Full wwPDB EM Validation Report

Dec 19, 2022 – 11:21 am GMT

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

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.38 Å.

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

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

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

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

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

2 Entry composition (i)

There are 79 unique types of molecules in this entry. The entry contains 122511 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a DNA chain called SCAFFOLD STRAND.

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

- Molecule 2 is a DNA chain called STAPLE STRAND.

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

- Molecule 3 is a DNA chain called STAPLE STRAND.

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

- Molecule 4 is a DNA chain called STAPLE STRAND.

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

- Molecule 5 is a DNA chain called STAPLE STRAND.

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

- Molecule 6 is a DNA chain called STAPLE STRAND.

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

- Molecule 7 is a DNA chain called STAPLE STRAND.

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

- Molecule 8 is a DNA chain called STAPLE STRAND.

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

- Molecule 9 is a DNA chain called STAPLE STRAND.

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

- Molecule 10 is a DNA chain called STAPLE STRAND.

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

- Molecule 11 is a DNA chain called STAPLE STRAND.

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

- Molecule 12 is a DNA chain called STAPLE STRAND.

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

- Molecule 13 is a DNA chain called STAPLE STRAND.

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

- Molecule 14 is a DNA chain called STAPLE STRAND.

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

- Molecule 15 is a DNA chain called STAPLE STRAND.

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

- Molecule 16 is a DNA chain called STAPLE STRAND.

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

- Molecule 17 is a DNA chain called STAPLE STRAND.

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

- Molecule 18 is a DNA chain called STAPLE STRAND.

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

- Molecule 19 is a DNA chain called STAPLE STRAND.

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

- Molecule 20 is a DNA chain called STAPLE STRAND.

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

- Molecule 21 is a DNA chain called STAPLE STRAND.

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

- Molecule 22 is a DNA chain called STAPLE STRAND.

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

- Molecule 23 is a DNA chain called STAPLE STRAND.

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

- Molecule 24 is a DNA chain called STAPLE STRAND.

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

- Molecule 25 is a DNA chain called STAPLE STRAND.

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

- Molecule 26 is a DNA chain called STAPLE STRAND.

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

- Molecule 27 is a DNA chain called STAPLE STRAND.

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

- Molecule 28 is a DNA chain called STAPLE STRAND.

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

- Molecule 29 is a DNA chain called STAPLE STRAND.

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

- Molecule 30 is a DNA chain called STAPLE STRAND.

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

- Molecule 31 is a DNA chain called STAPLE STRAND.

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

- Molecule 32 is a DNA chain called STAPLE STRAND.

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

- Molecule 33 is a DNA chain called STAPLE STRAND.

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

- Molecule 34 is a DNA chain called STAPLE STRAND.

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

- Molecule 35 is a DNA chain called STAPLE STRAND.

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

- Molecule 36 is a DNA chain called STAPLE STRAND.

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

- Molecule 37 is a DNA chain called STAPLE STRAND.

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

- Molecule 38 is a DNA chain called STAPLE STRAND.

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

- Molecule 39 is a DNA chain called STAPLE STRAND.

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

- Molecule 40 is a DNA chain called STAPLE STRAND.

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

- Molecule 41 is a DNA chain called STAPLE STRAND.

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

- Molecule 42 is a DNA chain called STAPLE STRAND.

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

- Molecule 43 is a DNA chain called STAPLE STRAND.

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

- Molecule 44 is a DNA chain called STAPLE STRAND.

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

- Molecule 45 is a DNA chain called STAPLE STRAND.

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

- Molecule 46 is a DNA chain called STAPLE STRAND.

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

- Molecule 47 is a DNA chain called STAPLE STRAND.

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

- Molecule 48 is a DNA chain called STAPLE STRAND.

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

- Molecule 49 is a DNA chain called STAPLE STRAND.

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

- Molecule 50 is a DNA chain called STAPLE STRAND.

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

- Molecule 51 is a DNA chain called STAPLE STRAND.

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

- Molecule 52 is a DNA chain called STAPLE STRAND.

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

- Molecule 53 is a DNA chain called STAPLE STRAND.

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

- Molecule 54 is a DNA chain called STAPLE STRAND.

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

- Molecule 55 is a DNA chain called STAPLE STRAND.

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

- Molecule 56 is a DNA chain called STAPLE STRAND.

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

- Molecule 57 is a DNA chain called STAPLE STRAND.

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

- Molecule 58 is a DNA chain called STAPLE STRAND.

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

- Molecule 59 is a DNA chain called STAPLE STRAND.

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

- Molecule 60 is a DNA chain called STAPLE STRAND.

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

- Molecule 61 is a DNA chain called STAPLE STRAND.

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

- Molecule 62 is a DNA chain called STAPLE STRAND.

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

- Molecule 63 is a DNA chain called STAPLE STRAND.

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

- Molecule 64 is a DNA chain called STAPLE STRAND.

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

- Molecule 65 is a DNA chain called STAPLE STRAND.

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

- Molecule 66 is a DNA chain called STAPLE STRAND.

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

- Molecule 67 is a DNA chain called STAPLE STRAND.

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

- Molecule 68 is a DNA chain called STAPLE STRAND.

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

- Molecule 69 is a DNA chain called STAPLE STRAND.

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

- Molecule 70 is a DNA chain called STAPLE STRAND.

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

- Molecule 71 is a DNA chain called STAPLE STRAND.

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

- Molecule 72 is a DNA chain called STAPLE STRAND.

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

- Molecule 73 is a DNA chain called STAPLE STRAND.

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

- Molecule 74 is a DNA chain called STAPLE STRAND.

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

- Molecule 75 is a DNA chain called STAPLE STRAND.

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

- Molecule 76 is a DNA chain called STAPLE STRAND.

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

- Molecule 77 is a DNA chain called STAPLE STRAND.

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

- Molecule 78 is a DNA chain called STAPLE STRAND.

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

- Molecule 79 is a DNA chain called STAPLE STRAND.

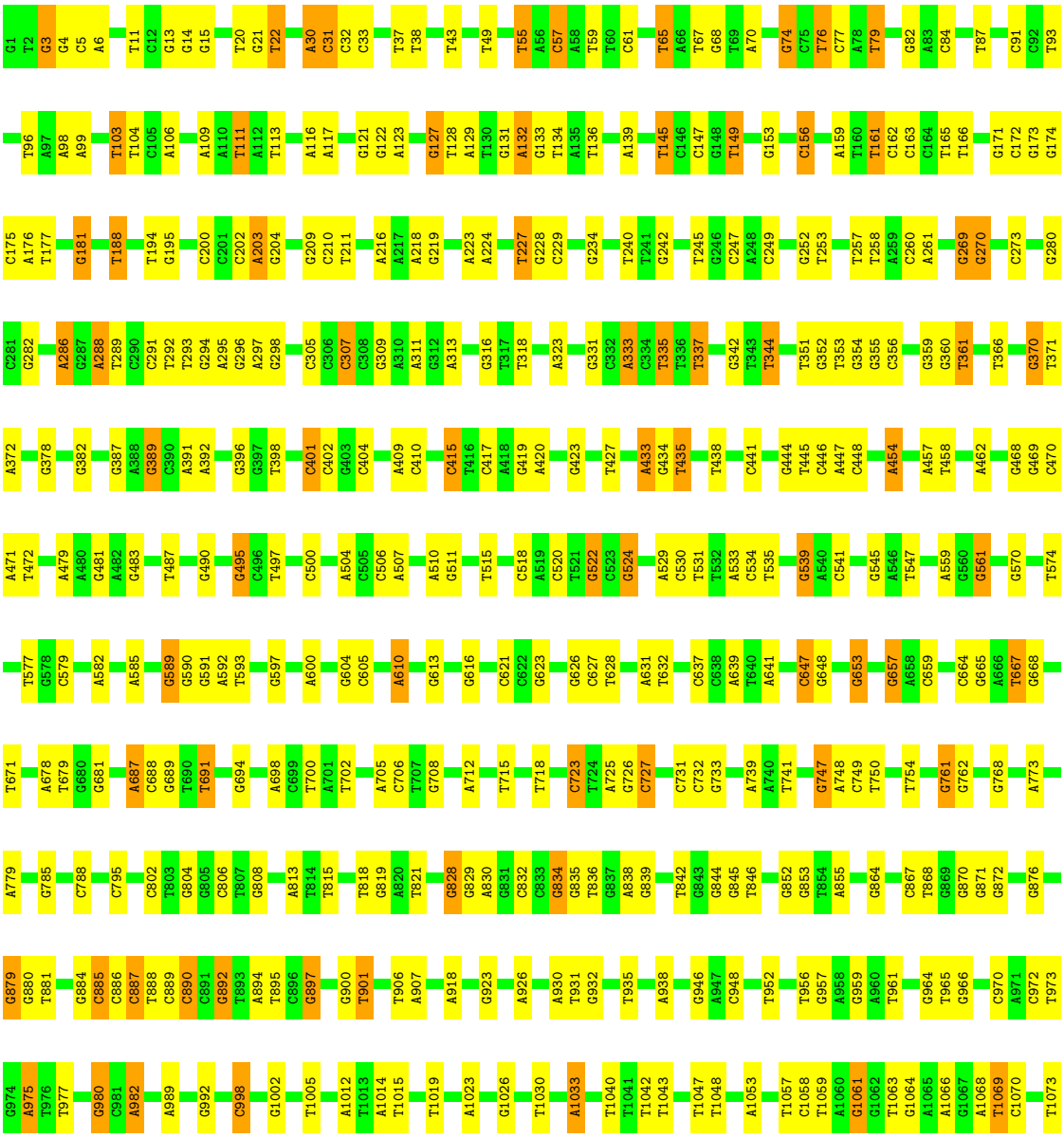
Mol	Chain	Residues	Atoms					AltConf	Trace
79	BQ	37	Total	C	N	O	P	0	0
			755	362	133	224	36		

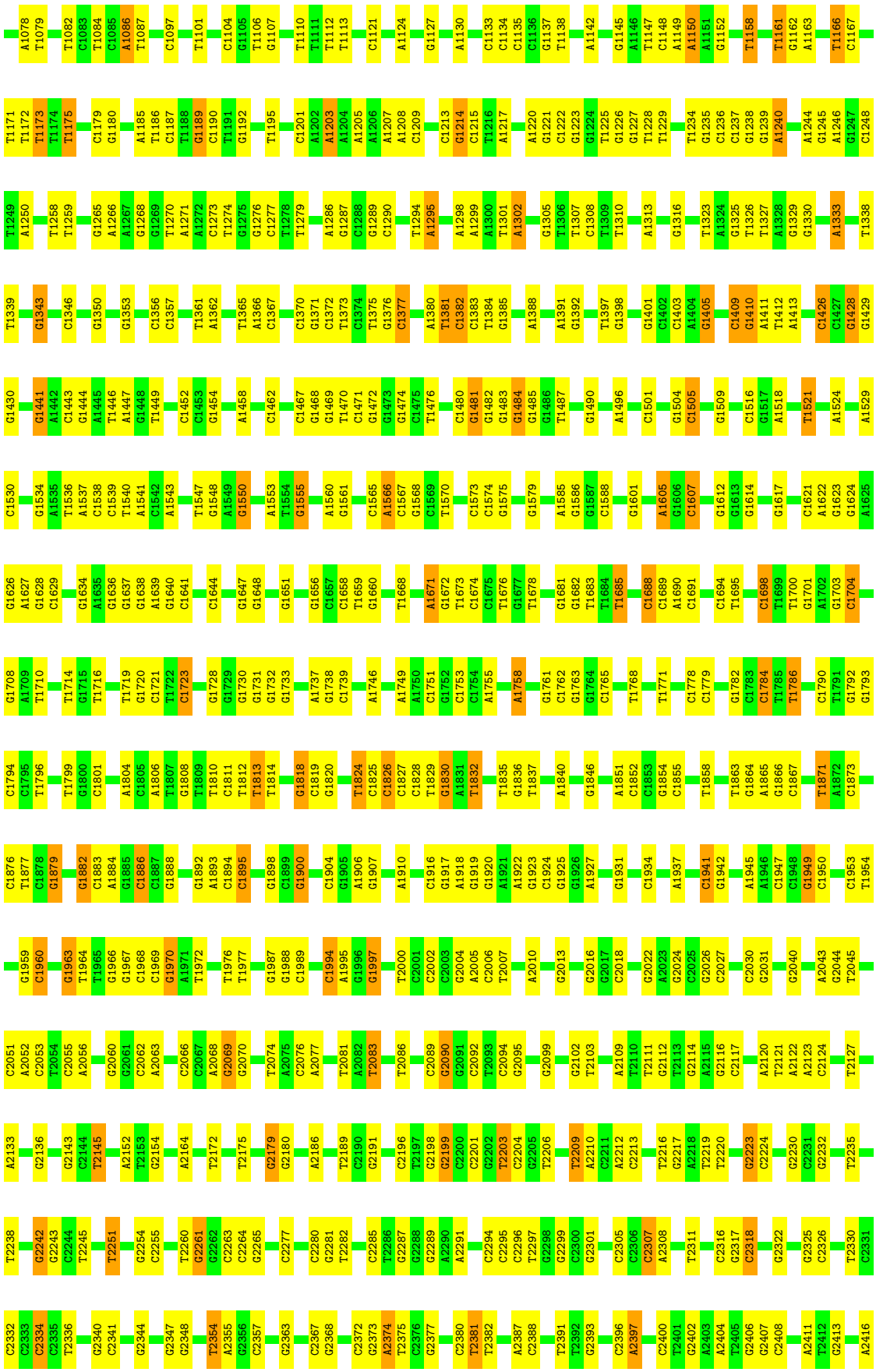
3 Residue-property plots (i)

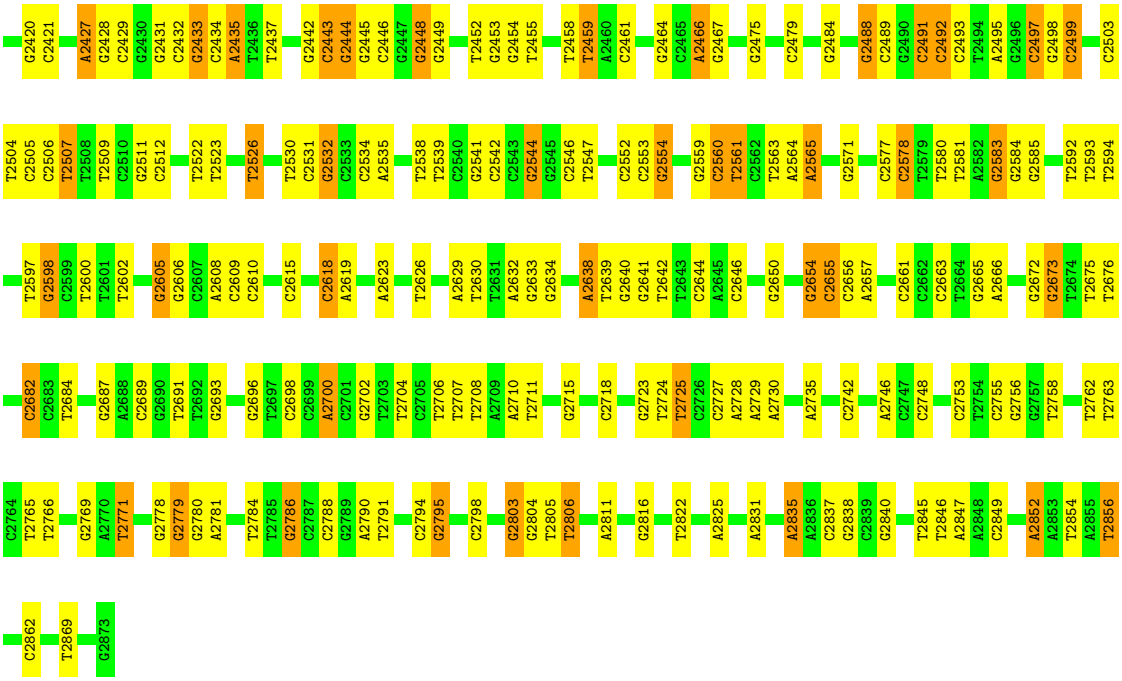
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: SCAFFOLD STRAND

