	48	65%	33%	•
186	С9	57	81%	16%	ó •
187	DA	45	62%	31%	7%
188	DB	32	72%	25%	•
189	DC	40	60%	38%	•
190	DD	45	100%	22%	7%
191	DE	48	94%	21%	•
192	DF	40	28%	22%	•



Mol	Chain	Length	Quality of chain				
193	DG	48	73%	25%	•		
194	DH	32	69%	25%	6%		
195	DI	32	72%	28%			



2 Entry composition (i)

There are 195 unique types of molecules in this entry. The entry contains 342569 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		At	\mathbf{oms}	AltConf	Trace		
2	AB	29	Total 582	C 282	N 90	0 182	Р 28	0	0

• Molecule 3 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
3	AC	48	Total 984	C 469	N 182	O 286	Р 47	0	0

• Molecule 4 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
4	AD	53	Total 1094	C 523	N 206	O 313	Р 52	0	0

• Molecule 5 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
5	AE	60	Total 1217	C 585	N 201	0 372	Р 59	0	0

• Molecule 6 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
6	AF	48	Total 982	C 469	N 179	0 287	Р 47	0	0

• Molecule 7 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
7	AG	48	Total 991	$\begin{array}{c} \mathrm{C} \\ 470 \end{array}$	N 193	0 281	Р 47	0	0

• Molecule 8 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
8	AH	60	Total 1224	C 593	N 196	O 376	Р 59	0	0

• Molecule 9 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
9	AI	42	Total 851	C 413	N 139	O 258	Р 41	0	0

• Molecule 10 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
10	AJ	60	Total 1218	C 593	N 193	0 373	Р 59	0	0

• Molecule 11 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	AltConf	Trace			
11	AK	32	Total 658	C 316	N 122	0 189	Р 31	0	0

• Molecule 12 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
12	AL	40	Total 815	C 393	N 138	0 245	Р 39	0	0

• Molecule 13 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
13	AM	48	Total 988	С 474	N 186	0 281	Р 47	0	0

• Molecule 14 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
14	AN	32	Total 662	C 317	N 130	0 184	Р 31	0	0

• Molecule 15 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
15	AO	48	Total 978	C 470	N 181	O 280	Р 47	0	0

• Molecule 16 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
16	AP	40	Total 817	C 390	N 159	O 229	Р 39	0	0

• Molecule 17 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
17	AQ	45	Total 914	C 443	N 151	0 276	Р 44	0	0

• Molecule 18 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
18	AR	48	Total 986	C 474	N 183	0 282	Р 47	0	0

• Molecule 19 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
19	AS	48	Total 988	C 471	N 192	0 278	Р 47	0	0

• Molecule 20 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}		AltConf	Trace		
20	AT	45	Total 928	C 443	N 166	0 275	Р 44	0	0

• Molecule 21 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
21	AU	48	Total 977	C 467	N 178	O 285	Р 47	0	0

• Molecule 22 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
22	AV	40	Total 817	C 387	N 165	O 226	Р 39	0	0

• Molecule 23 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
23	AW	58	Total 1155	C 556	N 185	O 357	Р 57	0	0

• Molecule 24 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
24	AX	60	Total 1225	C 590	N 214	O 362	Р 59	0	0

• Molecule 25 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
25	AY	32	Total 659	C 314	N 124	0 190	Р 31	0	0

• Molecule 26 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
26	AZ	48	Total 990	C 472	N 191	O 280	Р 47	0	0

• Molecule 27 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
27	Aa	40	Total 823	C 396	N 147	0 241	Р 39	0	0

• Molecule 28 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
28	Ab	48	Total 986	C 468	N 189	O 282	Р 47	0	0

• Molecule 29 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
29	Ac	40	Total 812	C 390	N 150	0 233	Р 39	0	0

• Molecule 30 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
30	Ad	53	Total 1091	C 522	N 204	0 313	Р 52	0	0

• Molecule 31 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
31	Ae	40	Total 830	C 392	N 163	O 236	Р 39	0	0

• Molecule 32 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
32	Af	32	Total 666	C 317	N 127	0 191	Р 31	0	0

• Molecule 33 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	Atoms					
33	Ag	58	Total 1173	C 571	N 185	O 360	Р 57	0	0		

• Molecule 34 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
34	Ah	60	Total 1233	C 594	N 216	0 364	Р 59	0	0

• Molecule 35 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
35	Ai	48	Total 979	$\begin{array}{c} \mathrm{C} \\ 467 \end{array}$	N 172	O 293	Р 47	0	0

• Molecule 36 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
36	Aj	48	Total 969	C 466	N 170	O 286	Р 47	0	0

• Molecule 37 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
37	Ak	32	Total 652	C 312	N 123	0 186	Р 31	0	0

• Molecule 38 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
38	Al	48	Total 982	C 471	N 183	0 281	Р 47	0	0

• Molecule 39 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
39	Am	58	Total 1175	C 569	N 187	O 362	Р 57	0	0

• Molecule 40 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
40	An	60	Total 1231	C 594	N 210	O 368	Р 59	0	0

• Molecule 41 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}		AltConf	Trace		
41	Ao	57	Total 1167	C 563	N 199	0 349	Р 56	0	0

• Molecule 42 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
42	Ap	60	Total 1217	C 590	N 187	O 381	Р 59	0	0

• Molecule 43 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
43	Aq	48	Total 985	C 468	N 183	0 287	Р 47	0	0

• Molecule 44 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
44	Ar	37	Total 752	C 361	N 137	0 218	Р 36	0	0

• Molecule 45 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
45	As	40	Total 817	C 396	N 138	0 244	Р 39	0	0

• Molecule 46 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
46	At	44	Total 899	C 432	N 168	O 256	Р 43	0	0

• Molecule 47 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
47	Au	40	Total 818	C 391	N 158	O 230	Р 39	0	0

• Molecule 48 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
48	Av	40	Total 814	C 387	N 153	O 235	Р 39	0	0

• Molecule 49 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
49	Aw	56	Total 1137	C 545	N 199	O 338	Р 55	0	0

• Molecule 50 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
50	Ax	40	Total 815	C 393	N 141	0 242	Р 39	0	0

• Molecule 51 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
51	Ау	48	Total 990	C 471	N 195	0 277	Р 47	0	0

• Molecule 52 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
52	Az	45	Total 900	C 432	N 156	0 268	Р 44	0	0

• Molecule 53 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
53	A0	32	Total 641	C 308	N 109	0 193	Р 31	0	0

• Molecule 54 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
54	A1	48	Total 992	C 472	N 191	0 282	Р 47	0	0

• Molecule 55 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
55	A2	48	Total 966	C 458	N 175	0 286	Р 47	0	0

• Molecule 56 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
56	A3	56	Total 1151	C 546	N 222	O 328	Р 55	0	0

• Molecule 57 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
57	A4	45	Total 931	C 445	N 170	0 272	Р 44	0	0

• Molecule 58 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
58	A5	48	Total 991	C 471	N 192	0 281	Р 47	0	0

• Molecule 59 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
59	A6	32	Total 655	C 313	N 119	0 192	Р 31	0	0

• Molecule 60 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
60	A7	32	Total 643	C 307	N 122	0 183	Р 31	0	0

• Molecule 61 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
61	A8	32	Total 658	C 312	N 129	0 186	Р 31	0	0

• Molecule 62 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
62	A9	48	Total 988	C 468	N 195	0 278	Р 47	0	0

• Molecule 63 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
63	ВА	45	Total 918	C 439	N 176	O 259	Р 44	0	0

• Molecule 64 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
64	BB	32	Total	С	Ν	Ο	Р	0	0
01	DD	02	659	311	133	184	31	0	0

• Molecule 65 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
65	BC	45	Total 910	C 438	N 153	O 275	Р 44	0	0

• Molecule 66 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
66	BD	57	Total 1156	C 561	N 183	O 356	Р 56	0	0

• Molecule 67 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
67	BE	57	Total 1155	$\begin{array}{c} \mathrm{C} \\ 559 \end{array}$	N 191	0 349	Р 56	0	0

• Molecule 68 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
68	BF	45	Total 911	C 436	N 158	0 273	Р 44	0	0

• Molecule 69 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
69	BG	40	Total 807	C 387	N 147	0 234	Р 39	0	0

• Molecule 70 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
70	BH	57	Total 1156	C 564	N 177	O 359	Р 56	0	0

• Molecule 71 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
71	BI	57	Total 1156	C 564	N 189	0 347	Р 56	0	0

• Molecule 72 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
72	BJ	45	Total 918	C 443	N 157	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	32	Total 655	C 313	N 119	0 192	Р 31	0	0

• Molecule 74 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
74	BL	56	Total 1142	C 548	N 199	0 340	Р 55	0	0

• Molecule 75 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
75	BM	32	Total 650	C 312	N 126	0 181	Р 31	0	0

• Molecule 76 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
76	BN	40	Total 832	C 394	N 173	0 226	Р 39	0	0

• Molecule 77 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms		AltConf	Trace	
77	BO	48	Total 974	C 464	N 181	O 282	Р 47	0	0

• Molecule 78 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
78	BP	58	Total 1175	$\begin{array}{c} \mathrm{C} \\ 569 \end{array}$	N 196	O 353	Р 57	0	0

• Molecule 79 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
79	BQ	57	Total 1147	C 558	N 183	O 350	Р 56	0	0

• Molecule 80 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
80	BR	48	Total 995	C 475	N 191	0 282	Р 47	0	0

• Molecule 81 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
81	BS	48	Total 975	C 470	N 169	0 289	Р 47	0	0

• Molecule 82 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
82	BT	48	Total 973	C 465	N 174	0 287	Р 47	0	0

• Molecule 83 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
83	BU	48	Total 981	C 466	N 182	0 286	Р 47	0	0

• Molecule 84 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
84	BV	58	Total 1186	$\begin{array}{c} \mathrm{C} \\ 573 \end{array}$	N 201	O 355	Р 57	0	0

• Molecule 85 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
85	BW	60	Total 1213	C 586	N 191	0 377	Р 59	0	0

• Molecule 86 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
86	BX	32	Total 657	C 311	N 127	0 188	Р 31	0	0

• Molecule 87 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
87	BY	40	Total 831	C 392	N 160	0 240	Р 39	0	0

• Molecule 88 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
88	BZ	40	Total 818	C 388	N 155	O 236	Р 39	0	0

• Molecule 89 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
89	Ba	48	Total 1002	C 476	N 205	0 274	Р 47	0	0

• Molecule 90 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}		AltConf	Trace		
90	Bb	48	Total 971	C 464	N 175	O 285	Р 47	0	0

• Molecule 91 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
91	Bc	32	Total	C 212	N 121	0	P 21	0	0
			660	313	131	183	31		

• Molecule 92 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
92	Bd	48	Total 992	С 473	N 202	O 270	Р 47	0	0

• Molecule 93 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
93	Be	48	Total 976	C 469	N 176	0 284	Р 47	0	0

• Molecule 94 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
94	Bf	48	Total 986	C 470	N 190	0 279	Р 47	0	0

• Molecule 95 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}		AltConf	Trace		
95	Bg	40	Total 812	C 389	N 142	0 242	Р 39	0	0

• Molecule 96 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
96	Bh	56	Total 1157	C 552	N 222	O 328	Р 55	0	0

• Molecule 97 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}		AltConf	Trace		
97	Bi	40	Total 805	C 390	N 132	0 244	Р 39	0	0

• Molecule 98 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms			AltConf	Trace
98	Bj	32	Total 653	C 313	N 125	O 184	Р 31	0	0

• Molecule 99 is a DNA chain called STAPLE STRAND.