Chain AA: 59% 34% 7%

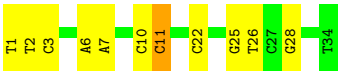






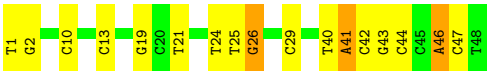
- Molecule 2: STAPLE STRAND

Chain AB:



- Molecule 3: STAPLE STRAND

Chain AC:

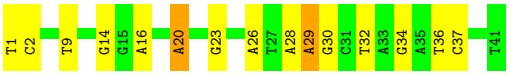


- Molecule 4: STAPLE STRAND

Chain AD:

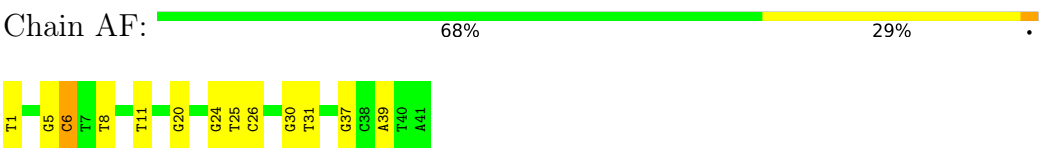
- Molecule 5: STAPLE STRAND

Chain AE:



- Molecule 6: STAPLE STRAND

Chain AF:

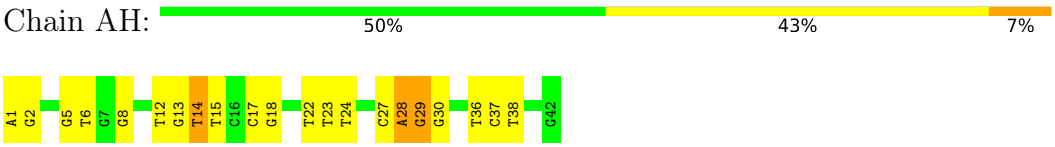


• Molecule 7: STAPLE STRAND

Chain AG:

• Molecule 8: STAPLE STRAND

Chain AH:

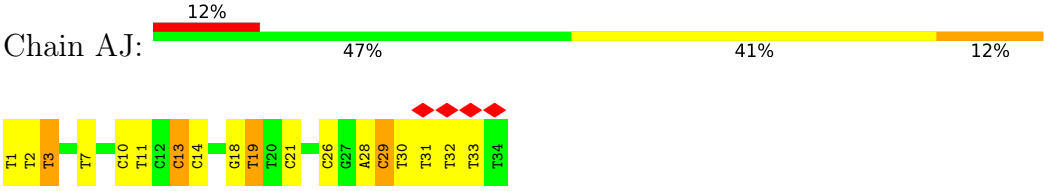


• Molecule 9: STAPLE STRAND

Chain AI:

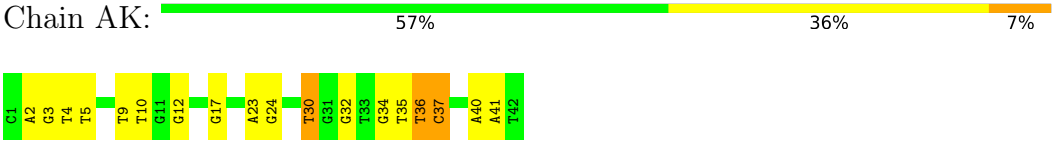
• Molecule 10: STAPLE STRAND

Chain AJ:



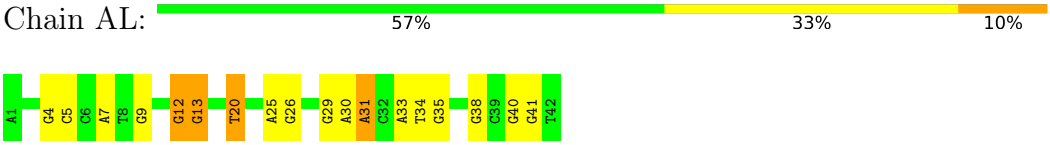
• Molecule 11: STAPLE STRAND

Chain AK:



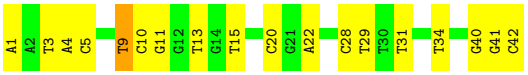
• Molecule 12: STAPLE STRAND

Chain AL:



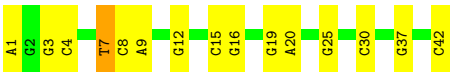
• Molecule 13: STAPLE STRAND

Chain AM:



• Molecule 14: STAPLE STRAND

Chain AN:

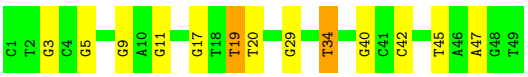


• Molecule 15: STAPLE STRAND

Chain AO:

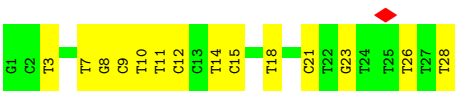
• Molecule 16: STAPLE STRAND

Chain AP:



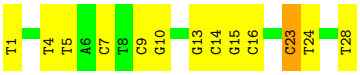
• Molecule 17: STAPLE STRAND

Chain AQ:



• Molecule 18: STAPLE STRAND

Chain AR:

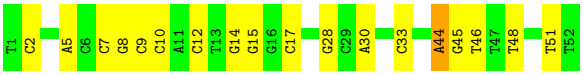


• Molecule 19: STAPLE STRAND

Chain AS:

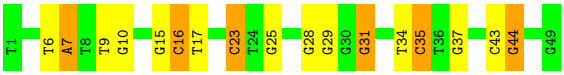
• Molecule 20: STAPLE STRAND

Chain AT:



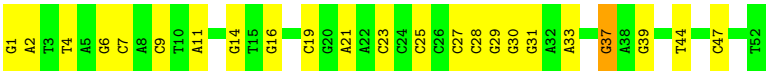
• Molecule 21: STAPLE STRAND

Chain AU:



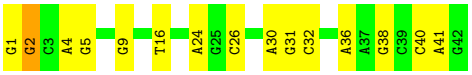
• Molecule 22: STAPLE STRAND

Chain AV:



• Molecule 23: STAPLE STRAND

Chain AW:



• Molecule 24: STAPLE STRAND

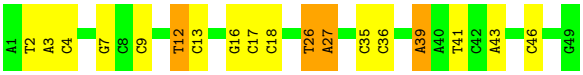
Chain AX:

• Molecule 25: STAPLE STRAND

Chain AY:

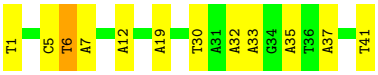
• Molecule 26: STAPLE STRAND

Chain AZ:



• Molecule 27: STAPLE STRAND

Chain Aa:



• Molecule 28: STAPLE STRAND

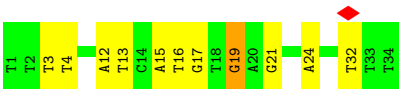
Chain Ab:

• Molecule 29: STAPLE STRAND

Chain Ac:

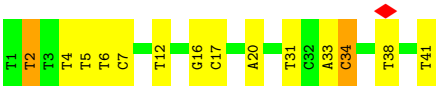
• Molecule 30: STAPLE STRAND

Chain Ad:



• Molecule 31: STAPLE STRAND

Chain Ae:

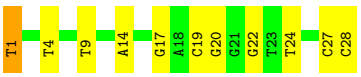


• Molecule 32: STAPLE STRAND

Chain Af:

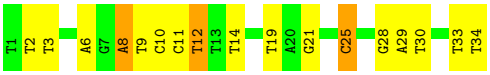
• Molecule 33: STAPLE STRAND

Chain Ag:



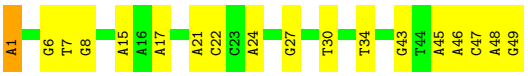
• Molecule 34: STAPLE STRAND

Chain Ah:



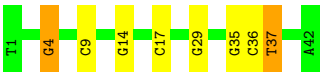
• Molecule 35: STAPLE STRAND

Chain Ai:



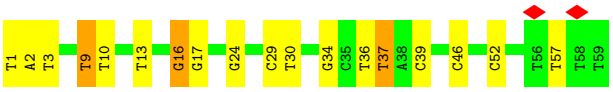
• Molecule 36: STAPLE STRAND

Chain Aj:



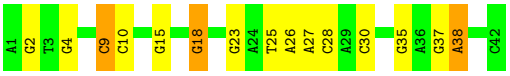
• Molecule 37: STAPLE STRAND

Chain Ak:



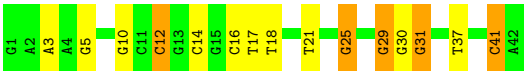
• Molecule 38: STAPLE STRAND

Chain Al:



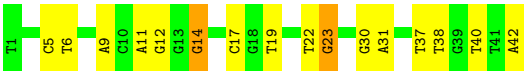
• Molecule 39: STAPLE STRAND

Chain Am:



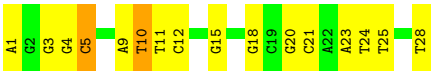
• Molecule 40: STAPLE STRAND

Chain An:



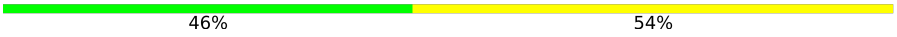
• Molecule 41: STAPLE STRAND

Chain Ao:



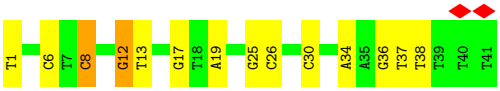
• Molecule 42: STAPLE STRAND

Chain Ap:



• Molecule 43: STAPLE STRAND

Chain Aq:

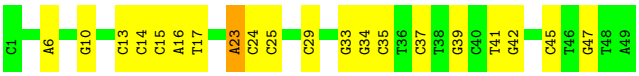


• Molecule 44: STAPLE STRAND

Chain Ar:

• Molecule 45: STAPLE STRAND

Chain As:

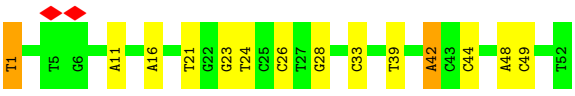


• Molecule 46: STAPLE STRAND

Chain At:

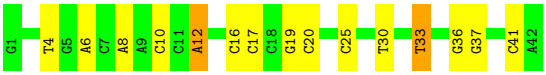
• Molecule 47: STAPLE STRAND

Chain Au:



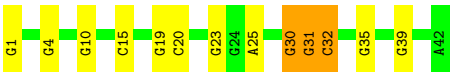
• Molecule 48: STAPLE STRAND

Chain Av:



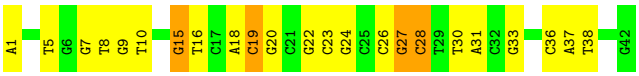
• Molecule 49: STAPLE STRAND

Chain Aw:



• Molecule 50: STAPLE STRAND

Chain Ax:

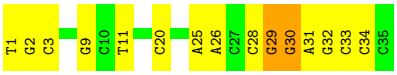


• Molecule 51: STAPLE STRAND

Chain Ay:

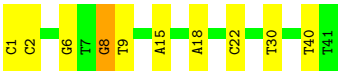
• Molecule 52: STAPLE STRAND

Chain Az:



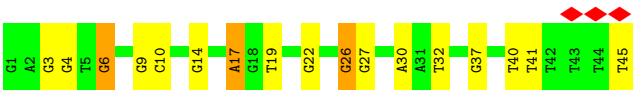
• Molecule 53: STAPLE STRAND

Chain A0:



• Molecule 54: STAPLE STRAND

Chain A1:

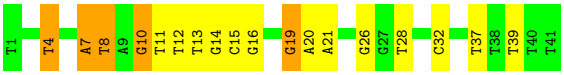


• Molecule 55: STAPLE STRAND

Chain A2:

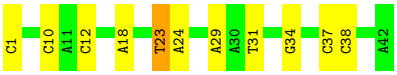
• Molecule 56: STAPLE STRAND

Chain A3:



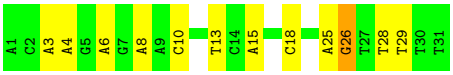
• Molecule 57: STAPLE STRAND

Chain A4:



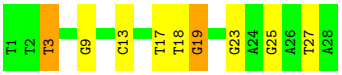
• Molecule 58: STAPLE STRAND

Chain A5:



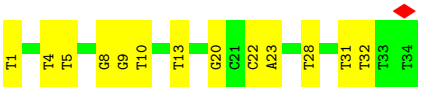
• Molecule 59: STAPLE STRAND

Chain A6:



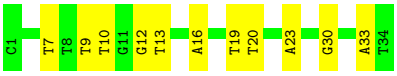
• Molecule 60: STAPLE STRAND

Chain A7:



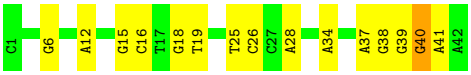
• Molecule 61: STAPLE STRAND

Chain A8:



• Molecule 62: STAPLE STRAND

Chain A9:

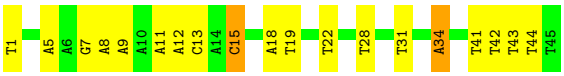


• Molecule 63: STAPLE STRAND

Chain BA:

• Molecule 64: STAPLE STRAND

Chain BB:

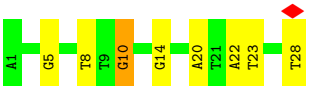


• Molecule 65: STAPLE STRAND

Chain BC:

• Molecule 66: STAPLE STRAND

Chain BD:

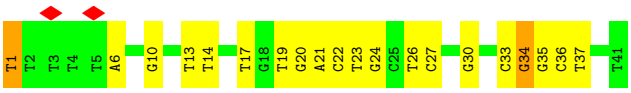


• Molecule 67: STAPLE STRAND

Chain BE:

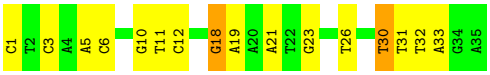
• Molecule 68: STAPLE STRAND

Chain BF:



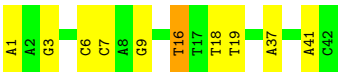
• Molecule 69: STAPLE STRAND

Chain BG:



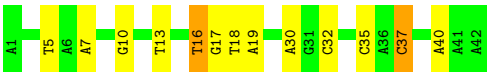
• Molecule 70: STAPLE STRAND

Chain BH:



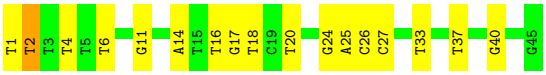
• Molecule 71: STAPLE STRAND

Chain BI:



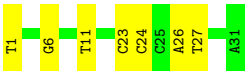
• Molecule 72: STAPLE STRAND

Chain BJ:



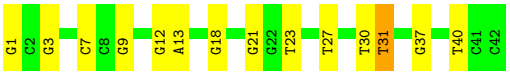
• Molecule 73: STAPLE STRAND

Chain BK:



• Molecule 74: STAPLE STRAND

Chain BL:

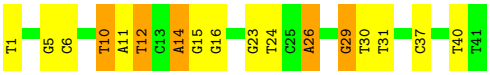


• Molecule 75: STAPLE STRAND

Chain BM:

• Molecule 76: STAPLE STRAND

Chain BN:

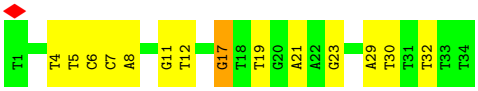


• Molecule 77: STAPLE STRAND

Chain BO:

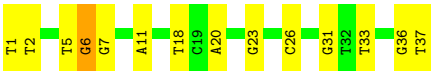
• Molecule 78: STAPLE STRAND

Chain BP:



• Molecule 79: STAPLE STRAND

Chain BQ:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42209	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.372	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.0628	Depositor
Map size (Å)	695.7, 695.7, 695.7	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.319, 2.319, 2.319	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	AA	1.23	5/66004 (0.0%)	1.43	971/101868 (1.0%)
2	AB	1.27	0/774	1.37	5/1192 (0.4%)
3	AC	1.22	0/1078	1.46	19/1660 (1.1%)
4	AD	1.19	0/790	1.49	11/1219 (0.9%)
5	AE	1.25	0/940	1.42	8/1449 (0.6%)
6	AF	1.22	0/929	1.41	11/1431 (0.8%)
7	AG	1.20	0/769	1.48	12/1184 (1.0%)
8	AH	1.27	0/958	1.47	18/1478 (1.2%)
9	AI	1.22	0/646	1.31	6/996 (0.6%)
10	AJ	1.22	0/746	1.68	24/1147 (2.1%)
11	AK	1.22	0/962	1.35	9/1484 (0.6%)
12	AL	1.22	0/971	1.36	11/1499 (0.7%)
13	AM	1.24	0/970	1.45	17/1497 (1.1%)
14	AN	1.31	0/990	1.38	11/1530 (0.7%)
15	AO	1.26	0/1132	1.43	17/1746 (1.0%)
16	AP	1.23	0/1119	1.33	10/1725 (0.6%)
17	AQ	1.23	0/623	1.42	5/959 (0.5%)
18	AR	1.23	0/628	1.56	16/967 (1.7%)
19	AS	1.22	0/957	1.38	13/1477 (0.9%)
20	AT	1.21	0/1172	1.28	3/1804 (0.2%)
21	AU	1.31	0/1134	1.44	12/1752 (0.7%)
22	AV	1.26	0/1193	1.52	27/1840 (1.5%)
23	AW	1.22	0/966	1.37	10/1489 (0.7%)
24	AX	1.21	0/847	1.35	7/1304 (0.5%)
25	AY	1.21	0/702	1.32	8/1081 (0.7%)
26	AZ	1.22	0/1122	1.38	11/1729 (0.6%)
27	Aa	1.16	0/936	1.37	10/1439 (0.7%)
28	Ab	1.31	1/961 (0.1%)	1.64	25/1480 (1.7%)
29	Ac	1.26	0/963	1.43	11/1486 (0.7%)
30	Ad	1.20	1/779 (0.1%)	1.21	3/1203 (0.2%)
31	Ae	1.22	1/920 (0.1%)	1.42	9/1417 (0.6%)
32	Af	1.24	0/970	1.42	16/1498 (1.1%)
33	Ag	1.19	0/635	1.29	7/979 (0.7%)
34	Ah	1.24	0/766	1.62	17/1181 (1.4%)

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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

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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1302	DA	C5'-C4'	5.50	1.57	1.51
30	Ad	32	DT	C5'-C4'	5.45	1.57	1.51
50	Ax	15	DG	C2-N2	-5.25	1.29	1.34
1	AA	2655	DC	C5'-C4'	5.23	1.57	1.51
1	AA	1452	DC	C5'-C4'	5.23	1.57	1.51
28	Ab	37	DT	O3'-P	-5.17	1.54	1.61
1	AA	828	DG	C4'-C3'	5.16	1.58	1.53
60	A7	4	DT	C5'-C4'	5.10	1.56	1.51
40	An	30	DG	C4'-C3'	5.09	1.58	1.53
1	AA	923	DG	C2-N2	-5.07	1.29	1.34
31	Ae	38	DT	C5'-C4'	5.05	1.56	1.51
52	Az	32	DG	C2-N2	-5.02	1.29	1.34
77	BO	38	DA	N9-C4	-5.01	1.34	1.37

All (1892) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Ah	12	DT	P-O3'-C3'	15.81	138.68	119.70
1	AA	1873	DC	P-O3'-C3'	15.25	138.00	119.70
1	AA	175	DC	P-O3'-C3'	15.17	137.90	119.70
54	A1	9	DG	P-O3'-C3'	15.13	137.85	119.70
1	AA	409	DA	P-O3'-C3'	14.92	137.60	119.70
1	AA	2803	DG	P-O3'-C3'	14.80	137.46	119.70
26	AZ	9	DC	P-O3'-C3'	14.64	137.27	119.70
1	AA	2682	DC	P-O3'-C3'	14.47	137.07	119.70
1	AA	1410	DG	P-O3'-C3'	14.45	137.04	119.70
39	Am	14	DC	P-O3'-C3'	14.21	136.75	119.70
1	AA	57	DC	P-O3'-C3'	14.16	136.69	119.70
71	BI	37	DC	P-O3'-C3'	14.07	136.59	119.70
77	BO	30	DA	P-O3'-C3'	13.99	136.49	119.70
38	Al	30	DC	P-O3'-C3'	13.96	136.46	119.70
78	BP	29	DA	P-O3'-C3'	13.92	136.40	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Ah	9	DT	P-O3'-C3'	13.83	136.29	119.70
28	Ab	37	DT	P-O3'-C3'	13.75	136.20	119.70
6	AF	11	DT	P-O3'-C3'	13.68	136.12	119.70
1	AA	1383	DC	P-O3'-C3'	13.67	136.11	119.70
1	AA	288	DA	P-O3'-C3'	13.61	136.03	119.70
46	At	47	DT	P-O3'-C3'	13.47	135.87	119.70
1	AA	610	DA	P-O3'-C3'	13.45	135.84	119.70
1	AA	2124	DC	P-O3'-C3'	13.43	135.82	119.70
1	AA	1778	DC	P-O3'-C3'	13.40	135.78	119.70
1	AA	1651	DG	P-O3'-C3'	13.38	135.75	119.70
17	AQ	28	DT	O4'-C4'-C3'	-13.38	97.97	106.00
1	AA	1540	DT	P-O3'-C3'	13.35	135.72	119.70
45	As	35	DC	P-O3'-C3'	13.35	135.72	119.70
42	Ap	5	DT	O4'-C4'-C3'	-13.32	98.00	106.00
1	AA	337	DT	P-O3'-C3'	13.32	135.68	119.70
78	BP	32	DT	P-O3'-C3'	13.08	135.40	119.70
1	AA	1205	DA	P-O3'-C3'	13.07	135.39	119.70
1	AA	2728	DA	P-O3'-C3'	13.07	135.38	119.70
4	AD	29	DA	P-O3'-C3'	12.98	135.28	119.70
52	Az	1	DT	P-O3'-C3'	12.98	135.27	119.70
1	AA	2053	DC	P-O3'-C3'	12.97	135.26	119.70
1	AA	2062	DC	P-O3'-C3'	12.94	135.23	119.70
1	AA	240	DT	P-O3'-C3'	12.89	135.17	119.70
1	AA	2382	DT	O4'-C4'-C3'	-12.86	98.28	106.00
39	Am	29	DG	P-O3'-C3'	12.81	135.07	119.70
22	AV	9	DC	P-O3'-C3'	12.78	135.04	119.70
64	BB	9	DA	P-O3'-C3'	12.71	134.96	119.70
45	As	37	DC	P-O3'-C3'	12.67	134.90	119.70
28	Ab	34	DT	O4'-C4'-C3'	-12.63	98.42	106.00
1	AA	1836	DG	O4'-C4'-C3'	-12.62	98.42	106.00
29	Ac	30	DG	P-O3'-C3'	12.54	134.75	119.70
72	BJ	26	DC	P-O3'-C3'	12.46	134.65	119.70
4	AD	22	DA	P-O3'-C3'	12.44	134.63	119.70
1	AA	1641	DC	P-O3'-C3'	12.44	134.62	119.70
1	AA	2639	DT	O4'-C4'-C3'	-12.39	98.56	106.00
1	AA	1441	DG	P-O3'-C3'	12.33	134.50	119.70
1	AA	2507	DT	O4'-C4'-C3'	-12.32	98.61	106.00
1	AA	2092	DC	P-O3'-C3'	12.26	134.41	119.70
5	AE	1	DT	O4'-C4'-C3'	-12.18	98.69	106.00
32	Af	8	DA	P-O3'-C3'	12.17	134.30	119.70
51	Ay	9	DA	P-O3'-C3'	12.16	134.29	119.70
1	AA	1628	DG	P-O3'-C3'	12.16	134.29	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1222	DC	P-O3'-C3'	12.15	134.28	119.70
1	AA	2355	DA	P-O3'-C3'	12.15	134.28	119.70
1	AA	269	DG	P-O3'-C3'	12.13	134.26	119.70
62	A9	34	DA	P-O3'-C3'	12.13	134.26	119.70
60	A7	4	DT	P-O3'-C3'	12.11	134.23	119.70
1	AA	2491	DC	P-O3'-C3'	12.11	134.23	119.70
14	AN	30	DC	P-O3'-C3'	12.10	134.22	119.70
62	A9	12	DA	P-O3'-C3'	12.07	134.18	119.70
1	AA	2673	DG	P-O3'-C3'	12.06	134.17	119.70
1	AA	1941	DC	P-O3'-C3'	12.01	134.11	119.70
1	AA	931	DT	O4'-C4'-C3'	-11.99	98.81	106.00
7	AG	22	DC	P-O3'-C3'	11.97	134.07	119.70
1	AA	1607	DC	P-O3'-C3'	11.97	134.06	119.70
1	AA	1540	DT	O4'-C4'-C3'	-11.94	98.83	106.00
1	AA	149	DT	P-O3'-C3'	11.93	134.02	119.70
41	Ao	21	DC	O4'-C4'-C3'	-11.92	98.85	106.00
36	Aj	37	DT	P-O3'-C3'	11.91	134.00	119.70
3	AC	21	DT	P-O3'-C3'	11.88	133.96	119.70
1	AA	845	DG	O4'-C4'-C3'	-11.86	98.89	106.00
1	AA	1033	DA	O4'-C4'-C3'	-11.84	98.90	106.00
75	BM	48	DA	P-O3'-C3'	11.81	133.87	119.70
1	AA	1575	DG	O4'-C4'-C3'	-11.81	98.92	106.00
34	Ah	25	DC	P-O3'-C3'	11.79	133.85	119.70
13	AM	1	DA	O4'-C4'-C3'	-11.76	98.94	106.00
1	AA	574	DT	P-O3'-C3'	11.73	133.78	119.70
1	AA	2781	DA	P-O3'-C3'	11.70	133.74	119.70
1	AA	1970	DG	P-O3'-C3'	11.68	133.72	119.70
21	AU	44	DG	P-O3'-C3'	11.66	133.70	119.70
1	AA	1064	DG	O4'-C4'-C3'	-11.66	99.00	106.00
32	Af	10	DG	O4'-C4'-C3'	-11.64	99.01	106.00
1	AA	2069	DG	P-O3'-C3'	11.63	133.66	119.70
12	AL	9	DG	O4'-C4'-C3'	-11.57	99.06	106.00
39	Am	31	DG	O4'-C4'-C3'	-11.52	99.09	106.00
1	AA	417	DC	P-O3'-C3'	11.52	133.52	119.70
1	AA	2638	DA	P-O3'-C3'	11.52	133.52	119.70
15	AO	43	DA	P-O3'-C3'	11.49	133.49	119.70
28	Ab	34	DT	P-O3'-C3'	11.47	133.46	119.70
1	AA	1565	DC	P-O3'-C3'	11.46	133.45	119.70
73	BK	1	DT	O4'-C4'-C3'	-11.40	99.16	106.00
53	A0	40	DT	P-O3'-C3'	11.37	133.34	119.70
67	BE	17	DG	O4'-C4'-C3'	-11.35	99.19	106.00
1	AA	541	DC	P-O3'-C3'	11.34	133.31	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1892	DG	O4'-C4'-C3'	-11.31	99.21	106.00
22	AV	29	DG	P-O3'-C3'	11.27	133.22	119.70
10	AJ	3	DT	O4'-C4'-C3'	-11.26	99.25	106.00
47	Au	1	DT	P-O3'-C3'	11.24	133.19	119.70
75	BM	23	DC	P-O3'-C3'	11.23	133.18	119.70
7	AG	1	DT	O4'-C4'-C3'	-11.18	99.30	106.00
59	A6	19	DG	P-O3'-C3'	11.17	133.10	119.70
1	AA	2040	DG	O4'-C4'-C3'	-11.16	99.30	106.00
1	AA	659	DC	P-O3'-C3'	11.16	133.09	119.70
1	AA	2702	DG	O4'-C4'-C3'	-11.16	99.31	106.00
46	At	21	DG	O4'-C4'-C3'	-11.13	99.32	106.00
31	Ae	17	DC	O4'-C4'-C3'	-11.10	99.34	106.00
1	AA	821	DT	P-O3'-C3'	11.09	133.00	119.70
22	AV	27	DC	P-O3'-C3'	11.08	133.00	119.70
65	BC	1	DA	P-O3'-C3'	11.06	132.98	119.70
1	AA	597	DG	O4'-C4'-C3'	-11.06	99.36	106.00
65	BC	29	DT	O4'-C4'-C3'	-11.04	99.37	106.00
1	AA	1732	DG	O4'-C4'-C3'	-11.04	99.38	106.00
11	AK	41	DA	P-O3'-C3'	11.02	132.93	119.70
1	AA	2791	DT	O4'-C4'-C3'	-11.00	99.40	106.00
1	AA	2296	DC	P-O3'-C3'	10.96	132.85	119.70
1	AA	2693	DG	O4'-C4'-C3'	-10.94	99.43	106.00
13	AM	40	DG	P-O3'-C3'	10.94	132.83	119.70
1	AA	1710	DT	O4'-C4'-C3'	-10.91	99.46	106.00
79	BQ	36	DG	P-O3'-C3'	10.90	132.78	119.70
1	AA	68	DG	O4'-C4'-C3'	-10.88	99.47	106.00
1	AA	2499	DC	P-O3'-C3'	10.88	132.75	119.70
1	AA	733	DG	P-O3'-C3'	10.86	132.73	119.70
1	AA	22	DT	P-O3'-C3'	10.83	132.70	119.70
1	AA	1804	DA	P-O3'-C3'	10.83	132.70	119.70
1	AA	665	DG	O4'-C4'-C3'	-10.82	99.51	106.00
1	AA	1879	DG	O4'-C4'-C3'	-10.77	99.54	106.00
49	Aw	25	DA	O4'-C4'-C3'	-10.71	99.57	106.00
1	AA	1836	DG	P-O3'-C3'	10.70	132.54	119.70
1	AA	1033	DA	P-O3'-C3'	10.69	132.53	119.70
35	Ai	1	DA	O4'-C4'-C3'	-10.69	99.59	106.00
3	AC	47	DC	P-O3'-C3'	10.67	132.50	119.70
49	Aw	32	DC	P-O3'-C3'	10.66	132.50	119.70
59	A6	27	DT	P-O3'-C3'	10.63	132.46	119.70
5	AE	37	DC	P-O3'-C3'	10.63	132.45	119.70
1	AA	881	DT	O4'-C4'-C3'	-10.57	99.66	106.00
1	AA	2223	DG	P-O3'-C3'	10.57	132.38	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2434	DC	P-O3'-C3'	10.51	132.31	119.70
1	AA	1723	DC	P-O3'-C3'	10.50	132.30	119.70
37	Ak	9	DT	O4'-C4'-C3'	-10.40	99.76	106.00
13	AM	40	DG	O4'-C4'-C3'	-10.40	99.76	106.00
1	AA	520	DC	P-O3'-C3'	10.38	132.16	119.70
56	A3	8	DT	O4'-C4'-C3'	-10.38	99.78	106.00
18	AR	1	DT	O4'-C4'-C3'	-10.34	99.80	106.00
1	AA	1365	DT	O4'-C4'-C3'	-10.33	99.80	106.00
22	AV	44	DT	O4'-C4'-C3'	-10.33	99.80	106.00
41	Ao	10	DT	O4'-C4'-C3'	-10.31	99.81	106.00
74	BL	18	DG	O4'-C4'-C3'	-10.31	99.81	106.00
78	BP	8	DA	O4'-C4'-C3'	-10.28	99.83	106.00
3	AC	26	DG	P-O3'-C3'	10.28	132.04	119.70
21	AU	23	DC	P-O3'-C3'	10.27	132.02	119.70
74	BL	37	DG	P-O3'-C3'	10.27	132.02	119.70
1	AA	520	DC	O4'-C4'-C3'	-10.21	99.87	106.00
38	Al	38	DA	P-O3'-C3'	10.20	131.94	119.70
1	AA	1444	DG	P-O3'-C3'	10.14	131.87	119.70
28	Ab	31	DG	O4'-C4'-C3'	-10.12	99.93	106.00
4	AD	16	DG	O4'-C4'-C3'	-10.10	99.94	106.00
70	BH	37	DA	P-O3'-C3'	10.08	131.79	119.70
1	AA	828	DG	P-O3'-C3'	10.07	131.78	119.70
1	AA	1521	DT	O4'-C4'-C3'	-10.04	99.98	106.00
1	AA	2526	DT	O4'-C4'-C3'	-10.02	99.99	106.00
31	Ae	2	DT	O4'-C4'-C3'	-10.00	100.00	106.00
1	AA	359	DG	O4'-C4'-C3'	-9.98	100.01	106.00
42	Ap	13	DG	O4'-C4'-C3'	-9.98	100.01	106.00
62	A9	18	DG	O4'-C4'-C3'	-9.96	100.02	106.00
1	AA	2341	DC	P-O3'-C3'	9.96	131.65	119.70
10	AJ	7	DT	O4'-C4'-C3'	-9.95	100.03	106.00
1	AA	1391	DA	P-O3'-C3'	9.93	131.62	119.70
61	A8	33	DA	P-O3'-C3'	9.89	131.57	119.70
4	AD	10	DT	O4'-C4'-C3'	-9.88	100.07	106.00
33	Ag	1	DT	O4'-C4'-C3'	-9.86	100.08	106.00
18	AR	23	DC	C2-N1-C1'	9.83	129.61	118.80
1	AA	1302	DA	O4'-C4'-C3'	-9.80	100.12	106.00
29	Ac	4	DT	O4'-C4'-C3'	-9.79	100.12	106.00
1	AA	1883	DC	P-O3'-C3'	9.78	131.44	119.70
27	Aa	1	DT	P-O3'-C3'	9.78	131.44	119.70
69	BG	19	DA	P-O3'-C3'	9.75	131.40	119.70
38	Al	25	DT	O4'-C4'-C3'	-9.74	100.16	106.00
61	A8	10	DT	P-O3'-C3'	9.71	131.35	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	901	DT	P-O3'-C3'	9.69	131.32	119.70
1	AA	1627	DA	P-O3'-C3'	9.66	131.29	119.70
54	A1	19	DT	O4'-C4'-C3'	-9.64	100.22	106.00
1	AA	389	DG	P-O3'-C3'	9.62	131.25	119.70
1	AA	2435	DA	P-O3'-C3'	9.61	131.24	119.70
17	AQ	3	DT	O4'-C4'-C3'	-9.61	100.23	106.00
1	AA	1626	DG	P-O3'-C3'	9.57	131.19	119.70
79	BQ	31	DG	O4'-C4'-C3'	-9.57	100.26	106.00
1	AA	200	DC	P-O3'-C3'	9.52	131.13	119.70
1	AA	1134	DC	O4'-C4'-C3'	-9.51	100.29	106.00
48	Av	4	DT	O4'-C4'-C3'	-9.51	100.30	106.00
48	Av	33	DT	P-O3'-C3'	9.49	131.08	119.70
69	BG	19	DA	O4'-C1'-C2'	-9.47	98.32	105.90
1	AA	616	DG	O4'-C4'-C3'	-9.41	100.35	106.00
1	AA	1723	DC	O4'-C1'-C2'	-9.38	98.39	105.90
1	AA	1941	DC	O4'-C1'-C2'	-9.38	98.40	105.90
1	AA	2260	DT	P-O3'-C3'	9.38	130.95	119.70
15	AO	41	DG	P-O3'-C3'	9.36	130.93	119.70
41	Ao	23	DA	P-O3'-C3'	9.36	130.93	119.70
56	A3	32	DC	P-O3'-C3'	9.35	130.91	119.70
1	AA	890	DC	P-O3'-C3'	9.33	130.90	119.70
15	AO	12	DA	P-O3'-C3'	9.30	130.86	119.70