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

• Molecule 100 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
100	Bl	48	Total 974	C 463	N 176	0 288	Р 47	0	0

• Molecule 101 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
101	Bm	56	Total 1148	C 548	N 205	0 340	Р 55	0	0

• Molecule 102 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
102	Bn	48	Total 971	C 466	N 173	0 285	Р 47	0	0

• Molecule 103 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
103	Во	48	Total 994	C 471	N 201	0 275	Р 47	0	0

• Molecule 104 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
104	Вр	40	Total 822	C 393	N 153	0 237	Р 39	0	0

• Molecule 105 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms			AltConf	Trace
105	Bq	48	Total 986	C 470	N 169	O 300	Р 47	0	0

• Molecule 106 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
106	Br	48	Total 992	C 471	N 189	0 285	Р 47	0	0

• Molecule 107 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
107	Bs	32	Total 653	C 312	N 129	0 181	Р 31	0	0

• Molecule 108 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
108	Bt	40	Total 823	C 391	N 158	O 235	Р 39	0	0

• Molecule 109 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
109	Bu	40	Total 819	C 391	N 158	0 231	Р 39	0	0

• Molecule 110 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
110	Bv	40	Total 812	C 388	N 149	O 236	Р 39	0	0

• Molecule 111 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
111	Bw	60	Total 1216	C 592	N 194	0 371	Р 59	0	0

• Molecule 112 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
112	Bx	45	Total 919	C 439	N 167	O 269	Р 44	0	0

• Molecule 113 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
113	Ву	40	Total 823	C 389	N 169	0 226	Р 39	0	0

• Molecule 114 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
114	Bz	32	Total 654	C 316	N 116	0 191	Р 31	0	0

• Molecule 115 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
115	B0	60	Total 1210	C 590	N 187	0 374	Р 59	0	0

• Molecule 116 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
116	B1	60	Total 1213	C 589	N 188	0 377	Р 59	0	0

• Molecule 117 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
117	B2	40	Total 823	C 393	N 162	O 229	Р 39	0	0

• Molecule 118 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
118	B3	32	Total 664	C 314	N 136	0 183	Р 31	0	0

• Molecule 119 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	AltConf	Trace			
119	B4	32	Total 663	C 314	N 130	O 188	Р 31	0	0

• Molecule 120 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
120	В5	60	Total 1223	C 590	N 214	O 360	Р 59	0	0

• Molecule 121 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
121	B6	53	Total 1077	C 516	N 195	0 314	Р 52	0	0

• Molecule 122 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
122	B7	48	Total 982	C 468	N 192	0 275	Р 47	0	0

• Molecule 123 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
123	B8	32	Total 658	C 313	N 131	0 183	Р 31	0	0

• Molecule 124 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
124	B9	48	Total 975	C 464	N 181	O 283	Р 47	0	0

• Molecule 125 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
125	CA	48	Total 977	C 465	N 177	0 288	Р 47	0	0

• Molecule 126 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
126	CB	60	Total 1223	C 592	N 212	O 360	Р 59	0	0

• Molecule 127 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
127	CC	37	Total 754	C 361	N 134	0 223	Р 36	0	0

• Molecule 128 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
128	CD	57	Total 1160	C 566	N 178	O 360	Р 56	0	0

• Molecule 129 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
129	CE	32	Total 667	C 313	N 134	0 189	Р 31	0	0

• Molecule 130 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
130	CF	40	Total 822	C 393	N 159	0 231	Р 39	0	0

• Molecule 131 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms	AltConf	Trace		
131	CG	32	Total 658	C 315	N 123	0 189	Р 31	0	0

• Molecule 132 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
132	CH	53	Total 1087	C 521	N 205	O 309	Р 52	0	0

• Molecule 133 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
133	CI	32	Total 646	C 314	N 109	O 192	Р 31	0	0

• Molecule 134 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
134	CJ	57	Total 1159	C 564	N 186	O 353	Р 56	0	0

• Molecule 135 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
135	СК	32	Total 650	C 313	N 119	0 187	Р 31	0	0

• Molecule 136 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
136	CL	40	Total 819	C 390	N 162	0 228	Р 39	0	0

• Molecule 137 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
137	СМ	32	Total 664	C 316	N 134	0 183	Р 31	0	0

• Molecule 138 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
138	CN	56	Total 1153	C 553	N 218	0 327	Р 55	0	0

• Molecule 139 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
139	СО	48	Total 979	C 467	N 190	0 275	Р 47	0	0

• Molecule 140 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
140	СР	48	Total 992	C 473	N 181	O 291	Р 47	0	0

• Molecule 141 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
141	CQ	57	Total 1162	C 564	N 189	O 353	Р 56	0	0

• Molecule 142 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
142	CR	60	Total 1225	C 594	N 204	O 368	Р 59	0	0

• Molecule 143 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
143	\mathbf{CS}	48	Total 968	C 468	N 159	0 294	Р 47	0	0

• Molecule 144 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
144	CT	56	Total 1158	C 554	N 220	O 329	Р 55	0	0

• Molecule 145 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
145	CU	37	Total 759	C 364	N 146	0 213	Р 36	0	0

• Molecule 146 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
146	CV	32	Total 656	C 314	N 124	0 187	Р 31	0	0

• Molecule 147 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms			AltConf	Trace
147	CW	32	Total 652	C 314	N 121	O 186	Р 31	0	0

• Molecule 148 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
148	CX	57	Total 1159	C 564	N 180	O 359	Р 56	0	0

• Molecule 149 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
149	CY	60	Total 1211	C 593	N 187	0 372	Р 59	0	0

• Molecule 150 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
150	CZ	48	Total 981	C 472	N 173	O 289	Р 47	0	0

• Molecule 151 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
151	Ca	48	Total 984	C 473	N 193	0 271	Р 47	0	0

• Molecule 152 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
152	Cb	40	Total 821	C 392	N 160	0 230	Р 39	0	0

• Molecule 153 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
153	Cc	32	Total 655	C 314	N 121	0 189	Р 31	0	0

• Molecule 154 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
154	Cd	40	Total 831	C 393	N 174	O 225	Р 39	0	0

• Molecule 155 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
155	Ce	40	Total 829	C 397	N 155	0 238	Р 39	0	0

• Molecule 156 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
156	Cf	32	Total 657	C 316	N 116	0 194	Р 31	0	0

• Molecule 157 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
157	Cg	40	Total 817	C 393	N 153	0 232	Р 39	0	0

• Molecule 158 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
158	Ch	40	Total 817	C 394	N 149	O 235	Р 39	0	0

• Molecule 159 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
159	Ci	48	Total 971	C 466	N 176	0 282	Р 47	0	0

• Molecule 160 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
160	Сј	40	Total 817	C 391	N 152	O 235	Р 39	0	0

• Molecule 161 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms	AltConf	Trace		
161	Ck	48	Total 985	C 474	N 171	O 293	Р 47	0	0

• Molecule 162 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
162	Cl	40	Total 821	C 393	N 159	O 230	Р 39	0	0

• Molecule 163 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
163	Cm	48	Total 980	C 471	N 174	0 288	Р 47	0	0

• Molecule 164 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
164	Cn	40	Total 819	C 393	N 150	0 237	Р 39	0	0

• Molecule 165 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
165	Со	40	Total 811	C 388	N 152	0 232	Р 39	0	0

• Molecule 166 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
166	Ср	37	Total 752	C 361	N 137	0 218	Р 36	0	0

• Molecule 167 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
167	Cq	37	Total 754	C 360	N 144	0 214	Р 36	0	0

• Molecule 168 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
168	Cr	40	Total 832	C 396	N 159	O 238	Р 39	0	0

• Molecule 169 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
169	Cs	40	Total 822	C 393	N 159	0 231	Р 39	0	0

• Molecule 170 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
170	Ct	45	Total 920	C 443	N 163	O 270	Р 44	0	0

• Molecule 171 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
171	Cu	37	Total 757	C 366	N 138	0 217	Р 36	0	0

• Molecule 172 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
172	Cv	40	Total 810	C 390	N 138	0 243	Р 39	0	0

• Molecule 173 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
173	Cw	40	Total 825	C 391	N 161	0 234	Р 39	0	0

• Molecule 174 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
174	Cx	32	Total 652	C 310	N 128	0 183	Р 31	0	0

• Molecule 175 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		A	toms			AltConf	Trace
175	Су	32	Total 652	C 309	N 129	O 183	Р 31	0	0

• Molecule 176 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
176	Cz	32	Total 667	C 316	N 131	0 189	Р 31	0	0

• Molecule 177 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
177	C0	57	Total 1148	C 554	N 190	0 348	Р 56	0	0

• Molecule 178 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
178	C1	57	Total 1166	C 566	N 187	0 357	Р 56	0	0

• Molecule 179 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
179	C2	32	Total 657	C 315	N 123	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	48	Total 979	C 466	N 188	0 278	Р 47	0	0

• Molecule 181 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
181	C4	48	Total 977	C 470	N 178	0 282	Р 47	0	0

• Molecule 182 is a DNA chain called STAPLE STRAND.


Mol	Chain	Residues		A	toms		AltConf	Trace	
182	C5	48	Total 976	C 470	N 169	O 290	Р 47	0	0

• Molecule 183 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
183	C6	48	Total 997	C 473	N 196	0 281	Р 47	0	0

• Molecule 184 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
184	C7	40	Total 803	C 388	N 134	0 242	Р 39	0	0

• Molecule 185 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms		AltConf	Trace	
185	C8	48	Total 991	C 472	N 194	0 278	Р 47	0	0

• Molecule 186 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms		AltConf	Trace	
186	C9	57	Total 1158	C 563	N 187	O 352	Р 56	0	0

• Molecule 187 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
187	DA	45	Total 917	C 440	N 163	О 270	Р 44	0	0

• Molecule 188 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
188	DB	32	Total 646	C 310	N 119	0 186	Р 31	0	0

• Molecule 189 is a DNA chain called STAPLE STRAND.



Mol	Chain	Residues		\mathbf{A}	toms	AltConf	Trace		
189	DC	40	Total 832	C 395	N 178	O 220	Р 39	0	0

• Molecule 190 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
190	DD	45	Total 910	C 435	N 159	0 272	Р 44	0	0

• Molecule 191 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
191	DE	48	Total 982	C 471	N 180	0 284	Р 47	0	0

• Molecule 192 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		A	toms			AltConf	Trace
192	DF	40	Total 817	C 389	N 154	O 235	Р 39	0	0

• Molecule 193 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}	toms		AltConf	Trace	
193	DG	48	Total 990	C 471	N 186	O 286	Р 47	0	0

• Molecule 194 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
194	DH	32	Total 654	C 312	N 132	0 179	Р 31	0	0

• Molecule 195 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms			AltConf	Trace
195	DI	32	Total 653	C 314	N 118	0 190	Р 31	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





C1107 T1108 A1109	G1112 G1113 G1114	T1119	C1123 C1124 G1125 C1126 C1126	A1134 T1140	T1146 T1146 T1147	11140 G1149 T1150 C1151	G1152 A1153 T1154	C1158 A1159 C1160	G1165 C1166 C1167	A1170	G1176 G1176	G1179 G1180 C1181	A1184 61188	C1189 A1190 G1191 A1192	T1197 A1198 A1199	G1200
G1204 A1205 T1206	C1207 G1212	T1217 G1220	T1221 C1222 T1223 C1224	C1231	61236 61236 71236	A1249	C1253 G1254 G1255 A1256	C1263 T1264	C1271	T1278 G1283	A1204 C1285 T1286	A1291 A1292 C1293	G1299 C1300 T1301	G1306 T1316	T1317 G1318 T1319	G1 <mark>327</mark> A1328
61329 11332	A1333 C1336 C1337	T1338 C1342	G1345 G1349 G1349	C1350 C1353	C1358 G1364 G1364	T1366 T1367 G1368	G1378 T1379 C1380	T1385	A1388 G1396 A1397	C1398 T1399	A1403 A1404 C1408	C1409 T1410	11416 A1417 C1418	A1421 A1422 A1426 A1426	T1427 T1428 C1429 G1430	C1431 C1432
T1433	T1443 C1444 C1444	G1453 C1454	T1459 G1460	G1463 A1468	A1473 G1474 A1475 C1475	T1488 C1489	G1490 C1491 C1492 C1493	G1508 C1509	T1533 G1534	C1535 C1536 T1537	G1538 G1539 T1540	T1541 T1542 C1543	G1546 C1547	A1548 C1549	01556 01557 01558 01558 01559	C1562 C1562 G1563 G1564 A1565
G1568	G1571 G1572 C1573 T1574	A1577	T1579	C1585 T1586 T1587	C1589	41592	(1594 1599 1599	G1606	C1611 C1614	A1617 A1618 A1619	C1620 T1621 G1622	G1623 C1630 A1631	C1632 A1637 C1638	G1639 A1640 T1641	A1648 C1659	G1662 T1666 A1672 ♦
T1673 T1674	A1675 C1676 G1677 C1677	G1693	C1696 C1697 C1698	61702 61702 A1703	G1704 A1705 A1706 T1707	G1710 G1718 G1718	C1722 C1722 T1723	C1/24 61725 C1726	A1731 T1732 T1733	T1740 G1741	G1744 G1748	C1/49 T1750 G1751	T1754 G1758	G1762 G1763	C1769 G1770 C1771	A1/74 A177
G1783	T1791	T1800	11801 A1802 A1803	A1804 A1805 A1806	A1807 G1811	T1817	T1832 G1833	T1838 T1839 T1840 T1841		A1853 T1857	11858 A1863	11864 T1865 A1868	A1869 T1870 A1871	T1878 A1881	T1885 C1886 T1887	11888 11891 11892 11892 11893 11894
T1895	G1899 G1909 A1910	T1911 A1917	C1918 C1919 G1922	A1925 C1926	G1931 A1932 T1933	1193 1 61935 A1936 C1937	A1943 G1944 T1945	T1946	T1948 A1949 C1950	41952 A1952 A1955	T1960	C1969 G1974 T1975	C1979	A1985 C1986 C1990	A1991 A1995	61998 41999 C2000 C2001
T2002 G2003 A2004	T2005 A2006 G2007	T2011 T2012 G2013	T2014 A2015 G2016 A2017	A2024	C2032	T2048	A2049 A2050 T2055	C2056 A2057 G2058	A2061 G2062 A2063	A2064 C2065 G2066	T2068	A2074 T2075	T2080	T2090	G2097	C2101
G2103 G2104 C2105	C2106 T2107 T2108 T2109	T2117	T2124 C2125 T2126 T2127	T2128 A2129 C2130 C2131	T2132 A2133 C2134	T2139 G2145	T2149 T2150 G2151	C2152 A2153 T2154 T2154	12155 A2160 T2161	A2162 T2163 A2164 T2164	42165 A2167	G2169 G2169 T2172	A2177 T2181	A2185 T2186	62191 C2192 G2193 T2194	1219 5 12196 62196
A2199 T2200	A2201 G2204	T2208 C2215	T2221 T2224	A2227 G2228 G2229	G2230 T2234	T2237 G2238 T2239	T2240 T2241 G2244	G2245 T2246	62253 A2254 T2255	G2259 T2262 T2763	12203 A2264 T2265	T2270 G2271	C2275 A2279 T2280	T2281 G2282 T2288	T2289 T2294 A2295	A2296
G2303 C2304 C2305	T2306 T2307 G2308 C2309	G2312	T2315 T2318	A2321 T2322	T2327 G2328 T2329	T2333 G2334	A2340 T2345 A2346	G2347 A2352	G2358 A2361	A2369 G2370 C7371	C2375 C2376 C2376	C2377 A2381	G2385 A2388	T2396 A2397	A2399 A2399 C2400 T7404	12407
A2410	G2419 G2424 T2425	A2426 T2432	G2433 A2439	A2442 A2443 A2444	A2448 C2449 T2450	C2455	G2456 C2457 A2458	T2462 A2471	T2474 T2477	A2478 T2479 A2480	T2481 G2482 G2483	A2484 A2500	A2505 C2506 T2507	12500 T2509 A2510 G2511	T2512 T2513 G2514 C2515	A2516 T2517 A2518



T2519	T2536	<mark>G2</mark> 540	T2543 T2544	A2545 T2546	C2 <mark>553</mark> A2554	A2555	A2558	A2579 A7580	T2581	T2586	T2589 17590	T2591	A2596	G2600	C2601	A2602 A2603	A2612	C2617	T2618 47619	A2620	C2622	T2632	G2634	A2635	62636	G2640 C2641	T2642	G2 <mark>651</mark>	<mark>G2656</mark>	G2664 C2665
A2670 T3671	1 20/1	G2680	A2681 T2682	A2083 T2684	<mark>G2687</mark>	<mark>G2690</mark>	T2702 C2703	C2704	C2712 T2713	T2714			12/30	G2733	T2736	C2741	T2742	A2745	G2749	A2752	G2754 G2755	T2756	A2761	C2762 C2763	T2764 G2765	A2766	T2770	A2777	G2779	T2781
T2784	G2789	T2793 C2794	A2798	G2801	C2809 A2810	T2811 T2812	T2813 G2814	A2815 G2816	G2817 G2818		A 2020		12831	T2835 A2836	T2837	G2841	A2842 T2843	T2844	A2849 C2850	T2851	G2855	42050 A2857	C2858 G2859	C2860 T2861	A2862 T2863	C2864	42866 A2866	T2868	A2872	A 2875 C 2874 A 2875
T2876	A2880 C2881	T2882 A2883	T2884 T2885	A2880 C2889	C2890	G2895 G2896	C2897	A2901 C2902	T2903	T2908	A2926 T70077	T2928	<mark>G2931</mark>	T2935		T2939 C2940	G2941 T2942	C2943 G2944	T2945	G2948	A2956	G2959	T2960 T2961	A2962 T2963	TORR	00021	G2970 T2971	T2972 G2973	C2974	T2978 G2984
	42909 T2990 A2991	A 2992 T 2993	T2999	13000 G3001 G3002	C3003	T3008	G3015	<mark>G3024</mark>	G3028	G3030	T3032	C3036	C3037 T3038	A3039	A3046	A3047 C3048	T3049 G3050	A3051 T3052	T3056				T3074 G3075	T3076	T3079	63083	1 30 85	63087 13087 13080	13089	T3093
T3098	G3102 T3103	A3104 G3105	T3114	T3122 C3123	C3124 T3125	T3134	G3138	43143	G3144	T3148	A3150	T3159	<mark>G3163</mark>	T3167		A3170	T3174 G3175	A3176 T3177	T3178 A3179		T3183	50101 50101	13190 A3191	A3192	C3195 A3196	T3197	T3199	A3207	T3209	13210 T3211 A3212
C3213	C3216	G3224 G3225	T3226 G3227	13229	C3233	T3235	A3237	63239 63239	G3244	C3245 C3246	T3247 T3248	A3249 T3250	A3253		63256 A3257	A3258 T3259	(3060			63270	A3273 C3274	G3275	T3 <mark>2</mark> 80 T3281	T3282 (3283	G3284		A3288 T3289	G 3290	T3295	T3300 G3305
	43310 A3311 T3312	T3313 A3314	C3315	63320 A3321 T3322	A3330	C3336	A3339	T3340 C3341	C3342 C3343		63348 13348 13340		A3354 C3355	(3359 (3359	T3360	13361 C3362	A3363 T3364	G3367	T3368 C3360		A3377	A3379 A3379	G3380 T3381	C3386	A3387 G3388			10094 T3395 79306		13399 T3400 A3401
T3402	40400 A3404	<mark>G34</mark> 07 A3408	G3417	G3422 T3423	T3424 C3425	<mark>C3426</mark> G3427	A3432	G 3433	C3437	G3440	A3442	A3445	G3450	G3453	A3454	134 5b	C3458 G3459	A3460 C3461	03464	V3V60	T3470	G3473	G3474 C3475	G 3476	G3479 A3480	T3481	T3487	C3488 T3489	G3495	T3496 A3497
T3503 T3503	1 3504 T 3505 C 3506	G3507 C3508	T3512	G3514 G3514 T3515	A3516 T3517	A3518	C3521	<mark>G3522</mark> C3523	T3524 G3525	G3526 G3527	G3528 G3529			T3546	G3550	13552 A3552	T3553	T3556	G3560	T3565	C3568	T3570	135/1 T3572	G3575	63580	C35.84	T3585 T3586	C3587	T3589	G3591 T3592 G3593
	G3601 T3602	A3603	C3609 C3610	T3615	A3621 A3622	A3623 C3624	T3625 T3626	C3627	A3631	A3638	T3640	A3645	G3646 T3647	C3648 C3649	T3650	<mark>C3659</mark>	T3660 G3661	T3662 A3663	G3664 C3665	C3666	<mark>G3670</mark>	A3673	C3675 C3675	G3679	T3680	G3684	T3686	G3690 T3601		1309 4 63697
<mark>C3698</mark>	G3703 A3704	G3705	G3709 A3710	A3713 T3714	G3718	<mark>C3719</mark> A3720	A3721	<mark>C3729</mark>	A3733 A3734	C3735	C3737	A3744	<mark>C3755</mark>	A 3758	A3759	13760 A3761	T3762 A3763	T3764	13768 13769	A3770	C3773	<mark>G3776</mark>	63783	G3787	T3788 T3789	T2704	13795 T3795	T3797	T3809	A3818
T3823	G3828 43829	A3830	A3835	13838 A3843	G3844 C3845	A3846	G3851	A3854	G3859 A3860	T3861	A3864 A3865	T3866	G3871	T3874		A3897 G3898	A3899 T3900	T3901	C3907 C3908	T3909		57 CC 4	A3919	A3922 T3923	T3924 C3925	H F F O O O T	C3932	T3934	T3940	T3946
T3952	A3957	<mark>C3960</mark> C3961	A3968	13970	T3 <mark>973</mark>	G3978 T3979	T3980	T3984	C3987 43988	A3989	A3991 T3007	1000H	13997 8998	A4004	A4005	900 1 .	A4013 C4014	T4015 A4016	A4017	G4023	G4028	A4023	A4036 A4037	C4038 T4039	G4047	T4048	44050	C4053	A4059	64061