78	BP	30	DT	O4'-C4'-C3'	-9.30	100.42	106.00
1	AA	836	DT	O4'-C4'-C3'	-9.29	100.43	106.00
28	Ab	13	DA	P-O3'-C3'	9.28	130.84	119.70
1	AA	2577	DC	P-O3'-C3'	9.28	130.83	119.70
1	AA	2069	DG	O4'-C1'-C2'	-9.27	98.48	105.90
1	AA	2532	DG	P-O3'-C3'	9.27	130.82	119.70
14	AN	9	DA	P-O3'-C3'	9.26	130.81	119.70
1	AA	2715	DG	O4'-C4'-C3'	-9.26	100.45	106.00
1	AA	240	DT	O4'-C1'-C2'	-9.25	98.50	105.90
50	Ax	19	DC	P-O3'-C3'	9.24	130.79	119.70
1	AA	821	DT	O4'-C1'-C2'	-9.23	98.51	105.90
42	Ap	11	DG	C5-C6-O6	-9.21	123.07	128.60
23	AW	5	DG	P-O3'-C3'	9.21	130.75	119.70
79	BQ	26	DC	P-O3'-C3'	9.18	130.72	119.70
1	AA	2092	DC	O4'-C1'-C2'	-9.15	98.58	105.90
1	AA	1333	DA	P-O3'-C3'	9.14	130.67	119.70
6	AF	11	DT	O4'-C1'-C2'	-9.14	98.59	105.90
18	AR	23	DC	O4'-C1'-N1	9.10	114.37	108.00
41	Ao	5	DC	P-O3'-C3'	9.05	130.56	119.70
14	AN	4	DC	P-O3'-C3'	9.03	130.53	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	24	DC	P-O3'-C3'	9.02	130.53	119.70
1	AA	885	DC	C6-N1-C2	-9.00	116.70	120.30
1	AA	1087	DT	P-O3'-C3'	9.00	130.50	119.70
10	AJ	19	DT	P-O3'-C3'	8.99	130.49	119.70
1	AA	2838	DG	P-O3'-C3'	8.98	130.48	119.70
1	AA	723	DC	P-O3'-C3'	8.97	130.47	119.70
51	Ay	27	DT	C6-C5-C7	-8.96	117.52	122.90
1	AA	2491	DC	O4'-C1'-C2'	-8.96	98.73	105.90
47	Au	11	DA	P-O3'-C3'	8.94	130.43	119.70
65	BC	1	DA	O4'-C1'-C2'	-8.93	98.75	105.90
1	AA	2242	DG	O4'-C1'-C2'	-8.93	98.76	105.90
1	AA	210	DC	O4'-C1'-C2'	-8.91	98.77	105.90
22	AV	37	DG	P-O3'-C3'	8.91	130.39	119.70
43	Aq	1	DT	O4'-C1'-C2'	-8.91	98.78	105.90
1	AA	1651	DG	O4'-C1'-C2'	-8.90	98.78	105.90
1	AA	1700	DT	O4'-C4'-C3'	-8.90	100.66	106.00
1	AA	2626	DT	P-O3'-C3'	8.88	130.36	119.70
22	AV	33	DA	O4'-C4'-C3'	-8.87	100.68	106.00
1	AA	2242	DG	P-O3'-C3'	8.87	130.34	119.70
1	AA	795	DC	P-O3'-C3'	8.86	130.34	119.70
1	AA	1960	DC	P-O3'-C3'	8.86	130.34	119.70
1	AA	2673	DG	O4'-C1'-C2'	-8.86	98.81	105.90
72	BJ	1	DT	O4'-C1'-C2'	-8.86	98.81	105.90
1	AA	980	DG	O4'-C4'-C3'	-8.85	100.69	106.00
1	AA	149	DT	O4'-C1'-C2'	-8.85	98.82	105.90
1	AA	2437	DT	P-O3'-C3'	8.80	130.26	119.70
63	BA	10	DC	P-O3'-C3'	8.79	130.24	119.70
1	AA	577	DT	O4'-C4'-C3'	-8.78	100.73	106.00
1	AA	1235	DG	O4'-C4'-C3'	-8.78	100.73	106.00
1	AA	446	DC	P-O3'-C3'	8.77	130.23	119.70
31	Ae	34	DC	O4'-C1'-N1	8.76	114.13	108.00
1	AA	1410	DG	O4'-C1'-C2'	-8.70	98.94	105.90
31	Ae	34	DC	O4'-C1'-C2'	-8.65	98.98	105.90
53	A0	8	DG	O4'-C4'-C3'	-8.65	100.81	106.00
40	An	30	DG	P-O3'-C3'	8.64	130.07	119.70
78	BP	30	DT	O4'-C1'-C2'	-8.64	98.99	105.90
65	BC	6	DC	P-O3'-C3'	8.63	130.06	119.70
1	AA	1970	DG	O4'-C1'-C2'	-8.62	99.00	105.90
68	BF	19	DT	P-O3'-C3'	8.62	130.05	119.70
70	BH	16	DT	P-O3'-C3'	8.59	130.01	119.70
3	AC	46	DA	N1-C6-N6	-8.59	113.45	118.60
1	AA	733	DG	O4'-C1'-C2'	-8.59	99.03	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	31	DG	O4'-C1'-C2'	-8.59	99.03	105.90
1	AA	2779	DG	P-O3'-C3'	8.57	129.98	119.70
1	AA	181	DG	O4'-C4'-C3'	-8.55	100.87	106.00
69	BG	1	DC	O4'-C1'-C2'	-8.55	99.06	105.90
1	AA	647	DC	P-O3'-C3'	8.54	129.95	119.70
1	AA	354	DG	P-O3'-C3'	8.53	129.94	119.70
55	A2	34	DT	O4'-C4'-C3'	-8.53	100.88	106.00
65	BC	14	DG	O4'-C1'-C2'	-8.52	99.08	105.90
1	AA	1377	DC	P-O3'-C3'	8.52	129.92	119.70
10	AJ	11	DT	O4'-C1'-C2'	-8.51	99.09	105.90
1	AA	161	DT	P-O3'-C3'	8.49	129.89	119.70
1	AA	1682	DG	O4'-C4'-C3'	-8.49	100.90	106.00
78	BP	4	DT	O4'-C4'-C3'	-8.49	100.91	106.00
1	AA	1391	DA	O4'-C4'-C3'	-8.49	100.91	106.00
6	AF	37	DG	O4'-C4'-C3'	-8.48	100.91	106.00
9	AI	19	DC	O4'-C1'-C2'	-8.48	99.12	105.90
28	Ab	14	DA	P-O3'-C3'	8.48	129.87	119.70
1	AA	733	DG	O4'-C4'-C3'	-8.46	100.92	106.00
10	AJ	26	DC	O4'-C1'-C2'	-8.46	99.13	105.90
43	Aq	38	DT	P-O3'-C3'	8.45	129.84	119.70
10	AJ	11	DT	P-O3'-C3'	8.45	129.84	119.70
52	Az	30	DG	P-O3'-C3'	8.44	129.83	119.70
1	AA	1441	DG	O4'-C1'-N9	8.44	113.91	108.00
1	AA	1970	DG	O4'-C4'-C3'	-8.44	100.94	106.00
3	AC	41	DA	P-O3'-C3'	8.44	129.82	119.70
13	AM	1	DA	P-O3'-C3'	8.40	129.78	119.70
63	BA	28	DG	O4'-C4'-C3'	-8.39	100.97	106.00
42	Ap	13	DG	P-O3'-C3'	8.37	129.75	119.70
71	BI	7	DA	O4'-C1'-C2'	-8.37	99.21	105.90
1	AA	1730	DG	O4'-C1'-C2'	-8.36	99.22	105.90
1	AA	417	DC	O4'-C1'-C2'	-8.34	99.23	105.90
1	AA	2654	DG	O4'-C1'-C2'	-8.34	99.23	105.90
18	AR	23	DC	C6-N1-C1'	-8.32	110.81	120.80
56	A3	19	DG	P-O3'-C3'	8.32	129.69	119.70
1	AA	2355	DA	O4'-C1'-C2'	-8.31	99.25	105.90
10	AJ	30	DT	O4'-C1'-C2'	-8.29	99.27	105.90
23	AW	9	DG	O4'-C1'-C2'	-8.29	99.27	105.90
1	AA	1804	DA	O4'-C1'-C2'	-8.29	99.27	105.90
78	BP	5	DT	O4'-C4'-C3'	-8.28	101.03	106.00
8	AH	14	DT	P-O3'-C3'	8.22	129.56	119.70
51	Ay	27	DT	C4-C5-C7	8.21	123.93	119.00
14	AN	30	DC	O4'-C1'-C2'	-8.20	99.34	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1751	DC	O4'-C4'-C3'	-8.20	101.08	106.00
67	BE	22	DG	O4'-C1'-C2'	-8.20	99.34	105.90
61	A8	9	DT	O4'-C4'-C3'	-8.19	101.08	106.00
73	BK	6	DG	O4'-C1'-C2'	-8.19	99.35	105.90
1	AA	98	DA	O4'-C1'-C2'	-8.18	99.36	105.90
41	Ao	10	DT	C1'-O4'-C4'	-8.18	101.92	110.10
1	AA	1444	DG	O4'-C4'-C3'	-8.17	101.10	106.00
31	Ae	34	DC	C1'-O4'-C4'	-8.17	101.93	110.10
1	AA	2554	DG	O4'-C1'-C2'	-8.15	99.38	105.90
1	AA	900	DG	O4'-C1'-C2'	-8.14	99.39	105.90
13	AM	1	DA	C1'-O4'-C4'	-8.13	101.97	110.10
13	AM	40	DG	O4'-C1'-C2'	-8.11	99.41	105.90
1	AA	252	DG	O4'-C1'-C2'	-8.11	99.41	105.90
1	AA	2069	DG	C1'-O4'-C4'	-8.11	102.00	110.10
34	Ah	12	DT	O4'-C1'-C2'	-8.11	99.42	105.90
1	AA	2051	DC	O4'-C1'-C2'	-8.10	99.42	105.90
1	AA	1401	DG	O4'-C1'-C2'	-8.09	99.42	105.90
1	AA	2092	DC	O4'-C4'-C3'	-8.09	101.14	106.00
78	BP	5	DT	O4'-C1'-C2'	-8.09	99.43	105.90
1	AA	2434	DC	O4'-C1'-C2'	-8.09	99.43	105.90
1	AA	1614	DG	O4'-C4'-C3'	-8.08	101.15	106.00
34	Ah	14	DT	O4'-C4'-C3'	-8.08	101.15	106.00
1	AA	1605	DA	O4'-C1'-C2'	-8.07	99.44	105.90
1	AA	2090	DG	O4'-C1'-C2'	-8.06	99.45	105.90
1	AA	2382	DT	C1'-O4'-C4'	-8.06	102.04	110.10
1	AA	1441	DG	O4'-C1'-C2'	-8.05	99.46	105.90
1	AA	828	DG	O4'-C1'-C2'	-8.05	99.46	105.90
1	AA	2296	DC	O4'-C4'-C3'	-8.04	101.18	106.00
8	AH	12	DT	C4'-C3'-C2'	-8.04	95.86	103.10
9	AI	19	DC	P-O3'-C3'	8.02	129.32	119.70
22	AV	39	DG	O4'-C1'-C2'	-8.02	99.49	105.90
1	AA	946	DG	O4'-C1'-C2'	-8.01	99.49	105.90
1	AA	659	DC	O4'-C1'-C2'	-8.00	99.50	105.90
32	Af	10	DG	C1'-O4'-C4'	-8.00	102.10	110.10
1	AA	269	DG	O4'-C1'-C2'	-7.99	99.51	105.90
1	AA	1372	DC	O4'-C1'-C2'	-7.98	99.51	105.90
1	AA	1033	DA	C1'-O4'-C4'	-7.98	102.12	110.10
34	Ah	8	DA	P-O3'-C3'	7.98	129.27	119.70
24	AX	33	DG	P-O3'-C3'	7.97	129.27	119.70
3	AC	47	DC	O4'-C1'-C2'	-7.97	99.53	105.90
28	Ab	40	DG	P-O3'-C3'	7.95	129.24	119.70
19	AS	1	DT	O4'-C4'-C3'	-7.94	101.24	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
72	BJ	24	DG	O4'-C1'-C2'	-7.93	99.55	105.90
74	BL	1	DG	O4'-C1'-C2'	-7.92	99.56	105.90
76	BN	1	DT	O4'-C1'-C2'	-7.92	99.56	105.90
22	AV	9	DC	O4'-C1'-C2'	-7.92	99.56	105.90
68	BF	26	DT	P-O3'-C3'	7.92	129.20	119.70
52	Az	34	DC	P-O3'-C3'	7.90	129.19	119.70
1	AA	337	DT	O4'-C1'-C2'	-7.90	99.58	105.90
19	AS	36	DT	O4'-C1'-C2'	-7.90	99.58	105.90
1	AA	454	DA	O4'-C1'-C2'	-7.89	99.58	105.90
1	AA	1605	DA	P-O3'-C3'	7.89	129.17	119.70
1	AA	1238	DG	O4'-C1'-C2'	-7.88	99.59	105.90
1	AA	2006	DC	O4'-C4'-C3'	-7.88	101.27	106.00
1	AA	1779	DC	O4'-C1'-C2'	-7.87	99.61	105.90
1	AA	2511	DG	O4'-C1'-C2'	-7.87	99.61	105.90
18	AR	28	DT	O4'-C1'-C2'	-7.85	99.62	105.90
1	AA	1391	DA	O4'-C1'-C2'	-7.84	99.63	105.90
1	AA	1629	DC	O4'-C1'-C2'	-7.83	99.63	105.90
1	AA	1487	DT	O4'-C4'-C3'	-7.83	101.30	106.00
1	AA	1626	DG	O4'-C1'-C2'	-7.83	99.64	105.90
1	AA	1441	DG	C1'-O4'-C4'	-7.83	102.27	110.10
41	Ao	21	DC	C1'-O4'-C4'	-7.83	102.27	110.10
58	A5	10	DC	O4'-C1'-C2'	-7.82	99.65	105.90
1	AA	589	DG	P-O3'-C3'	7.81	129.07	119.70
1	AA	1158	DT	P-O3'-C3'	7.80	129.06	119.70
1	AA	1370	DC	O4'-C1'-C2'	-7.80	99.66	105.90
1	AA	2285	DC	O4'-C4'-C3'	-7.79	101.33	106.00
1	AA	2444	DG	O4'-C1'-C2'	-7.79	99.67	105.90
1	AA	2341	DC	O4'-C1'-C2'	-7.78	99.67	105.90
31	Ae	34	DC	P-O3'-C3'	7.78	129.04	119.70
1	AA	1659	DT	C1'-O4'-C4'	-7.77	102.33	110.10
29	Ac	29	DA	O4'-C1'-C2'	-7.77	99.68	105.90
42	Ap	8	DG	O4'-C4'-C3'	-7.77	101.34	106.00
66	BD	20	DA	O4'-C1'-C2'	-7.77	99.68	105.90
1	AA	1614	DG	O4'-C1'-C2'	-7.76	99.69	105.90
35	Ai	43	DG	P-O3'-C3'	7.76	129.01	119.70
1	AA	2497	DC	C6-N1-C2	-7.75	117.20	120.30
1	AA	2522	DT	O4'-C4'-C3'	-7.75	101.35	106.00
1	AA	1428	DG	O4'-C1'-C2'	-7.75	99.70	105.90
55	A2	23	DA	O4'-C1'-C2'	-7.75	99.70	105.90
4	AD	22	DA	O4'-C1'-C2'	-7.74	99.71	105.90
1	AA	2781	DA	O4'-C1'-C2'	-7.73	99.71	105.90
46	At	40	DG	O4'-C1'-C2'	-7.73	99.72	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	BC	1	DA	O4'-C4'-C3'	-7.72	101.37	106.00
1	AA	2598	DG	O4'-C4'-C3'	-7.71	101.37	106.00
8	AH	12	DT	O4'-C4'-C3'	-7.71	101.37	106.00
29	Ac	16	DC	P-O3'-C3'	7.70	128.94	119.70
42	Ap	11	DG	N1-C6-O6	7.70	124.52	119.90
1	AA	1480	DC	O4'-C1'-C2'	-7.69	99.75	105.90
1	AA	705	DA	P-O3'-C3'	7.68	128.91	119.70
46	At	13	DG	O4'-C1'-C2'	-7.67	99.76	105.90
1	AA	1397	DT	O4'-C1'-C2'	-7.67	99.77	105.90
8	AH	28	DA	P-O3'-C3'	7.66	128.89	119.70
1	AA	610	DA	O4'-C1'-C2'	-7.66	99.77	105.90
29	Ac	30	DG	O4'-C1'-C2'	-7.65	99.78	105.90
1	AA	1047	DT	O4'-C1'-C2'	-7.64	99.79	105.90
65	BC	4	DG	P-O3'-C3'	7.64	128.87	119.70
7	AG	5	DG	O4'-C1'-C2'	-7.64	99.79	105.90
28	Ab	9	DA	O4'-C1'-C2'	-7.64	99.79	105.90
1	AA	2242	DG	C1'-O4'-C4'	-7.63	102.47	110.10
1	AA	76	DT	C4'-C3'-C2'	-7.63	96.23	103.10