G4064 G4065	C4066	T4067 G4068	T4069 C4070	T4071 04072		A4076	T4078	A4082	G4088	T4089	14090 G4091	T4092 A4093	14008	T4099	A4100	G4103	G4106	A410/ C4108	C4113	A4116	G4119	44100	C4123	G4124 G4125	T4126 A4127	C4128	64131 64132	G4133 G4133	14134	C4137	T4140 T4141	64142	j
G4163	A4164	G4165 G4166	G4167	G4169	G4170	C4176	G4182 T4183	G4184 C4185	C4186	A4194	T4198	G4199 G4200	C4201	64202	G4214	G4217	G4218 T4219	T4222	90042	04220	04230	64234	G4241 A4242	T4243	A4246 C4247	C4248 T4249		G4255 G4256	G4257	T4261 A4262	C4263	A4266 T4267	A4208
T4269 C4270	A4271	A4272 C4273	T4278	C4279 C4279		04200 A4286	C428/	A4290	G4294	G4298	G4299 T4300	A4301	G4306	A4310	A4319	A4320 T4321	C4322	A4326	T4333	C4334 T4335	64342	T4343	C4350	T4357	A4358	T4361	G4366 T4367	T4368	A4371	G4372	A4376 A4377	143/8	2
64393	C4394	A4395 G4396	G4397 G4398	G4399 C4400		A4400	64409	A4413	G4417	G4424	14470	C4428	G4433	C4435	A4436	C4441 C4442	C4443	A4448	A4449 A4450	T4456	G4462	T4463	C4465	A4460 C4467	G4472	T4475	44481		G4484 C4485	C4486 A4487	T4488	44491 T4492 G4493	2
G4496		T4499 A4500	G4503	G4504	G4508	G4520		G4524	T4 <mark>529</mark> T4530		A4533 T4534	T4535 C4536	TAGA3	A4544	A4545 T4546	G4547	A4551	T4553	T4554	G4559 T4560	T4561	T4564	A4572	G4575	G4582	T4583	G4586	G4591	C4593	T4594	C4598 C4599	14600 C4601 C4602	2>>
T4603 G4604	T4605	G4610	G4614	C4675	G4626	1402/ G4628 G4628	67.079	G4632	G4637 G4638	T4639	G4641 G4641	C4645	T4648		G4652 G4653	T4654 G4655		84959	G4664	G4674	G4 <mark>679</mark> A4680	G4681	C4692	14093 G4694	G4697	G4700	G4701 C4702		14/00	G4709	G4712 G4713	14/14 G4715	•
T4718 C4719	T4720	G4721 G4722	T4723	G4 <mark>7</mark> 30 44731	T4732	14/33 T4734	T4738	G4742	T4749		44 / 24	C4758 T4 759	A4760 A4761	T4762	A4763 A4764	G4767	G4768	G4770 C4770	C4777	44781	G4784	T4780		A4792 A4793	A4794	C4799	G4804	C4812	14813	A4816	T4825 G4826	A4827 T4828	•
C4836	G4841	T4844	G4850	C4851	C4854	G4859	C4867	A4868 T4869	G4877		14880 C4881	C4882 G4883	G4884 C4885	C4886	A4893	T4897		1.4300	T4903	A4914 T4915	T4918	G4919	T4921	649.22	A4928 A4929	T4930	C4934 44935	A4936	A493/ T4938	G4939	T4942 C4943	A4944 A4945 G4946	2
A4959		A4966 C4967	A4976	A4977 T4978	A4979	T4981	14982	G4986	A4992	T4995	A4390	C5001	T5008	T5012	G5015	T5016 T5017	G5018	A5020 A5020	C5024	CE028	T5029	<mark>G5033</mark>	T5037	15038 G5039	G5042	G5045	G5046 T5047			A5055	T5062 T5063		
T5068 G5069		T5074 G5075	A5078	A5/089	T5090		96069	G5099 T5100	GE 105		C5111 T5112	T5113	T5117	G5120	G5123	G5134		GD 138	G5153	C5158	A5161 C5162	T5163	A5168	G5174	T5180	A5185	T5186 G5187	C5188	T5195	G5 199	G5200 G5201	15202 A5203 T5204	4 2 2
T5205	T5210	A5211	A5214	C5223	G5227	T5229 T5229	19230	T5234 T5235	C5236 T5237	G5238	G5239 T5240	A5241	T5246 C5047	H 100	A5255	G5259 C5260	T5261	797.q.	T5270	A5275	G5278 G5279	TEORO	C5283	40.204	G5289	A5292 G5293	A5096	00704	T5301	T5303	C5306	T5312	-
35317	r5322	45323	T5324	15328	15333	15334 15335	000	r5345 r5346	35347 15348	35349	15351	r5352 r5353	A5354	15357	CD358	35362 15363	T5364	15366	15369	C5370 35371	05372 15373	15379	05380 15380	Toppo	C5389 15389	r5390 r5391	35392	45396	r5402	15403 55404	15407	1 34 08 4 5 4 09 1 5 4 10	-
T5424		T5429 T5430	C5431 25432	C5433	T5440	T5442	T5445	A5446 T5447	T5448	T5452	35455	T5456 45457	TEAGA		A5467	A5473	35482	15483 T5484	A5485 \5486	45489	A5490 A5491	45492 15493	A5494	35497	T5498	A5504 T5505	A5610	T5511	35513	G5514 G5515	A5516 T5517	45520 T5521	
A5522 A5523	T5524	G5527	G5528 C5529	T5530 G5531			(2040)	A5543	A5551	G5561	A5564	A5565 G5566	Т5571	C5572	G5573 T5574	T5575	T5590	T5596	A5597 A5598	T5601	T5602 (55603	15604 45605		60069	T5612	A5615	A5620 G5621		A5024	A5627	T5631 T5632	G5633 A5634 T5635	



G5640	G5641 C5642 T5643	A5648 A5649 C5650	C5653	A5658 A5659	G5663	G5664 G5665	G5668 T5669	T5670	C5681 C5682	G5685 C5686	G5687		A5698 C5699	65700 65701 65702	45705	A5706 G5707	T5715 A5716	T5717	T5723 T5724	G5725	T5733	C5738 G5739	G5742	•	
A5745 T5746	G5747 A5748 T5749 T5750	C5751 C5751 G5756	<mark>G5759</mark>	A5765 A5766	G5772	C5773 T5774 T5775	G5776 C5777 C5777	T5778 T5779	G5780 T5781	T5784	G5789 A5790	G5793 G5793	A5798	C5799	45807	A5808 T5809	C5812	G5814	C5817	(5820 (5821 4500	A5022 A5823	G5830 G5831	A5832 A5833	•	
A5836	G5842 T5847	T5852 G5853 G5854	T5863 G5864	A5875	A5878 T5879	T5884	T5889	T5895	A5901 G5902 G5903	A5904 C5905	T5906 T5907		A5912 T5913	T5914 G5915	G5918	A5921 A5922	A5923	A5925 G5926	G5927 C5928	G5929	A5938	G5942	G5945 A5946	A5947	
G5951	G5954 T5955 T5956	T5959 T5960 G5961	G5964	G5967	A5976 G5976 A5977	A5978 T5979 T5080	T5983	T5984	T5994 C5995 G5996	T6008	C6009 T6010	A6014 T6015	C6018	A6028 A6029	C6032	G6037	C6038	T6045 T6045	A6046 C6047	A6048 T6049 C6050	T6051	G6059	A6062	00000	
G6069 C6070	G6071 A6072 T6073 T6074	A6079 T6080	T6081 A6082 A6083	G6097	T6100 T6101	G6102	10107 A6108 T6109	G6113	G6114 T6115	T6 <mark>1</mark> 21	C6130 G6131 C6130	C0132 A6133 T6134	A6135 T6136	G6137 A6138 T6139	G6148	G6149 C6150	T6151 T6152	C6156 T6157	A6158	A6161 A6162	G6174 T6175	G6176	T6179 A6180	-	
C6183	A6186 T6187 T6188 T6189	A6190 C6194	A6198	A6202	T6211	T6215 A6216	T6217	C6224	T6227	16234 A6235 G6236	C6239	G6244	T6251 T6252	A6253	A6262 T6263 A6264	T6265	G6268 A6269		T6275 T6276 T6276	<mark>C6279</mark>	G6282	00200 G6284	T6288 T6289	T6290	
<mark>66308</mark>	T6311 46316	A6326	A6330 T6331 A6332	C6341	C6342 T6343	G6346 C6347 C6348	66349 66350	A6351 G6352	66353 66361	46 <u>3</u> 64	<mark>C6367</mark>	<mark>G6373</mark> A6374	C6375	G6380 A6381 T6382	T6383	G6386	A6389 A6390	G6401	C6405 T6406	A6411	G6412 G6413 G6414	T6415 C6416	T6417	A04.20	
T6421 C6422	G6432	T6438	T6440 G6445	G6446 A6447	16448 T6451	A6452	40450 A6457 A6458	A6459	A6463 A6464	A6467 A6468	T6469 A6470	G6471 C6472 G6473	A6477	T6478 T6479	C6482 A6483	G6484 A6485	G6491 G6492	T6493 T6494 T6494	A6495 T6496	Ce500	C6504	A6507	T6510 T6511 C6510	71000	
A6513 T6514	A6517 T6518	A6521 G6524	T6531 T6532 T6532	A6533 A6534	46539 G6539	A6543 T6544	A6552	T6555	T6558	16559 A6560 A6561	A0301 A6562	T6563 G6564	T6565 A6566	A6567	T6573	<mark>G6576</mark>	G6584 A6585	T6586 G6587	G6591 T6502	C6598	A6599 T6600	C6601 T6602	T6603	T6608	G6614
G6615	16619 G6626	T6629 A6630 A6631	T6632 T6633 C6634	C6637	C6644 G6645	G6651 T6652	C6655	G6658	T6663	A6667 G6668	C6669 A6670 A6671	A00/1 T6672 C6673	A6674 G6675	66676	C6682	<mark>(66690)</mark>	G6699 46700	T6701 G6702	T6703	G6708 G6709 TE710	G6714	A6717	G6720	-	
T6723	16/26 <mark>C6727</mark> A6728 T6729	C6730 C6730 G6735	T6736 T6737	A6738 A6739	A6740 C6741	C6742	A0740 A6746 A6747	A6748 T6749	C6750	T6758	T6766	16/6/ 16768 C6769	T6770 G6771	C6777	T6785 A6786	A6787 T6788	A6793 T6704	101 3 1 66797	G6798 T6799	A6800 G6801	C6805 T6806	A6807 A6808	C6809 C6810	T6813	
A6816 T6817	T6820 T6821	C6822 A6823 G6824	A6826	G6827 T6828	A6829 T6830	A6831 + A6832	T6833 • C6834	C6835	40030 T6842	C6843 A6844 C6045	G6846	A6850 T6851	A6852	66863 66863	A6866 TE867	10001 C6868	T6 <mark>875</mark>	G6881	A6884 T6885 A6886	T6887 G6888	G6891	A6892 T6893	A6894 A6895	C6903 C6904 T6905	T6906 C6907
T6908 G6909	G6912 G6913 T6914	T6915 T6916	T6919 T6920 G6921	T6922	6926 C6927 A6928	A6929 A6930 A6931	T6932	A6936	G6939 T6940 T6941	A6946	C6949	A6956 A6957	A6960	A6963 A6964	C6965	G6971 G6972	G6977	T6980 T6981	T6982 A6983	A6984 T6985 A 2082	A0900 C6987 G6988	A6989 (66990	T6991 T6992	06600	
<mark>66996</mark>	T6999 A7009	T7016	A7025 T7026 C7027	C7 028 T7 029	T7 034 G7 035	T7036 A7037	C7042 T7043	A7044	A7 048 C7 049 G7 050	T7053	A7056		T7 062 T7 063	A7 064 G7 065	T7066 T7067	G7068	T7070	G7072	G7 07 4	C7 07 8	T7 07 9 A7 080	A7081 A7082	G7083 A7084 TT7065	1/ 085 A7 086 T7 087	T7088





Chain AC:	75%	23% •
11 C2 A13 A13 A13 A13 C20 C20 C20 C20 C20 C20 C20 C20	C26 C27 G28 G28 C27 C27 C24 141 141 C47 C47 C47	
• Molecule 4: STA	PLE STRAND	
Chain AD:	62%	36% .
11 12 115 115 115 115 125 125 125 125 12	T29 630 630 135 135 135 136 136 136 136 136 136 146 046 046 046 046 046 046 046 046 046 0	
• Molecule 5: STA	PLE STRAND	
Chain AE:	52% 77%	20% ·
11 12 13 13 13 13 13 13 13 13 13 13 13 13 13	C18 719 720 721 721 725 725 726 728 733 732 733 733 733 733 733 733 733 733	138 640 641 640 641 151 151 155 155 156 156
• Molecule 6: STA	PLE STRAND	
Chain AF:	71%	19% 10%
41 44 65 65 66 77 8113 614 113 614 720	130 133 136 140 145 145 145 145 145 145 145	
• Molecule 7: STA	PLE STRAND	
Chain AG:	69%	25% 6%
A1 T7 C3 C3 C3 A1 A11 A11 A13 A14 A13 A14 A13 C25	6.20 633 633 633 633 633 635 635 635 645 645 645	
• Molecule 8: STA	PLE STRAND	
Chain AH:	85%	13% •
11 12 13 13 13 13 13 13 13 13 13 13 13 13 13	127 129 130 131 131 133 133 133 133 133 133 133	
• Molecule 9: STA	PLE STRAND	
Chain AI:	76%	21% •
A1 C2 C2 C3 C3 C3 C3 C3 C3 C3 C3 C3 C3	127 128 129 131 131 133 133 133 133 133 134	
• Molecule 10: STA	APLE STRAND	

WORLDWIDE PROTEIN DATA BANK

25%			
Chain AJ:	82%	17%	•
11 12 13 13 13 13 13 13 13 13 13 13	128 139 131 132 133 133 134 134 134 135 135 155 155 159		
• Molecule 11: STAP	LE STRAND		
Chain AK:	75%	19%	6%
11 46 715 716 716 716 716 724 724 724 724 725 725 725 725 725 725 725 725 725 725	A32		
• Molecule 12: STAP	LE STRAND		
Chain AL:	58%	35%	8%
A1 16 111 111 111 115 116 116 116 116 116	126 127 128 128 131 131 133 133 133 133 133 133 133 13		
• Molecule 13: STAP	LE STRAND		
Chain AM:	71%	27%	·
11 A2 G3 C3 14 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	A37 G38 A39 C40 C41 A45 C41 T45 C47 T48		
• Molecule 14: STAP	LE STRAND		
Chain AN:	66%	34%	
C1 15 15 16 16 16 14 16 115 115 115 115 115 115 115 115 115	625 626 632		
• Molecule 15: STAP	LE STRAND		
Chain AO:	73%	27%	
11 68 710 710 713 713 713 713 713 713 713 713 713 713	A32 A40 A40 A46 A46 A46 A46 A46 A46		
• Molecule 16: STAP	LE STRAND		
Chain AP:	70%	30%	_
C1 C7 A8 A11 A11 A11 A11 A12 A20 A20 A20 A20 A20 A20 A20 A20 A20 A2	T31 G32 G32 G33 G33 G34 G33 G34 G34 <td></td> <td></td>		
• Molecule 17: STAP	LE STRAND		







83%	13'	% •
	20%	
%	28%	
6	27%	•
-		
85%		15%
	25%	6%
	38%	·
4%	23%	•
	28%	10%
W O R L D W I D E		
		83% 13 83% 28% % 28% % 28% 85% 85% 25% 38% 38% 38%



• Molecule 32: STAPLE STRAND









• Molecule 46: STAPLE STRAND

Chain At:	75%	25%
T1 C8 A10 C11 C15 C15 C15	T18 A28 G34 T44 T44 T44	
• Molecule 4	7: STAPLE STRAND	
Chain Au:	68%	32%
G1 C2 T3 T5 T5 A10 A11 A11	G15 A23 A24 A34 C40 C40	
• Molecule 4	8: STAPLE STRAND	
Chain Av:	68%	32%
T1 67 410 611 611 715	A 20 C 21 C 22 C 23 C 22 C 23 C 22 C 23 C 23	
• Molecule 4	9: STAPLE STRAND	
Chain Aw:	71%	29%
T1 G6 A8 A9 T13 T13	616 617 726 726 734 734 734 734 734 741 741 741 742 745 745 75 745	
• Molecule 5	50: STAPLE STRAND	
Chain Ax:	55%	45%
A1 G5 A6 A7 T8 T9 G12	615 615 722 722 724 721 725 725 725 725 725 725 733 735 735 735 735 735 735 735 735 73	
• Molecule 5	51: STAPLE STRAND	
Chain Ay:	73%	23% •
C1 66 67 67 C15 C15 C15 C16 A18	A19 A20 C21 A36 A36 A37 C38 C48 C48 C48 C48	
• Molecule 5	52: STAPLE STRAND	
Chain Az:	82%	18%





• Molecule 53: STAPLE STRAND







• Molecule 60: STAPLE STRAND

Chain A7:	75%	22% •
T1 G5 A13 C18 C18 C18	A15 C20 G31 G31 G31 G31 G31 G31 G31 G31	
• Molecule 61	1: STAPLE STRAND	
Chain A8:	78%	22%
C1 45 45 45 45 45 45 45 45 45 45 45 45 45	A17 G31 G32 G32 G32 G32 G32 G32 G32 G32	
• Molecule 62	2: STAPLE STRAND	
Chain A9:	67%	33%
C1 G2 G3 A5 A5 A5 A15 A15 A15 A15	T17 117 22 22 23 23 23 23 23 23 23 23 23 23 23	
• Molecule 63	3: STAPLE STRAND	
Chain BA:	80%	18% •
A1 64 A16 A16 G21 C26 C26	A 27 A 4 T 4 4 T 4 2 T 4 2 T 4 2 T 4 6	
• Molecule 64	4: STAPLE STRAND	
Chain BB:	62%	25% 12%
A1 G4 A5 T6 G7 A8 C20 C20	624 825 625 631 631 631	
• Molecule 65	5: STAPLE STRAND	
Chain BC:	73%	27%
11 62 68 68 714 114 114 114 114	126 130 130 130 141 141 143 144 143 144 145 144 145	
• Molecule 66	5: STAPLE STRAND	
Chain BD:	[∞] 75%	23% •







• Molecule 74: STAPLE STRAND







• Molecule 81: STAPLE STRAND











• Molecule 95: STAPLE STRAND

Chain Bg:	50%	42%	8%
61 T6 T7 48 69 615 615 C16	017 017 019 019 020 020 020 020 123 123 124 125 123 126 123 131 131 131 131 137 138 039 039 140		
• Molecule 96	: STAPLE STRAND		
Chain Bh:	68%	29%	•
T1 G7 T14 G17 A18 A18 G21	124 22 22 22 22 22 22 22 22 22 22 22 22 2		
• Molecule 97	: STAPLE STRAND		
Chain Bi:	70%	20%	10%
61 62 C3 C5 C5 C12 A16 A16	122 123 123 124 123 137 137 137		
• Molecule 98	: STAPLE STRAND		
Chain Bj:	62%	34%	·
C1 C2 G3 G3 A4 A9 G12 A13 T14	d 18 7 23 7 24 7 25 7 25 7 31 7 31 7 31 7 31 7 31		
• Molecule 99	: STAPLE STRAND		
Chain Bk:	75%	25	%
A1 64 615 716 717 623 724	A25 A27 G32		
• Molecule 10	0: STAPLE STRAND		
Chain Bl:	73%	25%	·
G1 C6 C6 19 G13 C13 C13 C13 C13 C13 C14 C15 C13 C15 C15 C15 C15 C15 C15 C15 C15 C15 C15	C22 C31 C31 C31 C31 C34 C34 C33 C33 C33 C34 C44 C44 C44 C44		
• Molecule 10	1: STAPLE STRAND		
Chain Bm:	77%	20	•









• Molecule 109: STAPLE STRAND

Chain Bu:	72%	28%
d 1 C2 C5 C5 61 113 113 113 113 113 113 113 113 113	A 21 622 A 23 A 20 C 29 C 29 C 31 C 31 C 31 C 31 C 31 C 31 C 31 C 31	
• Molecule 110:	STAPLE STRAND	
Chain Bv:	68%	28% 5%
A1 62 63 63 48 48 48 19 11 41 41 41 5 41 6	116 173 123 123 124 140	
• Molecule 111:	STAPLE STRAND	
Chain Bw:	77%	17% 7%
11 12 13 44 44 410 126 126 127 128	120 120 151 151 153 154 154 156 156	
• Molecule 112:	STAPLE STRAND	
Chain Bx:	73%	24% •
11 13 14 17 17 11 115 115 115	117 A 20 6 21 6 21 6 25 6 45 0 45	
• Molecule 113:	STAPLE STRAND	
Chain By:	72%	28%
G1 A5 A9 A9 A9 A10 C18 A19 C23	<mark>80 - 80 - 80 - 80 - 80 - 80 - 80 - 80 -</mark>	
• Molecule 114:	STAPLE STRAND	
Chain Bz:	75%	25%
G1 16 10 110 114 114 114 114 114 114 114 116 116 117 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 116 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117 117	124 1724 A32	
• Molecule 115:	STAPLE STRAND	
Chain B0:	72%	28%







• Molecule 123: STAPLE STRAND







• Molecule 130: STAPLE STRAND







• Molecule 137: STAPLE STRAND



11 12 13 14 14 14 14 14 14 14 14 14 14 14 14 14	
• Molecule 144: STAPLE STRAND	
Chain CT: 75%	21% ·
A1 64 710 710 710 633 633 633 633 633 633 633 633 633 63	
• Molecule 145: STAPLE STRAND	
Chain CU: 78%	22%
A1 A7 A7 A1 C9 C9 C9 C18 C18 C18 C18 C18 C18 C18 C18	
• Molecule 146: STAPLE STRAND	
Chain CV: 75%	19% 6%
13 13 13 13 13 13 13 13 13 13 13 13 13 1	
• Molecule 147: STAPLE STRAND	
Chain CW: 62%	38%
A1 G5 G5 112 G14 G14 G14 G14 G14 G13 C32 C32 C32 C32 C32 C32	
• Molecule 148: STAPLE STRAND	
Chain CX: 74%	25% ·
11 12 15 15 15 15 15 13 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14	
• Molecule 149: STAPLE STRAND	
47% Chain CY: 80%	18% •
11 12 13 14 14 14 14 14 14 11 12 12 12 12 12 12 12 12 12 12 12 12	
• Molecule 150: STAPLE STRAND	
Chain CZ: 67%	31% •



• Molecule 151: STAPLE STRAND Chain Ca: 71% 27% • • • • • • • • • • • • • • • • • • •	
Chain Ca: 71% 27% a	
• • • • • • • • • • • • • • • • • • •	•
• Molecule 152: STAPLE STRAND Chain Cb: 60% 38% 0 2 0 8 6 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 2 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 8 8 8 7 2 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	
Chain Cb: 50% 38% 8 8 F 8 2 8 F 8 8 8 8 8 8 8 8 8 F 8 8 8 8 8 8 8 8 7 8 8 8 8 8 8 8 7 8 8 8 8 8 8 8 8 7 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	
8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8 8	•
• Molecule 153: STAPLE STRAND 9% Chain Cc: 59% • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • • •	
9% 41% 2 8 8 8 8 8 2 8 8	
2 8 8 5 8 8 8 2 9 3 2 9 8 8 2 9 3 2 9 8 8 2 9 3 2 9 8 8 2 9 2 3 3 9 3 3 3 9	
 Molecule 154: STAPLE STRAND Chain Cd: 62% 25% Chain Cd: 62% 25% Molecule 155: STAPLE STRAND Chain Ce: 70% 25% Molecule 156: STAPLE STRAND Chain Cf: 69% 28% Chain Cf: 69% 28% Molecule 157: STAPLE STRAND 	
Chain Cd: 62% 25% Image: State in the st	
	12%
 Molecule 155: STAPLE STRAND Chain Ce: 70% 25% Chain Ce: 8 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2	
Chain Ce: 70% 25% # # #################################	
 a b b b b b b b b b b b b b b b b b b b	5%
 Molecule 156: STAPLE STRAND Chain Cf: 69% 28% Chain Cf: 59% 28% Chain Cf: 59% 28% Chain Cf: 57: STAPLE STRAND 	
Chain Cf: 69% 28% 888 88	
الق	·
• Molecule 157: STAPLE STRAND	
Chain Cg: 70% 30%	, D







C1 A2 A7 A7 A7 A7 A7 A7 A7 A7 A7 A7		
• Molecule 165: STAPLE STRAND		
Chain Co: 65%	30%	5%
C1 C2 C3 C3 C4 C4 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1		
• Molecule 166: STAPLE STRAND		
Chain Cp: 70%	27%	•
T1 T2 T3 T4 T4 13 A13 A13 A27 C24 C28 A23 A26 C28 A36 A26 A36 A27		
• Molecule 167: STAPLE STRAND		
Chain Cq: 86%		11% •
T1 T2 T3 A7 A7 A17 C16 C16 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2		
• Molecule 168: STAPLE STRAND		
Chain Cr: 68%	25%	8%
A1 16 16 76 71 713 713 713 713 713 713 731 732 733 733 733 733 733 733 733 733 733		
• Molecule 169: STAPLE STRAND		
Chain Cs: 68%	32%	
A1 66 77 69 61 111 122 132 132 132 132 132 132 132 13		
• Molecule 170: STAPLE STRAND		
Chain Ct: 69%	24%	7%
T1 T2 T4 T4 C13 C13 C13 C13 C13 C13 C13 C13 C13 C13		
• Molecule 171: STAPLE STRAND		
Chain Cu: 59%	41%	







11 12 13 14 15 66 86 A10 612 612 613	114 615 615 617 617 418 419 620 620 622 723 724 725 725 726	127 128 129 130 131 132 133 135 135 136 136 136 136 136	A40 A41 A41 A42 A44 A44 A45 A45 A45 A48 A48 A48 A48 A48 A48 A48 A48 C47 C53 C53 C53	T55 C56 G57
• Molecule 179: STAP	LE STRAND			
Chain C2:	72%	22%	6%	
G1 A6 C11 C11 C13 C13 C13 C13 C13 C13 C22 C22 C22 C22 C22 C22 C22 C22 C22 C2				
• Molecule 180: STAP	LE STRAND			
Chain C3:	63%	35%	.	
C1 13 13 14 14 14 15 15 15 15 15 15 15 15 15 15 15 15 15	624 624 735 735 735 740 741 741 742 743 748			
• Molecule 181: STAP	LE STRAND			
Chain C4:	71%	23%	6%	
C1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	G37 C40 T41 A42 G48 G48			
• Molecule 182: STAP	LE STRAND			
Chain C5:	73%	25%	·	
A1 14 15 16 115 115 115 115 115 115 24 224 224 224 225 226 224 225 226 224 225 235 235 235 235 235 235 235 235 235	138 (442 (442 (448			
• Molecule 183: STAP	LE STRAND			
Chain C6:	67%	31%		
C1 65 65 66 69 613 614 714 612 620 620 621	27 131 132 133 133 136 136 136 136 142 142 142 142 148 148			
• Molecule 184: STAP	LE STRAND			
Chain C7:	68%	30%		
T1 C2 C2 C3 C3 A1 A1 A1 A1 A1 A1 A1 A1 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2 C2	A34 G38 T39 T40			
• Molecule 185: STAP	LE STRAND			
Chain C8:	65%	33%	.	