63	BA	8	DC	P-O3'-C3'	7.63	128.85	119.70
1	AA	1659	DT	O4'-C4'-C3'	-7.62	101.42	106.00
1	AA	2495	DA	O4'-C1'-C2'	-7.62	99.80	105.90
59	A6	13	DC	O4'-C1'-C2'	-7.62	99.80	105.90
1	AA	2673	DG	C1'-O4'-C4'	-7.62	102.48	110.10
42	Ap	8	DG	C5-C6-O6	-7.62	124.03	128.60
1	AA	2216	DT	O4'-C1'-C2'	-7.61	99.81	105.90
1	AA	2230	DG	O4'-C1'-C2'	-7.60	99.82	105.90
1	AA	1636	DG	O4'-C1'-C2'	-7.60	99.82	105.90
1	AA	472	DT	O4'-C1'-C2'	-7.60	99.82	105.90
60	A7	22	DC	P-O3'-C3'	7.59	128.81	119.70
49	Aw	35	DG	O4'-C1'-C2'	-7.59	99.83	105.90
1	AA	1372	DC	O4'-C4'-C3'	-7.59	101.45	106.00
1	AA	76	DT	O4'-C4'-C3'	-7.58	101.45	106.00
1	AA	1087	DT	O4'-C1'-C2'	-7.58	99.83	105.90
52	Az	31	DA	P-O3'-C3'	7.58	128.79	119.70
10	AJ	3	DT	C1'-O4'-C4'	-7.57	102.53	110.10
8	AH	22	DT	P-O3'-C3'	7.57	128.78	119.70
19	AS	36	DT	O4'-C4'-C3'	-7.57	101.46	106.00
1	AA	1371	DG	O4'-C1'-C2'	-7.56	99.85	105.90
1	AA	691	DT	C4'-C3'-C2'	-7.56	96.30	103.10
3	AC	29	DC	P-O3'-C3'	7.56	128.77	119.70
25	AY	4	DT	P-O3'-C3'	7.55	128.77	119.70
53	A0	1	DC	O4'-C4'-C3'	-7.55	101.47	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1659	DT	O4'-C1'-C2'	-7.55	99.86	105.90
18	AR	14	DC	O4'-C1'-C2'	-7.55	99.86	105.90
64	BB	43	DT	C4'-C3'-C2'	-7.54	96.31	103.10
27	Aa	1	DT	O4'-C4'-C3'	-7.54	101.47	106.00
1	AA	1454	DG	O4'-C1'-C2'	-7.54	99.87	105.90
1	AA	1487	DT	C4'-C3'-C2'	-7.54	96.32	103.10
1	AA	1064	DG	C1'-O4'-C4'	-7.53	102.57	110.10
1	AA	2374	DA	P-O3'-C3'	7.53	128.73	119.70
1	AA	1238	DG	P-O3'-C3'	7.52	128.73	119.70
1	AA	2673	DG	O4'-C1'-N9	7.52	113.27	108.00
75	BM	30	DG	O4'-C4'-C3'	-7.52	101.49	106.00
17	AQ	28	DT	C1'-O4'-C4'	-7.52	102.58	110.10
10	AJ	1	DT	O4'-C1'-C2'	-7.52	99.89	105.90
1	AA	2223	DG	O4'-C4'-C3'	-7.51	101.49	106.00
1	AA	409	DA	O4'-C1'-N9	7.51	113.26	108.00
1	AA	879	DG	O4'-C1'-C2'	-7.51	99.89	105.90
1	AA	2006	DC	P-O3'-C3'	7.51	128.71	119.70
1	AA	1222	DC	O4'-C1'-C2'	-7.50	99.90	105.90
7	AG	29	DG	O4'-C1'-N9	7.50	113.25	108.00
42	Ap	21	DC	O4'-C1'-C2'	-7.49	99.91	105.90
75	BM	30	DG	O4'-C1'-C2'	-7.48	99.92	105.90
55	A2	34	DT	O4'-C1'-C2'	-7.48	99.92	105.90
1	AA	1058	DC	O4'-C4'-C3'	-7.47	101.51	104.50
1	AA	2583	DG	P-O3'-C3'	7.47	128.67	119.70
1	AA	1723	DC	O4'-C4'-C3'	-7.47	101.51	104.50
1	AA	2220	DT	C4'-C3'-C2'	-7.47	96.38	103.10
76	BN	16	DG	P-O3'-C3'	7.46	128.66	119.70
76	BN	29	DG	O4'-C1'-C2'	-7.46	99.93	105.90
1	AA	2602	DT	O4'-C4'-C3'	-7.46	101.52	104.50
1	AA	3	DG	O4'-C1'-C2'	-7.45	99.94	105.90
1	AA	378	DG	O4'-C4'-C3'	-7.44	101.53	104.50
1	AA	2180	DG	O4'-C1'-C2'	-7.43	99.95	105.90
75	BM	13	DG	O4'-C1'-C2'	-7.42	99.96	105.90
19	AS	1	DT	P-O3'-C3'	-7.42	110.80	119.70
69	BG	19	DA	C1'-O4'-C4'	-7.41	102.69	110.10
46	At	46	DG	P-O3'-C3'	7.41	128.59	119.70
16	AP	9	DG	O4'-C1'-C2'	-7.41	99.97	105.90
37	Ak	52	DC	O4'-C1'-C2'	-7.41	99.98	105.90
70	BH	16	DT	O4'-C1'-C2'	-7.41	99.97	105.90
1	AA	1836	DG	C1'-O4'-C4'	-7.40	102.70	110.10
28	Ab	40	DG	O4'-C1'-C2'	-7.39	99.98	105.90
78	BP	6	DC	O4'-C1'-C2'	-7.39	99.99	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Aw	4	DG	O4'-C1'-C2'	-7.38	99.99	105.90
35	Ai	43	DG	O4'-C1'-C2'	-7.38	100.00	105.90
72	BJ	2	DT	P-O3'-C3'	7.38	128.55	119.70
7	AG	24	DT	O4'-C4'-C3'	-7.38	101.55	104.50
77	BO	30	DA	O4'-C1'-C2'	-7.38	100.00	105.90
1	AA	1518	DA	P-O3'-C3'	7.37	128.55	119.70
68	BF	20	DG	O4'-C1'-C2'	-7.37	100.00	105.90
1	AA	1186	DT	P-O3'-C3'	7.37	128.54	119.70
68	BF	10	DG	O4'-C1'-C2'	-7.37	100.01	105.90
1	AA	561	DG	O4'-C1'-C2'	-7.37	100.01	105.90
58	A5	28	DT	O4'-C1'-C2'	-7.37	100.01	105.90
1	AA	2341	DC	O4'-C4'-C3'	-7.36	101.56	104.50
1	AA	1238	DG	C1'-O4'-C4'	-7.35	102.75	110.10
1	AA	55	DT	O4'-C4'-C3'	-7.35	101.56	104.50
1	AA	2263	DC	P-O3'-C3'	7.34	128.51	119.70
15	AO	1	DC	O4'-C1'-C2'	-7.34	100.02	105.90
1	AA	2199	DG	O4'-C1'-C2'	-7.34	100.03	105.90
34	Ah	30	DT	O4'-C4'-C3'	-7.34	101.56	104.50
14	AN	30	DC	O4'-C4'-C3'	-7.34	101.56	104.50
62	A9	16	DC	P-O3'-C3'	7.33	128.50	119.70
7	AG	17	DG	O4'-C1'-C2'	-7.33	100.04	105.90
1	AA	3	DG	P-O3'-C3'	7.31	128.47	119.70
1	AA	55	DT	C4'-C3'-C2'	-7.29	96.54	103.10
1	AA	2795	DG	P-O3'-C3'	7.29	128.45	119.70
55	A2	34	DT	C1'-O4'-C4'	-7.29	102.81	110.10
9	AI	19	DC	C1'-O4'-C4'	-7.29	102.81	110.10
1	AA	2301	DG	C4'-C3'-C2'	-7.28	96.55	103.10
15	AO	44	DG	P-O3'-C3'	7.27	128.43	119.70
1	AA	1963	DG	O4'-C1'-C2'	-7.27	100.09	105.90
1	AA	2592	DT	C4'-C3'-C2'	-7.26	96.56	103.10
1	AA	2069	DG	O4'-C4'-C3'	-7.24	101.61	104.50
56	A3	8	DT	C1'-O4'-C4'	-7.24	102.86	110.10
61	A8	9	DT	C4'-C3'-C2'	-7.23	96.59	103.10
1	AA	1481	DG	C1'-O4'-C4'	-7.22	102.88	110.10
1	AA	2488	DG	O4'-C1'-C2'	-7.22	100.12	105.90
72	BJ	26	DC	O4'-C1'-C2'	-7.22	100.12	105.90
1	AA	132	DA	P-O3'-C3'	7.22	128.36	119.70
1	AA	2835	DA	P-O3'-C3'	7.22	128.36	119.70
3	AC	40	DT	C4'-C3'-C2'	-7.21	96.61	103.10
1	AA	2069	DG	O4'-C1'-N9	7.21	113.04	108.00
43	Aq	26	DC	O4'-C1'-C2'	-7.20	100.14	105.90
1	AA	980	DG	C4'-C3'-C2'	-7.20	96.62	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1621	DC	O4'-C4'-C3'	-7.20	101.62	104.50
8	AH	8	DG	C4'-C3'-C2'	-7.20	96.62	103.10
1	AA	462	DA	P-O3'-C3'	7.19	128.33	119.70
1	AA	1166	DT	C4'-C3'-C2'	-7.19	96.63	103.10
1	AA	2491	DC	O4'-C4'-C3'	-7.18	101.63	104.50
1	AA	2301	DG	O4'-C4'-C3'	-7.18	101.63	104.50
38	Al	9	DC	O4'-C1'-N1	7.18	113.03	108.00
1	AA	2179	DG	O4'-C1'-C2'	-7.18	100.16	105.90
1	AA	247	DC	O4'-C4'-C3'	-7.17	101.63	104.50
1	AA	715	DT	C4'-C3'-C2'	-7.17	96.65	103.10
43	Aq	17	DG	O4'-C1'-C2'	-7.16	100.17	105.90
1	AA	1444	DG	O4'-C1'-C2'	-7.16	100.17	105.90
3	AC	21	DT	O4'-C1'-C2'	-7.15	100.18	105.90
6	AF	11	DT	O4'-C4'-C3'	-7.15	101.64	104.50
1	AA	1521	DT	P-O3'-C3'	7.15	128.28	119.70
69	BG	19	DA	O4'-C4'-C3'	-7.15	101.64	104.50
1	AA	1484	DG	O4'-C1'-C2'	-7.15	100.18	105.90
59	A6	19	DG	O4'-C1'-C2'	-7.13	100.19	105.90
78	BP	30	DT	P-O3'-C3'	7.13	128.26	119.70
27	Aa	37	DA	C4'-C3'-C2'	-7.12	96.69	103.10
74	BL	1	DG	C1'-O4'-C4'	-7.12	102.98	110.10
1	AA	1922	DA	O4'-C1'-C2'	-7.10	100.22	105.90
1	AA	541	DC	O4'-C1'-C2'	-7.10	100.22	105.90
1	AA	1945	DA	P-O3'-C3'	7.08	128.20	119.70
28	Ab	16	DC	O4'-C4'-C3'	-7.08	101.67	104.50
39	Am	12	DC	C2-N1-C1'	7.08	126.59	118.80
1	AA	2526	DT	C4'-C3'-C2'	-7.08	96.73	103.10
1	AA	1430	DG	O4'-C1'-C2'	-7.06	100.25	105.90
1	AA	2318	DC	O4'-C1'-C2'	-7.06	100.25	105.90
7	AG	24	DT	C4'-C3'-C2'	-7.06	96.75	103.10
59	A6	23	DG	O4'-C1'-C2'	-7.06	100.25	105.90
1	AA	2164	DA	P-O3'-C3'	7.06	128.17	119.70
1	AA	1804	DA	O4'-C4'-C3'	-7.05	101.68	104.50
1	AA	2728	DA	O4'-C1'-C2'	-7.05	100.26	105.90
44	Ar	37	DA	P-O3'-C3'	7.05	128.16	119.70
1	AA	653	DG	C4'-C3'-C2'	-7.05	96.76	103.10
28	Ab	42	DG	O4'-C1'-C2'	-7.05	100.26	105.90
1	AA	1898	DG	O4'-C4'-C3'	-7.05	101.68	104.50
1	AA	2136	DG	O4'-C1'-C2'	-7.05	100.26	105.90
1	AA	2786	DG	C4'-C3'-C2'	-7.05	96.76	103.10
1	AA	1481	DG	O4'-C1'-C2'	-7.04	100.27	105.90
1	AA	547	DT	O4'-C1'-C2'	-7.04	100.27	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2189	DT	O4'-C4'-C3'	-7.04	101.68	104.50
54	A1	3	DG	O4'-C1'-C2'	-7.04	100.27	105.90
32	Af	5	DA	O4'-C1'-C2'	-7.03	100.28	105.90
1	AA	2672	DG	O4'-C1'-C2'	-7.02	100.28	105.90
51	Ay	39	DG	O4'-C1'-C2'	-7.01	100.29	105.90
1	AA	1793	DG	C4'-C3'-C2'	-7.00	96.80	103.10
45	As	24	DC	P-O3'-C3'	6.99	128.09	119.70
72	BJ	20	DT	O4'-C1'-C2'	-6.99	100.31	105.90
1	AA	145	DT	C4'-C3'-C2'	-6.99	96.81	103.10
6	AF	37	DG	C4'-C3'-C2'	-6.99	96.81	103.10
75	BM	23	DC	O4'-C1'-C2'	-6.99	100.31	105.90
10	AJ	26	DC	O4'-C1'-N1	6.99	112.89	108.00
1	AA	1629	DC	O4'-C1'-N1	6.98	112.89	108.00
1	AA	1148	DC	P-O3'-C3'	6.98	128.08	119.70
1	AA	121	DG	O4'-C1'-C2'	-6.98	100.32	105.90
1	AA	409	DA	O4'-C1'-C2'	-6.98	100.32	105.90
54	A1	26	DG	O4'-C1'-C2'	-6.97	100.32	105.90
1	AA	589	DG	O4'-C1'-C2'	-6.97	100.32	105.90
1	AA	181	DG	C4'-C3'-C2'	-6.96	96.83	103.10
1	AA	1073	DT	C4'-C3'-C2'	-6.96	96.84	103.10
79	BQ	36	DG	O4'-C1'-C2'	-6.96	100.33	105.90
28	Ab	37	DT	O4'-C1'-C2'	-6.96	100.33	105.90
1	AA	1904	DC	O4'-C1'-C2'	-6.96	100.33	105.90
1	AA	2585	DG	P-O3'-C3'	6.96	128.05	119.70
45	As	34	DG	O4'-C1'-C2'	-6.96	100.33	105.90
1	AA	361	DT	C4'-C3'-C2'	-6.96	96.84	103.10
1	AA	1851	DA	P-O3'-C3'	6.95	128.04	119.70
1	AA	852	DG	P-O3'-C3'	6.95	128.03	119.70
1	AA	487	DT	O4'-C4'-C3'	-6.94	101.72	104.50
59	A6	25	DG	O4'-C1'-C2'	-6.94	100.35	105.90
75	BM	36	DT	O4'-C1'-C2'	-6.94	100.35	105.90
1	AA	161	DT	C4'-C3'-C2'	-6.94	96.86	103.10
1	AA	998	DC	C4'-C3'-C2'	-6.94	96.86	103.10
1	AA	70	DA	O4'-C1'-C2'	-6.93	100.35	105.90
39	Am	25	DG	P-O3'-C3'	6.93	128.02	119.70
2	AB	7	DA	O4'-C1'-C2'	-6.92	100.36	105.90
27	Aa	1	DT	O4'-C1'-C2'	-6.92	100.36	105.90
1	AA	2561	DT	C4-C5-C7	-6.92	114.85	119.00
64	BB	9	DA	O4'-C1'-C2'	-6.92	100.36	105.90
29	Ac	41	DC	P-O3'-C3'	6.92	128.00	119.70
46	At	40	DG	P-O3'-C3'	6.92	128.00	119.70
13	AM	11	DG	P-O3'-C3'	6.91	127.99	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1614	DG	C1'-O4'-C4'	-6.91	103.19	110.10
1	AA	2114	DG	O4'-C1'-C2'	-6.91	100.37	105.90
1	AA	1339	DT	C4'-C3'-C2'	-6.91	96.88	103.10
1	AA	1555	DG	O4'-C1'-C2'	-6.90	100.38	105.90
43	Aq	34	DA	O4'-C1'-C2'	-6.90	100.38	105.90
1	AA	2665	DG	O4'-C1'-C2'	-6.89	100.39	105.90
1	AA	2673	DG	O4'-C4'-C3'	-6.89	101.75	104.50
1	AA	1628	DG	O4'-C1'-C2'	-6.89	100.39	105.90
45	As	13	DC	P-O3'-C3'	6.89	127.96	119.70
39	Am	31	DG	C1'-O4'-C4'	-6.88	103.22	110.10
39	Am	12	DC	O4'-C1'-N1	6.88	112.82	108.00
56	A3	19	DG	O4'-C1'-N9	6.88	112.81	108.00
26	AZ	12	DT	C4'-C3'-C2'	-6.87	96.92	103.10