4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	509812	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 $(e^-/\text{\AA}^2)$	55	Depositor
Minimum defocus (nm)	260.5	Depositor
Maximum defocus (nm)	3692	Depositor
Magnification	47000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.401	Depositor
Minimum map value	-0.217	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.051	Depositor
Map size (Å)	644.96, 644.96, 644.96	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3900001, 1.3900001, 1.3900001	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	Bond		ond lengths		Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	AA	1.17	6/184801~(0.0%)	1.35	2299/285260~(0.8%)
2	AB	1.15	0/647	1.17	5/996~(0.5%)
3	AC	1.19	0/1104	1.35	14/1703~(0.8%)
4	AD	1.18	0/1230	1.39	17/1899~(0.9%)
5	AE	1.18	0/1358	1.39	15/2094~(0.7%)
6	AF	1.19	0/1101	1.41	18/1698~(1.1%)
7	AG	1.22	0/1115	1.37	16/1721~(0.9%)
8	AH	1.16	0/1366	1.22	10/2109~(0.5%)
9	AI	1.17	0/950	1.28	5/1464~(0.3%)
10	AJ	1.11	0/1359	1.21	9/2096~(0.4%)
11	AK	1.18	0/739	1.32	8/1140~(0.7%)
12	AL	1.14	0/911	1.35	13/1405~(0.9%)
13	AM	1.13	0/1111	1.29	9/1714~(0.5%)
14	AN	1.18	0/746	1.41	9/1151~(0.8%)
15	AO	1.12	0/1098	1.25	10/1691~(0.6%)
16	AP	1.18	0/919	1.27	8/1415~(0.6%)
17	AQ	1.13	0/1021	1.34	12/1574~(0.8%)
18	AR	1.20	1/1108~(0.1%)	1.29	9/1709~(0.5%)
19	AS	1.17	0/1112	1.24	7/1715~(0.4%)
20	AT	1.18	0/1040	1.35	14/1607~(0.9%)
21	AU	1.18	0/1095	1.34	9/1687~(0.5%)
22	AV	1.16	0/920	1.39	13/1416~(0.9%)
23	AW	1.16	0/1285	1.41	23/1975~(1.2%)
24	AX	1.15	0/1372	1.25	9/2116~(0.4%)
25	AY	1.18	0/740	1.22	5/1142~(0.4%)
26	AZ	1.17	0/1114	1.34	10/1719~(0.6%)
27	Aa	1.14	0/923	1.19	3/1425~(0.2%)
28	Ab	1.17	0/1108	1.32	14/1709~(0.8%)
29	Ac	1.20	1/911 (0.1%)	1.27	5/1402~(0.4%)
30	Ad	1.14	$0/1\overline{226}$	1.29	16/1892~(0.8%)
31	Ae	1.20	0/934	1.51	19/1443~(1.3%)
32	Af	1.19	0/749	1.25	$8\overline{/1158}~(0.7\%)$
33	Ag	1.12	0/1308	1.24	11/2016~(0.5%)
34	Ah	1.14	0/1382	1.24	9/2134~(0.4%)



Mal	Chain	B	ond lengths	-	Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
35	Ai	1.20	0/1095	1.25	8/1689~(0.5%)
36	Aj	1.16	0/1084	1.34	10/1668~(0.6%)
37	Ak	1.15	0/732	1.33	10/1127~(0.9%)
38	Al	1.13	0/1103	1.25	11/1700~(0.6%)
39	Am	1.17	0/1310	1.23	9/2020~(0.4%)
40	An	1.14	0/1378	1.19	8/2128~(0.4%)
41	Ao	1.16	0/1306	1.22	7/2016~(0.3%)
42	Ap	1.17	0/1355	1.33	21/2091~(1.0%)
43	Aq	1.19	0/1105	1.31	10/1705~(0.6%)
44	Ar	1.15	0/843	1.20	6/1298~(0.5%)
45	As	1.13	0/914	1.33	11/1410 (0.8%)
46	At	1.13	0/1010	1.26	7/1556~(0.4%)
47	Au	1.15	0/920	1.39	9/1417~(0.6%)
48	Av	1.18	0/913	1.43	11/1406~(0.8%)
49	Aw	1.17	1/1272~(0.1%)	1.42	16/1960~(0.8%)
50	Ax	1.13	0/912	1.41	16/1406~(1.1%)
51	Ay	1.15	0/1115	1.35	17/1720~(1.0%)
52	Az	1.15	0/1005	1.24	3/1544~(0.2%)
53	A0	1.19	0/715	1.50	13/1099~(1.2%)
54	A1	1.18	0/1116	1.39	14/1723~(0.8%)
55	A2	1.20	1/1080~(0.1%)	1.44	21/1661~(1.3%)
56	A3	1.21	0/1294	1.43	24/1996~(1.2%)
57	A4	1.17	0/1045	1.26	10/1615~(0.6%)
58	A5	1.19	0/1115	1.35	14/1721~(0.8%)
59	A6	1.18	0/734	1.27	7/1132~(0.6%)
60	A7	1.17	0/721	1.33	8/1107~(0.7%)
61	A8	1.16	0/740	1.21	4/1141~(0.4%)
62	A9	1.20	0/1112	1.41	13/1715~(0.8%)
63	BA	1.14	0/1032	1.23	4/1589~(0.3%)
64	BB	1.18	0/742	1.35	8/1144~(0.7%)
65	BC	1.17	0/1016	1.26	9/1565~(0.6%)
66	BD	1.16	0/1289	1.38	15/1988~(0.8%)
67	BE	1.18	0/1290	1.31	13/1988~(0.7%)
68	BF	1.16	0/1018	1.36	14/1568~(0.9%)
69	BG	1.19	1/904~(0.1%)	1.41	14/1390~(1.0%)
70	BH	1.12	0/1288	1.16	2/1987~(0.1%)
71	BI	1.13	0/1292	1.27	10/1991~(0.5%)
72	BJ	1.15	0/1027	1.33	12/1584~(0.8%)
73	BK	1.19	0/734	1.36	8/1132~(0.7%)
74	BL	1.18	0/1278	1.36	17/1971~(0.9%)
75	BM	1.12	0/731	1.25	3/1124~(0.3%)
76	BN	1.17	0/940	1.29	7/1451~(0.5%)
77	BO	1.18	0/1092	1.43	16/1681~(1.0%)



Mal	Chain	Be	ond lengths	-	Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
78	BP	1.15	0/1313	1.28	11/2023~(0.5%)
79	BQ	1.13	0/1279	1.27	10/1969~(0.5%)
80	BR	1.15	0/1120	1.28	7/1730(0.4%)
81	BS	1.16	0/1091	1.30	11/1681 (0.7%)
82	BT	1.17	0/1089	1.34	15/1677 (0.9%)
83	BU	1.16	0/1100	1.33	10/1696 (0.6%)
84	BV	1.15	0/1327	1.26	8/2048 (0.4%)
85	BW	1.17	0/1351	1.44	18/2083~(0.9%)
86	BX	1.21	0/738	1.35	7/1138~(0.6%)
87	BY	1.20	0/934	1.38	9/1444~(0.6%)
88	BZ	1.18	0/918	1.40	14/1415 (1.0%)
89	Ba	1.16	0/1132	1.32	14/1749~(0.8%)
90	Bb	1.23	0/1087	1.60	28/1673~(1.7%)
91	Bc	1.16	0/741	1.36	9/1142 (0.8%)
92	Bd	1.16	0/1120	1.36	15/1727~(0.9%)
93	Be	1.17	0/1094	1.41	16/1685~(0.9%)
94	Bf	1.15	0/1109	1.34	15/1710~(0.9%)
95	Bg	1.22	0/908	1.56	21/1399~(1.5%)
96	Bh	1.18	0/1302	1.31	16/2010~(0.8%)
97	Bi	1.14	0/898	1.39	11/1382~(0.8%)
98	Bj	1.20	0/734	1.56	13/1130~(1.2%)
99	Bk	1.12	0/742	1.35	11/1145~(1.0%)
100	Bl	1.18	0/1090	1.33	12/1679~(0.7%)
101	Bm	1.21	0/1286	1.46	15/1985~(0.8%)
102	Bn	1.17	1/1087~(0.1%)	1.36	14/1673~(0.8%)
103	Bo	1.18	0/1121	1.31	12/1730~(0.7%)
104	Bp	1.17	0/923	1.42	15/1424~(1.1%)
105	Bq	1.21	0/1102	1.35	14/1703~(0.8%)
106	Br	1.20	0/1115	1.39	15/1722~(0.9%)
107	Bs	1.16	0/735	1.28	5/1131~(0.4%)
108	Bt	1.18	0/925	1.39	14/1427~(1.0%)
109	Bu	1.16	0/921	1.31	9/1419~(0.6%)
110	Bv	1.20	0/910	1.38	11/1401~(0.8%)
111	Bw	1.13	0/1357	1.27	12/2092~(0.6%)
112	Bx	1.16	0/1030	1.35	14/1588~(0.9%)
113	By	1.18	0/928	1.36	11/1430~(0.8%)
114	Bz	1.15	0/733	1.20	3/1130~(0.3%)
115	B0	1.13	0/1348	1.30	12/2077~(0.6%)
116	B1	1.18	0/1351	1.22	5/2083~(0.2%)
117	B2	1.17	0/927	1.36	15/1429~(1.0%)
118	B3	1.17	0/749	1.19	4/1156~(0.3%)
119	B4	1.17	0/746	1.37	12/1152~(1.0%)
120	B5	1.14	0/1370	1.22	9/2112~(0.4%)