68	BF	33	DC	O4'-C1'-C2'	-6.87	100.40	105.90
28	Ab	31	DG	C4'-C3'-C2'	-6.87	96.92	103.10
35	Ai	1	DA	C4'-C3'-C2'	-6.87	96.92	103.10
1	AA	2532	DG	O4'-C1'-N9	6.87	112.81	108.00
4	AD	22	DA	O4'-C4'-C3'	-6.86	101.75	104.50
47	Au	33	DC	O4'-C1'-C2'	-6.86	100.41	105.90
61	A8	16	DA	C4'-C3'-C2'	-6.86	96.93	103.10
1	AA	1888	DG	O4'-C1'-C2'	-6.86	100.42	105.90
19	AS	24	DA	O4'-C1'-C2'	-6.86	100.42	105.90
50	Ax	9	DG	O4'-C1'-C2'	-6.86	100.42	105.90
1	AA	1678	DT	O4'-C1'-C2'	-6.85	100.42	105.90
1	AA	639	DA	C4'-C3'-C2'	-6.84	96.94	103.10
1	AA	1941	DC	O4'-C4'-C3'	-6.84	101.76	104.50
1	AA	2728	DA	O4'-C1'-N9	6.84	112.79	108.00
1	AA	657	DG	P-O3'-C3'	6.84	127.90	119.70
69	BG	23	DG	O4'-C1'-C2'	-6.83	100.44	105.90
1	AA	1779	DC	C1'-O4'-C4'	-6.82	103.28	110.10
1	AA	2199	DG	O4'-C1'-N9	6.82	112.78	108.00
1	AA	966	DG	C4'-C3'-C2'	-6.82	96.96	103.10
1	AA	1086	DA	N1-C6-N6	-6.81	114.51	118.60
28	Ab	34	DT	C1'-O4'-C4'	-6.81	103.29	110.10
61	A8	16	DA	O4'-C4'-C3'	-6.81	101.78	104.50
1	AA	487	DT	C4'-C3'-C2'	-6.80	96.98	103.10
56	A3	19	DG	C1'-O4'-C4'	-6.80	103.30	110.10
16	AP	20	DT	C4'-C3'-C2'	-6.80	96.98	103.10
1	AA	965	DT	C4'-C3'-C2'	-6.80	96.98	103.10
1	AA	1201	DC	P-O3'-C3'	6.79	127.85	119.70
28	Ab	16	DC	C4'-C3'-C2'	-6.79	96.99	103.10
1	AA	288	DA	O4'-C1'-C2'	-6.79	100.47	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2427	DA	O4'-C1'-N9	6.79	112.75	108.00
1	AA	378	DG	O4'-C1'-C2'	-6.78	100.47	105.90
1	AA	2646	DC	O4'-C1'-C2'	-6.78	100.48	105.90
1	AA	1061	DG	O4'-C1'-C2'	-6.78	100.48	105.90
78	BP	29	DA	O4'-C1'-C2'	-6.78	100.48	105.90
1	AA	2294	DC	C4'-C3'-C2'	-6.77	97.00	103.10
31	Ae	33	DA	O4'-C1'-C2'	-6.77	100.49	105.90
53	A0	30	DT	C4'-C3'-C2'	-6.76	97.01	103.10
1	AA	1220	DA	O4'-C1'-C2'	-6.76	100.49	105.90
34	Ah	14	DT	C4'-C3'-C2'	-6.76	97.02	103.10
42	Ap	5	DT	C1'-O4'-C4'	-6.75	103.35	110.10
58	A5	10	DC	C1'-O4'-C4'	-6.75	103.35	110.10
37	Ak	16	DG	O4'-C1'-C2'	-6.75	100.50	105.90
1	AA	1516	DC	O4'-C1'-C2'	-6.75	100.50	105.90
1	AA	1444	DG	C1'-O4'-C4'	-6.75	103.35	110.10
1	AA	218	DA	O4'-C1'-C2'	-6.74	100.51	105.90
1	AA	163	DC	O4'-C1'-C2'	-6.74	100.51	105.90
1	AA	1560	DA	O4'-C1'-C2'	-6.73	100.51	105.90
1	AA	1073	DT	O4'-C4'-C3'	-6.73	101.81	104.50
1	AA	1097	DC	O4'-C1'-C2'	-6.72	100.52	105.90
1	AA	1688	DC	O4'-C1'-C2'	-6.72	100.53	105.90
1	AA	1799	DT	C4'-C3'-C2'	-6.72	97.06	103.10
56	A3	19	DG	O4'-C1'-C2'	-6.71	100.53	105.90
1	AA	2189	DT	C4'-C3'-C2'	-6.71	97.06	103.10
38	Al	18	DG	C5-C6-O6	-6.71	124.57	128.60
1	AA	522	DG	O4'-C4'-C3'	-6.71	101.82	104.50
1	AA	372	DA	O4'-C1'-C2'	-6.71	100.53	105.90
8	AH	14	DT	O4'-C1'-C2'	-6.71	100.54	105.90
1	AA	1813	DT	O4'-C1'-C2'	-6.70	100.54	105.90
52	Az	29	DG	O4'-C1'-C2'	-6.69	100.54	105.90
28	Ab	18	DG	O4'-C1'-C2'	-6.69	100.55	105.90
12	AL	31	DA	C4'-C3'-C2'	-6.69	97.08	103.10
1	AA	1079	DT	O4'-C1'-C2'	-6.69	100.55	105.90
18	AR	23	DC	O4'-C1'-C2'	-6.69	100.55	105.90
1	AA	1053	DA	O4'-C1'-C2'	-6.68	100.55	105.90
5	AE	16	DA	P-O3'-C3'	6.68	127.72	119.70
34	Ah	19	DT	O4'-C1'-C2'	-6.68	100.55	105.90
54	A1	6	DG	O4'-C1'-C2'	-6.68	100.55	105.90
1	AA	623	DG	O4'-C1'-C2'	-6.68	100.56	105.90
1	AA	1644	DC	P-O5'-C5'	6.67	131.58	120.90
53	A0	30	DT	O4'-C4'-C3'	-6.67	101.83	104.50
1	AA	828	DG	C1'-O4'-C4'	-6.67	103.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1906	DA	O4'-C1'-C2'	-6.67	100.57	105.90
1	AA	2598	DG	C4'-C3'-C2'	-6.66	97.10	103.10
1	AA	1175	DT	C4'-C3'-C2'	-6.66	97.11	103.10
1	AA	1621	DC	C4'-C3'-C2'	-6.66	97.11	103.10
26	AZ	13	DC	P-O3'-C3'	6.66	127.69	119.70
1	AA	1248	DC	P-O3'-C3'	6.66	127.69	119.70
65	BC	6	DC	C4'-C3'-C2'	-6.66	97.11	103.10
1	AA	415	DC	P-O3'-C3'	6.65	127.68	119.70
1	AA	1235	DG	C4'-C3'-C2'	-6.65	97.12	103.10
79	BQ	26	DC	O4'-C1'-C2'	-6.65	100.58	105.90
13	AM	5	DC	P-O3'-C3'	6.65	127.67	119.70
15	AO	1	DC	O4'-C4'-C3'	-6.65	101.84	104.50
3	AC	1	DT	O4'-C4'-C3'	-6.64	101.84	104.50
9	AI	14	DG	O4'-C1'-C2'	-6.64	100.59	105.90
26	AZ	27	DA	P-O3'-C3'	6.64	127.66	119.70
8	AH	37	DC	O4'-C1'-C2'	-6.63	100.59	105.90
1	AA	2602	DT	C4'-C3'-C2'	-6.63	97.13	103.10
74	BL	23	DT	P-O3'-C3'	6.63	127.66	119.70
1	AA	1682	DG	C4'-C3'-C2'	-6.63	97.13	103.10
1	AA	1925	DG	O4'-C1'-C2'	-6.62	100.60	105.90
48	Av	16	DC	O4'-C1'-C2'	-6.62	100.60	105.90
69	BG	18	DG	O4'-C1'-C2'	-6.62	100.60	105.90
33	Ag	1	DT	C4'-C3'-C2'	-6.62	97.14	103.10
1	AA	1295	DA	P-O3'-C3'	6.62	127.64	119.70
1	AA	2654	DG	O4'-C1'-N9	6.62	112.63	108.00
8	AH	1	DA	O4'-C1'-C2'	-6.62	100.61	105.90
32	Af	30	DT	O4'-C1'-C2'	-6.61	100.61	105.90
1	AA	2406	DG	O4'-C1'-C2'	-6.61	100.61	105.90
12	AL	26	DG	O4'-C1'-C2'	-6.61	100.61	105.90
1	AA	885	DC	O4'-C1'-C2'	-6.61	100.61	105.90
72	BJ	1	DT	O4'-C4'-C3'	-6.61	101.86	104.50
1	AA	22	DT	O4'-C4'-C3'	-6.61	101.86	104.50
1	AA	653	DG	O4'-C4'-C3'	-6.61	101.86	104.50
25	AY	5	DT	O4'-C4'-C3'	-6.61	101.86	104.50
50	Ax	18	DA	N1-C6-N6	-6.61	114.64	118.60
76	BN	37	DC	O4'-C1'-C2'	-6.61	100.61	105.90
18	AR	9	DC	O4'-C1'-C2'	-6.60	100.62	105.90
42	Ap	8	DG	C4'-C3'-C2'	-6.60	97.16	103.10
1	AA	591	DG	O4'-C1'-C2'	-6.59	100.62	105.90
42	Ap	13	DG	C1'-O4'-C4'	-6.59	103.51	110.10
52	Az	26	DA	C4'-C3'-C2'	-6.59	97.17	103.10
1	AA	2492	DC	P-O5'-C5'	6.59	131.44	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
61	A8	33	DA	O4'-C1'-C2'	-6.59	100.63	105.90
1	AA	754	DT	O4'-C4'-C3'	-6.58	101.87	104.50
1	AA	2634	DG	P-O3'-C3'	6.58	127.60	119.70
1	AA	479	DA	O4'-C1'-C2'	-6.58	100.63	105.90
22	AV	9	DC	O4'-C4'-C3'	-6.58	101.87	104.50
71	BI	35	DC	P-O3'-C3'	6.58	127.60	119.70
68	BF	17	DT	C4'-C3'-C2'	-6.57	97.19	103.10
1	AA	715	DT	O4'-C4'-C3'	-6.56	101.88	104.50
1	AA	1152	DG	O4'-C1'-C2'	-6.56	100.65	105.90
4	AD	22	DA	C1'-O4'-C4'	-6.56	103.54	110.10
49	Aw	4	DG	P-O3'-C3'	6.56	127.57	119.70
1	AA	22	DT	O4'-C1'-C2'	-6.56	100.65	105.90
1	AA	2684	DT	C4'-C3'-C2'	-6.56	97.20	103.10
1	AA	2771	DT	O4'-C1'-C2'	-6.55	100.66	105.90
1	AA	1295	DA	O4'-C1'-C2'	-6.55	100.66	105.90
68	BF	24	DG	O4'-C1'-C2'	-6.55	100.66	105.90
1	AA	316	DG	O4'-C1'-C2'	-6.55	100.66	105.90
1	AA	2199	DG	C1'-O4'-C4'	-6.53	103.57	110.10
34	Ah	34	DT	O4'-C1'-C2'	-6.53	100.67	105.90
15	AO	2	DA	P-O3'-C3'	6.53	127.54	119.70
1	AA	900	DG	O4'-C4'-C3'	-6.53	101.89	104.50
74	BL	18	DG	C1'-O4'-C4'	-6.53	103.57	110.10
79	BQ	18	DT	O4'-C4'-C3'	-6.53	101.89	104.50
49	Aw	35	DG	O4'-C4'-C3'	-6.53	101.89	104.50
1	AA	2619	DA	P-O3'-C3'	6.52	127.53	119.70
1	AA	68	DG	C1'-O4'-C4'	-6.52	103.58	110.10
63	BA	31	DC	P-O3'-C3'	6.52	127.52	119.70
24	AX	20	DG	O4'-C1'-C2'	-6.51	100.69	105.90
1	AA	975	DA	P-O3'-C3'	6.51	127.51	119.70
1	AA	2769	DG	P-O3'-C3'	6.51	127.52	119.70
1	AA	2280	DC	O4'-C1'-C2'	-6.50	100.70	105.90
1	AA	2532	DG	O4'-C1'-C2'	-6.50	100.70	105.90
8	AH	23	DT	P-O3'-C3'	6.50	127.50	119.70
19	AS	31	DA	O4'-C1'-C2'	-6.50	100.70	105.90
1	AA	2420	DG	O4'-C4'-C3'	-6.49	101.90	104.50
68	BF	20	DG	P-O3'-C3'	6.48	127.48	119.70
1	AA	210	DC	C1'-O4'-C4'	-6.48	103.62	110.10
1	AA	754	DT	C4'-C3'-C2'	-6.48	97.27	103.10
1	AA	359	DG	C1'-O4'-C4'	-6.48	103.62	110.10
1	AA	2355	DA	O4'-C4'-C3'	-6.48	101.91	104.50
26	AZ	41	DT	O4'-C4'-C3'	-6.47	101.91	104.50
1	AA	1714	DT	C4'-C3'-C2'	-6.46	97.28	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	BI	7	DA	C1'-O4'-C4'	-6.46	103.64	110.10
75	BM	30	DG	P-O3'-C3'	6.46	127.45	119.70
1	AA	1401	DG	P-O3'-C3'	6.46	127.45	119.70
4	AD	1	DT	O4'-C1'-C2'	-6.46	100.73	105.90
1	AA	65	DT	O4'-C1'-C2'	-6.45	100.74	105.90
1	AA	845	DG	C1'-O4'-C4'	-6.45	103.65	110.10
37	Ak	16	DG	C1'-O4'-C4'	-6.45	103.65	110.10
1	AA	894	DA	O4'-C1'-C2'	-6.45	100.74	105.90
1	AA	1970	DG	C1'-O4'-C4'	-6.45	103.65	110.10
14	AN	9	DA	O4'-C1'-C2'	-6.45	100.74	105.90
1	AA	2285	DC	O4'-C1'-C2'	-6.45	100.74	105.90
1	AA	2223	DG	C4'-C3'-C2'	-6.44	97.30	103.10
5	AE	1	DT	C1'-O4'-C4'	-6.44	103.66	110.10
1	AA	923	DG	O4'-C1'-C2'	-6.44	100.75	105.90
19	AS	16	DT	C4'-C3'-C2'	-6.44	97.30	103.10
22	AV	19	DC	P-O3'-C3'	6.44	127.43	119.70
44	Ar	47	DG	C5-C6-O6	-6.43	124.74	128.60
22	AV	33	DA	C1'-O4'-C4'	-6.43	103.67	110.10
46	At	26	DA	O4'-C1'-C2'	-6.43	100.76	105.90
69	BG	30	DT	C4'-C3'-C2'	-6.43	97.31	103.10
4	AD	29	DA	O4'-C1'-C2'	-6.43	100.76	105.90
73	BK	6	DG	O4'-C4'-C3'	-6.42	101.93	104.50
1	AA	946	DG	C1'-O4'-C4'	-6.42	103.68	110.10
7	AG	10	DG	O4'-C1'-C2'	-6.42	100.77	105.90
1	AA	1851	DA	O4'-C1'-C2'	-6.42	100.77	105.90
1	AA	2212	DA	P-O3'-C3'	6.42	127.40	119.70
1	AA	1265	DG	P-O3'-C3'	6.41	127.40	119.70
1	AA	247	DC	C4'-C3'-C2'	-6.41	97.33	103.10
44	Ar	23	DA	C1'-O4'-C4'	-6.41	103.69	110.10
1	AA	1133	DC	O4'-C1'-C2'	-6.41	100.78	105.90
1	AA	2541	DG	P-O3'-C3'	6.41	127.39	119.70
51	Ay	9	DA	O4'-C1'-C2'	-6.41	100.78	105.90
1	AA	139	DA	N1-C6-N6	-6.40	114.76	118.60
5	AE	20	DA	O4'-C1'-N9	-6.40	103.52	108.00
32	Af	32	DT	C4'-C3'-C2'	-6.40	97.34	103.10
1	AA	298	DG	O4'-C1'-C2'	-6.40	100.78	105.90
1	AA	404	DC	O4'-C1'-C2'	-6.40	100.78	105.90
26	AZ	9	DC	O4'-C1'-C2'	-6.40	100.78	105.90
1	AA	396	DG	O4'-C1'-C2'	-6.39	100.78	105.90
44	Ar	7	DC	O4'-C1'-C2'	-6.39	100.78	105.90
23	AW	16	DT	O4'-C4'-C3'	-6.39	101.94	104.50
1	AA	468	DG	O4'-C1'-C2'	-6.39	100.79	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1409	DC	P-O3'-C3'	6.39	127.37	119.70
12	AL	20	DT	C4'-C3'-C2'	-6.39	97.35	103.10
62	A9	40	DG	N1-C6-O6	6.38	123.73	119.90
1	AA	2443	DC	P-O3'-C3'	6.38	127.36	119.70
1	AA	2657	DA	C4'-C3'-C2'	-6.38	97.36	103.10
42	Ap	14	DA	O4'-C1'-C2'	-6.38	100.80	105.90