	Chain	Be	ond lengths	-	Bond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
121	B6	1.16	0/1207	1.31	10/1859~(0.5%)
122	B7	1.16	0/1105	1.42	15/1702~(0.9%)
123	B8	1.16	0/741	1.24	2/1142~(0.2%)
124	B9	1.18	0/1093	1.48	24/1683~(1.4%)
125	CA	1.15	0/1094	1.34	12/1686~(0.7%)
126	CB	1.13	0/1370	1.20	8/2112~(0.4%)
127	CC	1.19	0/844	1.34	7/1301~(0.5%)
128	CD	1.12	0/1293	1.27	9/1996~(0.5%)
129	CE	1.21	0/751	1.46	17/1161~(1.5%)
130	CF	1.17	0/925	1.40	12/1426~(0.8%)
131	CG	1.17	0/739	1.29	9/1140~(0.8%)
132	CH	1.16	0/1222	1.34	12/1884~(0.6%)
133	CI	1.15	0/722	1.32	5/1111~(0.5%)
134	CJ	1.12	0/1294	1.38	20/1996~(1.0%)
135	CK	1.13	0/729	1.40	11/1122~(1.0%)
136	CL	1.20	0/922	1.45	10/1420~(0.7%)
137	CM	1.16	0/749	1.23	6/1156~(0.5%)
138	CN	1.14	0/1297	1.25	10/2001~(0.5%)
139	CO	1.15	0/1101	1.37	10/1695~(0.6%)
140	CP	1.18	0/1113	1.40	15/1720~(0.9%)
141	CQ	1.16	1/1298~(0.1%)	1.31	14/2003~(0.7%)
142	CR	1.14	0/1370	1.20	5/2114~(0.2%)
143	CS	1.13	0/1080	1.28	9/1663~(0.5%)
144	CT	1.16	0/1303	1.34	17/2012~(0.8%)
145	CU	1.13	0/854	1.37	8/1316~(0.6%)
146	CV	1.17	0/737	1.34	9/1136~(0.8%)
147	CW	1.15	0/732	1.29	10/1127~(0.9%)
148	CX	1.14	0/1292	1.32	14/1994~(0.7%)
149	CY	1.13	0/1350	1.18	6/2080~(0.3%)
150	CZ	1.16	0/1099	1.37	$16/1695 \ (0.9\%)$
151	Ca	1.13	0/1109	1.32	14/1708 (0.8%)
152	Cb	1.19	0/924	1.32	8/1424 (0.6%)
153	Cc	1.16	0/735	1.31	8/1133 (0.7%)
154	Cd	1.18	0/939	1.58	22/1449 (1.5%)
155	Ce	1.13	0/932	1.27	13/1440 (0.9%)
156	Cf	1.17	0/736	1.29	6/1136 (0.5%)
157	Cg	1.15	0/918	1.36	12/1414 (0.8%)
158	Ch	1.11	0/917	1.36	16/1413 (1.1%)
159	Ci	1.16	0/1088	1.33	12/1674 (0.7%)
160	Cj	1.15	0/917	1.36	9/1413(0.6%)
161	Ck	1.17	0/1103	1.32	$\frac{14}{1703}(0.8\%)$
162	CI	1.14	0/924	1.24	6/1424 (0.4%)
163	Cm	1.17	0/1098	1.36	12/1693~(0.7%)



Mal	Chain	B	ond lengths		Bond angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
164	Cn	1.17	0/919	1.40	19/1417~(1.3%)
165	Со	1.15	0/910	1.44	15/1400~(1.1%)
166	Ср	1.15	0/843	1.34	6/1298~(0.5%)
167	Cq	1.15	0/847	1.35	6/1304~(0.5%)
168	Cr	1.18	0/936	1.37	11/1447~(0.8%)
169	Cs	1.15	0/925	1.32	10/1426~(0.7%)
170	Ct	1.15	0/1031	1.35	10/1590~(0.6%)
171	Cu	1.15	0/850	1.41	11/1310~(0.8%)
172	Cv	1.15	0/905	1.31	8/1394~(0.6%)
173	Cw	1.19	0/928	1.36	12/1432~(0.8%)
174	Cx	1.19	0/733	1.40	9/1128~(0.8%)
175	Су	1.20	0/733	1.37	10/1128~(0.9%)
176	Cz	1.14	0/751	1.15	2/1161~(0.2%)
177	C0	1.18	1/1281~(0.1%)	1.41	17/1972~(0.9%)
178	C1	1.12	0/1302	1.23	9/2011~(0.4%)
179	C2	1.15	0/738	1.33	9/1138~(0.8%)
180	C3	1.17	0/1100	1.35	14/1694~(0.8%)
181	C4	1.14	0/1096	1.34	16/1688~(0.9%)
182	C5	1.14	0/1092	1.40	14/1683~(0.8%)
183	C6	1.20	0/1123	1.34	13/1735~(0.7%)
184	C7	1.13	0/896	1.40	11/1378~(0.8%)
185	C8	1.18	0/1116	1.39	16/1722~(0.9%)
186	C9	1.13	0/1293	1.21	7/1994~(0.4%)
187	DA	1.20	0/1027	1.35	12/1583~(0.8%)
188	DB	1.15	0/724	1.34	8/1113~(0.7%)
189	DC	1.17	0/942	1.43	13/1453~(0.9%)
190	DD	1.16	0/1017	1.31	9/1566~(0.6%)
191	DE	1.11	0/1102	1.26	13/1699~(0.8%)
192	DF	1.15	0/917	1.31	8/1413~(0.6%)
193	DG	1.13	0/1112	1.25	8/1717~(0.5%)
194	DH	1.17	$0/\overline{737}$	1.40	8/1134~(0.7%)
195	DI	1.15	0/732	1.30	7/1128~(0.6%)
All	All	1.16	14/383925~(0.0%)	1.34	$4478/5922\overline{51}\ (0.8\%)$

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	1	1140
3	AC	0	3



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



Mol	Chain	#Chirality outliers	#Planarity outliers
46	At	0	7
47	Au	0	7
48	Av	0	3
49	Aw	0	6
50	Ax	0	9
51	Ay	0	4
52	Az	0	5
53	A0	0	5
54	A1	0	8
55	A2	0	11
56	A3	0	9
57	A4	0	6
58	A5	0	5
59	A6	0	7
60	A7	0	2
61	A8	0	3
62	A9	0	6
63	BA	0	6
64	BB	0	9
65	BC	0	6
66	BD	0	4
67	BE	0	10
68	BF	0	7
69	BG	0	9
70	BH	0	14
71	BI	0	12
72	BJ	0	5
73	BK	0	3
74	BL	0	4
75	BM	0	3
76	BN	0	7
77	BO	0	7
78	BP	0	10
79	BQ	0	9
80	BR	0	4
81	BS	0	6
82	BT	0	5
83	BU	0	4
84	BV	0	7
85	BW	0	12
86	BX	0	4
87	BY	0	9



Mol	Chain	#Chirality outliers	#Planarity outliers
88	BZ	0	7
89	Ba	0	9
90	Bb	0	11
91	Bc	0	3
92	Bd	0	1
93	Be	0	4
94	Bf	0	5
95	Bg	0	12
96	Bh	0	10
97	Bi	0	8
98	Bj	0	4
99	Bk	0	2
100	Bl	0	6
101	Bm	0	7
102	Bn	0	3
103	Bo	0	5
104	Bp	0	4
105	Bq	0	4
106	Br	0	5
107	Bs	0	3
108	Bt	0	5
109	Bu	0	3
110	Bv	0	6
111	Bw	0	9
112	Bx	0	6
113	By	0	2
114	Bz	0	5
115	B0	0	7
116	B1	0	11
117	B2	0	4
118	B3	0	5
119	B4	0	3
120	B5	0	8
121	B6	0	11
122	B7	0	4
123	B8	0	4
124	B9	0	9
125	CA	0	10
126	CB	0	11
127	CC	0	4
128	CD	0	9
129	CE	0	2



Mol	Chain	#Chirality outliers	#Planarity outliers
130	CF	0	7
131	CG	0	6
132	СН	0	12
133	CI	0	3
134	CJ	0	7
135	CK	0	4
136	CL	0	6
137	CM	0	5
138	CN	0	7
139	СО	0	8
140	CP	0	11
141	CQ	0	10
142	CR	0	13
143	CS	0	8
144	CT	0	4
145	CU	0	4
146	CV	0	3
147	CW	0	4
148	CX	0	6
149	CY	0	9
150	CZ	0	6
151	Ca	0	5
152	Cb	0	10
153	Cc	0	6
154	Cd	0	8
155	Ce	0	5
156	Cf	0	6
157	Cg	0	2
158	Ch	0	6
159	Ci	0	6
160	Cj	0	5
161	Ck	0	5
162	Cl	0	6
163	Cm	0	11
164	Cn	0	7
165	Co	0	7
166	Ср	0	8
167	Cq	0	2
168	Cr	0	7
169	Cs	0	6
170	Ct	0	11
171	Cu	0	5



Mol	Chain	#Chirality outliers	#Planarity outliers
172	Cv	0	9
173	Cw	0	4
174	Cx	0	6
175	Су	0	3
176	Cz	0	3
177	C0	0	8
178	C1	0	13
179	C2	0	5
180	C3	0	10
181	C4	0	6
182	C5	0	5
183	C6	0	6
184	C7	0	5
185	C8	0	7
186	C9	0	8
187	DA	0	11
188	DB	0	4
189	DC	0	6
190	DD	0	11
191	DE	0	4
192	DF	0	4
193	DG	0	8
194	DH	0	6
195	DI	0	3
All	All	1	2388

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
55	A2	8	DC	C5'-C4'	5.42	1.57	1.51
1	AA	2168	DG	C5'-C4'	5.39	1.57	1.51
18	AR	40	DA	N9-C4	5.34	1.41	1.37
1	AA	2816	DG	C2'-C1'	5.33	1.57	1.52
177	C0	4	DT	C5'-C4'	5.32	1.57	1.51

The worst 5 of 4478 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	AA	601	DC	P-O3'-C3'	18.83	142.30	119.70
1	AA	4222	DT	P-O3'-C3'	18.05	141.36	119.70
1	AA	486	DC	P-O3'-C3'	15.05	137.76	119.70
84	BV	39	DA	P-O3'-C3'	15.05	137.76	119.70



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Mol	Chain	\mathbf{Res}	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	AA	6047	DC	P-O3'-C3'	14.93	137.62	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1863	DA	C3'

5 of 2388 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	31	DG	Sidechain
1	AA	40	DT	Sidechain
1	AA	67	DA	Sidechain
1	AA	71	DG	Sidechain
1	AA	78	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	91301	0	0
2	AB	582	0	334	0	0
3	AC	984	0	542	0	0
4	AD	1094	0	600	0	0
5	AE	1217	0	685	0	0
6	AF	982	0	543	0	0
7	AG	991	0	539	0	0
8	AH	1224	0	692	0	0
9	AI	851	0	483	0	0
10	AJ	1218	0	693	0	0
11	AK	658	0	364	0	0
12	AL	815	0	458	0	0
13	AM	988	0	544	0	0
14	AN	662	0	362	0	0
15	AO	978	0	543	0	0
16	AP	817	0	449	0	0
17	AQ	914	0	517	0	0



Conti	Continuea from previous page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
18	AR	986	0	545	0	0		
19	AS	988	0	540	0	0		
20	AT	928	0	512	0	0		
21	AU	977	0	542	0	0		
22	AV	817	0	445	0	0		
23	AW	1155	0	659	0	0		
24	AX	1225	0	684	0	0		
25	AY	659	0	362	0	0		
26	AZ	990	0	541	0	0		
27	Aa	823	0	457	0	0		
28	Ab	986	0	539	0	0		
29	Ac	812	0	452	0	0		
30	Ad	1091	0	600	0	0		
31	Ae	830	0	449	0	0		
32	Af	666	0	363	0	0		
33	Ag	1173	0	669	0	0		
34	Ah	1233	0	686	0	0		
35	Ai	979	0	544	0	0		
36	Aj	969	0	544	0	0		
37	Ak	652	0	361	0	0		
38	Al	982	0	543	0	0		
39	Am	1175	0	667	0	0		
40	An	1231	0	688	0	0		
41	Ao	1167	0	653	0	0		
42	Ap	1217	0	693	0	0		
43	Aq	985	0	541	0	0		
44	Ar	752	0	419	0	0		
45	As	817	0	460	0	0		
46	At	899	0	498	0	0		
47	Au	818	0	450	0	0		
48	Av	814	0	449	0	0		
49	Aw	1137	0	635	0	0		
50	Ax	815	0	457	0	0		
51	Ay	990	0	539	0	0		
52	Az	900	0	508	0	0		
53	A0	641	0	363	0	0		
54	A1	992	0	541	0	0		
55	A2	966	0	537	0	0		
56	A3	1151	0	628	0	0		
57	A4	931	0	512	0	0		
58	A5	991	0	540	0	0		
59	A6	655	0	363	0	0		



Conti	Continuea from previous page							
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
60	A7	643	0	358	0	0		
61	A8	658	0	359	0	0		
62	A9	988	0	537	0	0		
63	BA	918	0	506	0	0		
64	BB	659	0	357	0	0		
65	BC	910	0	513	0	0		
66	BD	1156	0	657	0	0		
67	BE	1155	0	653	0	0		
68	BF	911	0	510	0	0		
69	BG	807	0	451	0	0		
70	BH	1156	0	661	0	0		
71	BI	1156	0	657	0	0		
72	BJ	918	0	515	0	0		
73	BK	655	0	363	0	0		
74	BL	1142	0	637	0	0		
75	BM	650	0	360	0	0		
76	BN	832	0	447	0	0		
77	BO	974	0	539	0	0		
78	BP	1175	0	664	0	0		
79	BQ	1147	0	655	0	0		
80	BR	995	0	543	0	0		
81	BS	975	0	547	0	0		
82	BT	973	0	542	0	0		
83	BU	981	0	540	0	0		
84	BV	1186	0	665	0	0		
85	BW	1213	0	689	0	0		
86	BX	657	0	359	0	0		
87	BY	831	0	450	0	0		
88	BZ	818	0	449	0	0		
89	Ba	1002	0	539	0	0		
90	Bb	971	0	541	0	0		
91	Bc	658	0	359	0	0		
92	Bd	992	0	538	0	0		
93	Be	976	0	544	0	0		
94	Bf	986	0	540	0	0		
95	Bg	812	0	454	0	0		
96	Bh	1157	0	632	0	0		
97	Bi	805	0	458	0	0		
98	Bj	653	0	361	0	0		
99	Bk	660	0	363	0	0		
100	Bl	974	0	540	0	0		
101	Bm	1148	0	635	0	0		



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
102	Bn	971	0	543	0	0
103	Bo	994	0	537	0	0
104	Bp	822	0	453	0	0
105	Bq	986	0	547	0	0
106	Br	992	0	541	0	0
107	Bs	653	0	359	0	0
108	Bt	823	0	450	0	0
109	Bu	819	0	450	0	0
110	Bv	812	0	451	0	0
111	Bw	1216	0	692	0	0
112	Bx	919	0	509	0	0
113	By	823	0	445	0	0
114	Bz	654	0	366	0	0
115	B0	1210	0	693	0	0
116	B1	1213	0	692	0	0
117	B2	823	0	450	0	0
118	B3	664	0	358	0	0
119	B4	663	0	360	0	0
120	B5	1223	0	684	0	0
121	B6	1077	0	599	0	0
122	B7	982	0	538	0	0
123	B8	658	0	359	0	0
124	B9	975	0	539	0	0
125	CA	977	0	541	0	0
126	CB	1223	0	686	0	0
127	CC	754	0	420	0	0
128	CD	1160	0	662	0	0
129	CE	667	0	358	0	0
130	CF	822	0	451	0	0
131	CG	658	0	363	0	0
132	CH	1087	0	599	0	0
133	CI	646	0	367	0	0
134	CJ	1159	0	658	0	0
135	CK	650	0	363	0	0
136	CL	819	0	448	0	0
137	CM	664	0	360	0	0
138	CN	1153	0	634	0	0
139	CO	979	0	538	0	0
140	CP	992	0	545	0	0
141	CQ	1162	0	657	0	0
142	CR	1225	0	690	0	0
143	CS	968	0	549	0	0



Conti	nuea fron	n previous	page			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
144	CT	1158	0	634	0	0
145	CU	759	0	418	0	0
146	CV	656	0	362	0	0
147	CW	652	0	363	0	0
148	CX	1159	0	660	0	0
149	CY	1211	0	695	0	0
150	CZ	981	0	547	0	0
151	Ca	984	0	541	0	0
152	Cb	821	0	450	0	0
153	Cc	655	0	363	0	0
154	Cd	831	0	446	0	0
155	Се	829	0	455	0	0
156	Cf	657	0	366	0	0
157	Cg	817	0	453	0	0
158	Ch	817	0	455	0	0
159	Ci	971	0	542	0	0
160	Cj	817	0	452	0	0
161	Ck	985	0	549	0	0
162	Cl	821	0	451	0	0
163	Cm	980	0	546	0	0
164	Cn	819	0	454	0	0
165	Со	811	0	450	0	0
166	Ср	752	0	419	0	0
167	Cq	754	0	416	0	0
168	Cr	832	0	453	0	0
169	Cs	822	0	451	0	0
170	Ct	920	0	513	0	0
171	Cu	757	0	422	0	0
172	Cv	810	0	456	0	0
173	Cw	825	0	449	0	0
174	Cx	652	0	358	0	0
175	Су	652	0	357	0	0
176	Cz	667	0	361	0	0
177	CO	1148	0	650	0	0
178	C1	1166	0	659	0	0
179	C2	657	0	363	0	0
180	C3	979	0	538	0	0
181	C4	977	0	544	0	0
182	C5	976	0	547	0	0
183	C6	997	0	540	0	0
184	C7	803	0	456	0	0
185	C8	991	0	540	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
186	C9	1158	0	657	0	0
187	DA	917	0	511	0	0
188	DB	646	0	361	0	0
189	DC	832	0	446	0	0
190	DD	910	0	509	0	0
191	DE	982	0	544	0	0
192	DF	817	0	450	0	0
193	DG	990	0	542	0	0
194	DH	654	0	358	0	0
195	DI	653	0	364	0	0
All	All	342569	0	189904	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-11379. 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: 232



Y Index: 232



Z Index: 232



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: 247

Y Index: 179

Z Index: 222

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 0.051. 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 $6695~{\rm nm^3};$ this corresponds to an approximate mass of 6048 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 0.135 ${\rm \AA^{-1}}$



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 0.135 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estim	Estimation criterion (FSC cut-off)				
resolution estimate (A)	0.143	0.5	Half-bit			
Reported by author	7.40	-	-			
Author-provided FSC curve	7.69	10.03	7.86			
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-11379 and PDB model 7ARV. Per-residue inclusion information can be found in section 3 on page 39.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.051 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 (0.051).



9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.



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9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.051) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8382	0.1400
A0	0.8549	0.1250
A1	0.8417	0.1350
A2	0.7909	0.1050
A3	0.8775	0.1380
A4	0.9076	0.1430
A5	0.9223	0.1410
A6	0.8290	0.1290
A7	0.9238	0.1500
A8	0.8967	0.1500
A9	0.8887	0.1580
AA	0.8580	0.1440
AB	0.6409	0.1130
AC	0.8476	0.1330
AD	0.9132	0.1160
AE	0.4174	0.0720
AF	0.8503	0.1350
AG	0.8517	0.1320
AH	0.6683	0.0900
AI	0.7321	0.1060
AJ	0.6593	0.0950
AK	0.9012	0.1330
AL	0.8859	0.1230
AM	0.9241	0.1490
AN	0.8912	0.1610
AO	0.8926	0.1330
AP	0.7479	0.1310
AQ	0.8085	0.1340
AR	0.7150	0.1330
AS	0.7966	0.1190
AT	0.8103	0.1200
AU	0.8997	0.1440
AV	0.8874	0.1470
AW	0.8926	0.1000
AX	0.5535	0.0770



Chain	Atom inclusion	Q-score
AY	0.8756	0.1660
AZ	0.9364	0.1560
Aa	0.8724	0.1230
Ab	0.9067	0.1490
Ac	0.8571	0.1400
Ad	0.9038	0.1360
Ae	0.9193	0.1140
Af	0.8859	0.1400
Ag	0.8721	0.1170
Ah	0.6577	0.1130
Ai	0.8100	0.1550
Aj	0.8731	0.1360
Ak	0.8865	0.1490
Al	0.9043	0.1500
Am	0.8706	0.1120
An	0.6824	0.1130
Ao	0.8586	0.1130
Ар	0.6565	0.1070
Aq	0.9249	0.1520
Ar	0.7367	0.1160
As	0.9106	0.1510
At	0.9333	0.1460
Au	0.8863	0.1290
Av	0.8980	0.1450
Aw	0.8294	0.1380
Ax	0.8748	0.1450
Ay	0.9010	0.1530
Az	0.8722	0.1260
B0	0.7983	0.1190
B1	0.6208	0.1200
B2	0.8809	0.1560
B3	0.8795	0.1700
B4	0.8748	0.1730
B5	0.8070	0.1210
B6	0.8217	0.1520
B7	0.9165	0.1540
B8	0.9012	0.1820
B9	0.9190	0.1720
BA	0.9477	0.1560
BB	0.9135	0.1510
BC	0.8648	0.1270
BD	0.8979	0.1340



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Chain	Atom inclusion	Q-score
BE	0.6848	0.1030
BF	0.8211	0.1210
BG	0.8910	0.1630
BH	0.7976	0.1220
BI	0.7050	0.1170
BJ	0.8126	0.1590
BK	0.8382	0.1540
BL	0.9186	0.1460
BM	0.8554	0.1250
BN	0.8930	0.1460
BO	0.8737	0.1470
BP	0.8536	0.1230
BQ	0.6818	0.1040
BR	0.8593	0.1320
BS	0.8862	0.1560
BT	0.9168	0.1510
BU	0.8909	0.1610
BV	0.8381	0.1220
BW	0.7238	0.1110
BX	0.9209	0.1620
BY	0.9254	0.1430
BZ	0.9315	0.1660
Ba	0.8802	0.1400
Bb	0.8579	0.1450
Bc	0.8131	0.1300
Bd	0.8589	0.1450
Be	0.8320	0.1450
Bf	0.8509	0.1520
Bg	0.9187	0.1720
Bh	0.9170	0.1450
Bi	0.9217	0.1330
Bj	0.8208	0.1380
Bk	0.9379	0.1790
BI	0.8881	0.1470
Bm	0.9477	0.1570
Bn	0.9053	0.1410
Bo	0.9346	0.1550
Bp	0.8710	0.1410
Bq	0.8337	0.1290
Br	0.8700	0.1520
Bs	0.8545	0.1590
Bt	0.9465	0.1650



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Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
Bu	0.8962	0.1400
Bv	0.8645	0.1460
Bw	0.8651	0.1180
Bx	0.8455	0.1460
By	0.8967	0.1590
Bz	0.8318	0.1490
C0	0.8319	0.1070
C1	0.0000	0.0300
C2	0.9346	0.1800
C3	0.9203	0.1710
C4	0.9232	0.1580
C5	0.9580	0.1710
C6	0.9087	0.1650
C7	0.8780	0.1600
C8	0.8819	0.1660
C9	0.8653	0.1280
CA	0.8618	0.1670
CB	0.6574	0.1090
CC	0.8316	0.1460
CD	0.2474	0.0510
CE	0.9250	0.1660
CF	0.9148	0.1600
CG	0.8040	0.1370
CH	0.8970	0.1760
CI	0.9226	0.1710
CJ	0.3236	0.0600
CK	0.8477	0.1330
CL	0.8840	0.1640
CM	0.9277	0.1890
CN	0.6505	0.1250
CO	0.8458	0.1480
CP	0.8508	0.1460
CQ	0.8124	0.1190
CR	0.4620	0.0650
CS	0.8409	0.1460
CT	0.8558	0.1630
CU	0.8999	0.1630
CV	0.8796	0.1640
CW	0.9479	0.1740
CX	0.7903	0.1210
CY	0.5070	0.0830
CZ	0.8879	0.1460



Chain	Atom inclusion	Q-score
Ca	0.9065	0.1390
Cb	0.9391	0.1670
Cc	0.7939	0.1270
Cd	0.9410	0.1670
Ce	0.8951	0.1500
Cf	0.8919	0.1430
Cg	0.9364	0.1670
Ch	0.9400	0.1680
Ci	0.9228	0.1670
Сј	0.9584	0.1670
Ck	0.9360	0.1530
Cl	0.9440	0.1540
Cm	0.9082	0.1700
Cn	0.8864	0.1650
Со	0.7448	0.1320
Ср	0.8378	0.1520
Cq	0.7241	0.1270
Cr	0.9147	0.1890
Cs	0.8637	0.1220
Ct	0.9174	0.1710
Cu	0.6526	0.1260
Cv	0.9494	0.1760
Cw	0.8897	0.1630
Cx	0.8850	0.1560
Су	0.8742	0.1580
Cz	0.0000	0.0480
DA	0.8441	0.1520
DB	0.9520	0.1760
DC	0.8798	0.1530
DD	0.0000	0.0360
DE	0.0611	0.0430
DF	0.6083	0.1130
DG	0.7364	0.1190
DH	0.9388	0.1710
DI	0.9587	0.1760