72	BJ	17	DG	O4'-C1'-C2'	-6.38	100.80	105.90
1	AA	454	DA	C1'-O4'-C4'	-6.37	103.73	110.10
13	AM	40	DG	C1'-O4'-C4'	-6.37	103.73	110.10
1	AA	531	DT	P-O3'-C3'	6.37	127.34	119.70
1	AA	1910	DA	O4'-C1'-C2'	-6.37	100.80	105.90
49	Aw	35	DG	C1'-O4'-C4'	-6.37	103.73	110.10
1	AA	2504	DT	P-O3'-C3'	6.37	127.34	119.70
1	AA	1195	DT	C4'-C3'-C2'	-6.36	97.38	103.10
32	Af	30	DT	C1'-O4'-C4'	-6.36	103.74	110.10
1	AA	1538	DC	O4'-C4'-C3'	-6.36	101.96	104.50
1	AA	1826	DC	C6-N1-C2	-6.36	117.76	120.30
1	AA	705	DA	O4'-C1'-C2'	-6.35	100.82	105.90
1	AA	989	DA	O4'-C1'-C2'	-6.35	100.82	105.90
1	AA	1784	DC	C6-N1-C2	-6.34	117.76	120.30
1	AA	2199	DG	P-O3'-C3'	6.34	127.31	119.70
58	A5	28	DT	P-O3'-C3'	6.33	127.30	119.70
61	A8	20	DT	C4'-C3'-C2'	-6.33	97.40	103.10
1	AA	1286	DA	P-O3'-C3'	6.33	127.30	119.70
15	AO	41	DG	N1-C6-O6	6.33	123.70	119.90
65	BC	6	DC	O4'-C4'-C3'	-6.33	101.97	104.50
1	AA	1898	DG	C4'-C3'-C2'	-6.33	97.41	103.10
1	AA	2090	DG	C5-C6-O6	-6.32	124.81	128.60
71	BI	10	DG	O4'-C1'-C2'	-6.32	100.84	105.90
1	AA	1818	DG	O4'-C1'-C2'	-6.32	100.84	105.90
41	Ao	10	DT	P-O3'-C3'	6.32	127.28	119.70
54	A1	17	DA	O4'-C1'-C2'	-6.32	100.85	105.90
1	AA	881	DT	C1'-O4'-C4'	-6.31	103.79	110.10
3	AC	10	DC	P-O3'-C3'	6.31	127.28	119.70
1	AA	2296	DC	O4'-C1'-C2'	-6.31	100.85	105.90
1	AA	2340	DG	O4'-C1'-C2'	-6.31	100.85	105.90
1	AA	779	DA	O4'-C1'-C2'	-6.31	100.85	105.90
60	A7	8	DG	O4'-C1'-C2'	-6.31	100.85	105.90
1	AA	123	DA	P-O3'-C3'	6.30	127.27	119.70
1	AA	918	DA	O4'-C1'-C2'	-6.30	100.86	105.90
1	AA	2791	DT	C4'-C3'-C2'	-6.30	97.43	103.10
68	BF	22	DC	P-O3'-C3'	6.30	127.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2479	DC	P-O3'-C3'	6.30	127.26	119.70
1	AA	1624	DG	P-O3'-C3'	6.30	127.26	119.70
1	AA	15	DG	O4'-C1'-C2'	-6.29	100.86	105.90
10	AJ	3	DT	O4'-C1'-C2'	-6.29	100.87	105.90
41	Ao	21	DC	O4'-C1'-N1	6.29	112.41	108.00
1	AA	1947	DC	P-O3'-C3'	6.28	127.23	119.70
5	AE	29	DA	P-O3'-C3'	6.28	127.24	119.70
1	AA	1305	DG	O4'-C1'-C2'	-6.28	100.88	105.90
16	AP	9	DG	C1'-O4'-C4'	-6.28	103.82	110.10
1	AA	511	DG	O4'-C1'-C2'	-6.28	100.88	105.90
27	Aa	30	DT	O4'-C1'-C2'	-6.28	100.88	105.90
43	Aq	1	DT	C1'-O4'-C4'	-6.28	103.83	110.10
27	Aa	41	DT	O4'-C4'-C3'	-6.27	101.99	104.50
1	AA	2280	DC	O4'-C1'-N1	6.27	112.39	108.00
19	AS	12	DG	C4'-C3'-C2'	-6.27	97.46	103.10
10	AJ	19	DT	O4'-C1'-C2'	-6.26	100.89	105.90
1	AA	1430	DG	P-O3'-C3'	6.26	127.22	119.70
1	AA	435	DT	P-O3'-C3'	6.26	127.22	119.70
1	AA	1203	DA	N1-C6-N6	-6.26	114.84	118.60
1	AA	2285	DC	C1'-O4'-C4'	-6.25	103.84	110.10
79	BQ	18	DT	C4'-C3'-C2'	-6.25	97.47	103.10
1	AA	1994	DC	O4'-C1'-C2'	-6.25	100.90	105.90
1	AA	433	DA	P-O3'-C3'	6.24	127.18	119.70
63	BA	22	DA	O4'-C1'-C2'	-6.24	100.91	105.90
40	An	14	DG	O4'-C4'-C3'	-6.24	102.01	104.50
1	AA	2822	DT	C4'-C3'-C2'	-6.23	97.49	103.10
38	Al	18	DG	N1-C6-O6	6.23	123.64	119.90
1	AA	1671	DA	O4'-C1'-C2'	-6.23	100.92	105.90
45	As	16	DA	P-O3'-C3'	6.23	127.18	119.70
76	BN	12	DT	C4'-C3'-C2'	-6.23	97.49	103.10
1	AA	1150	DA	P-O3'-C3'	6.23	127.17	119.70
1	AA	2026	DG	O4'-C1'-C2'	-6.23	100.92	105.90
1	AA	2461	DC	O4'-C1'-C2'	-6.23	100.92	105.90
42	Ap	25	DT	P-O3'-C3'	6.22	127.17	119.70
1	AA	2491	DC	C1'-O4'-C4'	-6.22	103.88	110.10
70	BH	16	DT	C1'-O4'-C4'	-6.22	103.88	110.10
1	AA	1540	DT	C1'-O4'-C4'	-6.22	103.88	110.10
42	Ap	8	DG	N1-C6-O6	6.22	123.63	119.90
71	BI	30	DA	C4'-C3'-C2'	-6.22	97.50	103.10
44	Ar	47	DG	N1-C6-O6	6.22	123.63	119.90
9	AI	23	DC	O4'-C1'-C2'	-6.21	100.93	105.90
1	AA	2393	DG	C4'-C3'-C2'	-6.21	97.51	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2242	DG	O4'-C4'-C3'	-6.21	102.02	104.50
1	AA	980	DG	N1-C6-O6	6.21	123.62	119.90
1	AA	2318	DC	C1'-O4'-C4'	-6.20	103.90	110.10
1	AA	1365	DT	C1'-O4'-C4'	-6.20	103.90	110.10
28	Ab	9	DA	P-O3'-C3'	6.20	127.14	119.70
27	Aa	37	DA	O4'-C4'-C3'	-6.19	102.02	104.50
69	BG	6	DC	P-O5'-C5'	6.19	130.81	120.90
1	AA	2388	DC	O4'-C1'-C2'	-6.19	100.95	105.90
37	Ak	37	DT	C4'-C3'-C2'	-6.19	97.53	103.10
11	AK	30	DT	C4'-C3'-C2'	-6.18	97.54	103.10
16	AP	5	DG	O4'-C1'-C2'	-6.18	100.96	105.90
60	A7	10	DT	C4'-C3'-C2'	-6.18	97.54	103.10
12	AL	5	DC	O4'-C4'-C3'	-6.17	102.03	104.50
27	Aa	1	DT	C1'-O4'-C4'	-6.17	103.93	110.10
1	AA	2074	DT	C4'-C3'-C2'	-6.17	97.55	103.10
1	AA	387	DG	O4'-C1'-C2'	-6.17	100.97	105.90
61	A8	30	DG	O4'-C1'-C2'	-6.16	100.97	105.90
74	BL	31	DT	O4'-C4'-C3'	-6.16	102.03	104.50
46	At	34	DG	O4'-C1'-C2'	-6.16	100.97	105.90
1	AA	1900	DG	O4'-C4'-C3'	-6.16	102.04	104.50
50	Ax	9	DG	C1'-O4'-C4'	-6.16	103.94	110.10
1	AA	761	DG	O4'-C1'-C2'	-6.16	100.97	105.90
43	Aq	19	DA	O4'-C1'-C2'	-6.16	100.97	105.90
1	AA	1504	DG	C4'-C3'-C2'	-6.15	97.56	103.10
57	A4	10	DC	P-O3'-C3'	6.15	127.08	119.70
10	AJ	30	DT	O4'-C1'-N1	6.14	112.30	108.00
35	Ai	27	DG	O4'-C1'-C2'	-6.14	100.99	105.90
1	AA	1518	DA	O4'-C1'-N9	6.13	112.30	108.00
1	AA	1057	DT	C6-C5-C7	-6.13	119.22	122.90
1	AA	2539	DT	O4'-C4'-C3'	-6.13	102.05	104.50
21	AU	10	DG	O4'-C1'-C2'	-6.13	101.00	105.90
40	An	12	DG	O4'-C1'-C2'	-6.13	101.00	105.90
1	AA	2488	DG	P-O3'-C3'	6.13	127.06	119.70
54	A1	45	DT	O4'-C1'-N1	6.13	112.29	108.00
74	BL	31	DT	C4'-C3'-C2'	-6.13	97.58	103.10
22	AV	37	DG	O4'-C1'-C2'	-6.13	101.00	105.90
1	AA	20	DT	C4'-C3'-C2'	-6.13	97.59	103.10
1	AA	2798	DC	O4'-C1'-C2'	-6.13	101.00	105.90
49	Aw	30	DG	O4'-C1'-N9	6.12	112.29	108.00
1	AA	832	DC	P-O5'-C5'	6.12	130.69	120.90
18	AR	28	DT	C1'-O4'-C4'	-6.12	103.98	110.10
1	AA	547	DT	P-O3'-C3'	6.12	127.04	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	AO	41	DG	C5-C6-O6	-6.11	124.93	128.60
74	BL	9	DG	O4'-C1'-C2'	-6.11	101.01	105.90
1	AA	2434	DC	O4'-C4'-C3'	-6.11	102.06	104.50
58	A5	13	DT	C4'-C3'-C2'	-6.10	97.61	103.10
1	AA	879	DG	O4'-C1'-N9	6.10	112.27	108.00
49	Aw	4	DG	C1'-O4'-C4'	-6.10	104.00	110.10
60	A7	20	DG	O4'-C1'-C2'	-6.10	101.02	105.90
72	BJ	24	DG	O4'-C4'-C3'	-6.10	102.06	104.50
24	AX	23	DG	O4'-C1'-C2'	-6.10	101.02	105.90
1	AA	1019	DT	C4'-C3'-C2'	-6.10	97.61	103.10
1	AA	1470	DT	P-O3'-C3'	6.09	127.01	119.70
13	AM	34	DT	O4'-C4'-C3'	-6.09	102.06	104.50
42	Ap	16	DA	O4'-C1'-C2'	-6.09	101.03	105.90
2	AB	2	DT	O4'-C1'-C2'	-6.09	101.03	105.90
1	AA	2778	DG	O4'-C1'-C2'	-6.09	101.03	105.90
65	BC	29	DT	C1'-O4'-C4'	-6.09	104.01	110.10
70	BH	37	DA	O4'-C1'-C2'	-6.08	101.04	105.90
1	AA	1994	DC	P-O3'-C3'	6.08	127.00	119.70
68	BF	1	DT	O4'-C1'-C2'	-6.08	101.04	105.90
1	AA	1410	DG	O4'-C1'-N9	6.07	112.25	108.00
60	A7	1	DT	O4'-C1'-N1	6.07	112.25	108.00
1	AA	1265	DG	O4'-C1'-C2'	-6.07	101.05	105.90
1	AA	166	DT	C4'-C3'-C2'	-6.06	97.64	103.10
19	AS	16	DT	O4'-C4'-C3'	-6.06	102.07	104.50
1	AA	836	DT	P-O3'-C3'	6.06	126.97	119.70
1	AA	2532	DG	C5-C6-O6	-6.06	124.96	128.60
47	Au	24	DT	C4'-C3'-C2'	-6.06	97.64	103.10
1	AA	1189	DG	O4'-C1'-N9	6.06	112.24	108.00
1	AA	1886	DC	C6-N1-C2	-6.05	117.88	120.30
1	AA	1895	DC	C6-N1-C2	-6.05	117.88	120.30
62	A9	40	DG	C5-C6-O6	-6.05	124.97	128.60
6	AF	1	DT	O4'-C1'-C2'	-6.05	101.06	105.90
2	AB	22	DC	O4'-C1'-C2'	-6.04	101.07	105.90
1	AA	156	DC	P-O3'-C3'	6.04	126.95	119.70
1	AA	631	DA	C4'-C3'-C2'	-6.04	97.66	103.10
1	AA	956	DT	C4'-C3'-C2'	-6.04	97.67	103.10
1	AA	1474	DG	C4'-C3'-C2'	-6.04	97.67	103.10
1	AA	1524	DA	C4'-C3'-C2'	-6.04	97.67	103.10
28	Ab	40	DG	C1'-O4'-C4'	-6.04	104.06	110.10
63	BA	10	DC	O4'-C4'-C3'	-6.03	102.09	104.50
56	A3	14	DG	O4'-C1'-C2'	-6.03	101.08	105.90
75	BM	39	DC	P-O3'-C3'	6.02	126.93	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
78	BP	19	DT	P-O3'-C3'	6.02	126.93	119.70
1	AA	84	DC	O4'-C1'-C2'	-6.02	101.09	105.90
1	AA	2099	DG	O4'-C1'-C2'	-6.02	101.09	105.90
10	AJ	30	DT	C1'-O4'-C4'	-6.02	104.08	110.10
1	AA	2605	DG	O4'-C1'-C2'	-6.01	101.09	105.90
23	AW	16	DT	C4'-C3'-C2'	-6.01	97.69	103.10
46	At	40	DG	C1'-O4'-C4'	-6.01	104.09	110.10
1	AA	1005	DT	C4'-C3'-C2'	-6.00	97.69	103.10
1	AA	2090	DG	N1-C6-O6	6.00	123.50	119.90
77	BO	16	DC	O4'-C1'-C2'	-6.00	101.10	105.90
1	AA	2639	DT	C1'-O4'-C4'	-6.00	104.10	110.10
1	AA	33	DC	C4'-C3'-C2'	-5.99	97.71	103.10
1	AA	952	DT	C4'-C3'-C2'	-5.99	97.71	103.10
15	AO	43	DA	O4'-C1'-C2'	-5.99	101.11	105.90
1	AA	417	DC	O4'-C4'-C3'	-5.99	102.11	104.50
1	AA	1871	DT	O4'-C1'-C2'	-5.99	101.11	105.90
1	AA	1279	DT	C4'-C3'-C2'	-5.98	97.72	103.10
67	BE	23	DT	O4'-C1'-C2'	-5.98	101.11	105.90
1	AA	2654	DG	C1'-O4'-C4'	-5.98	104.12	110.10
12	AL	20	DT	O4'-C4'-C3'	-5.98	102.11	104.50
25	AY	19	DT	O4'-C4'-C3'	-5.98	102.11	104.50
1	AA	935	DT	C4'-C3'-C2'	-5.97	97.72	103.10
1	AA	1207	DA	O4'-C4'-C3'	-5.97	102.11	104.50
1	AA	889	DC	O4'-C1'-C2'	-5.97	101.12	105.90
1	AA	1685	DT	P-O3'-C3'	5.97	126.87	119.70
63	BA	9	DG	O4'-C1'-C2'	-5.97	101.12	105.90
34	Ah	9	DT	O4'-C1'-N1	5.97	112.18	108.00
1	AA	2626	DT	O4'-C1'-C2'	-5.97	101.13	105.90
35	Ai	15	DA	P-O3'-C3'	5.97	126.86	119.70
64	BB	34	DA	O4'-C1'-C2'	-5.96	101.13	105.90
65	BC	23	DT	C4'-C3'-C2'	-5.96	97.73	103.10
33	Ag	14	DA	O4'-C1'-C2'	-5.96	101.13	105.90
65	BC	14	DG	C1'-O4'-C4'	-5.96	104.14	110.10
1	AA	1410	DG	C1'-O4'-C4'	-5.96	104.14	110.10
1	AA	2263	DC	C4'-C3'-C2'	-5.96	97.74	103.10
68	BF	19	DT	O4'-C1'-C2'	-5.95	101.14	105.90
1	AA	261	DA	N1-C6-N6	-5.95	115.03	118.60
1	AA	1950	DC	O4'-C1'-C2'	-5.95	101.14	105.90
77	BO	30	DA	O4'-C4'-C3'	-5.95	102.12	104.50
1	AA	2154	DG	C5-C6-O6	-5.95	125.03	128.60
13	AM	22	DA	P-O3'-C3'	5.95	126.84	119.70
1	AA	1864	DG	P-O3'-C3'	5.95	126.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	11	DA	O4'-C1'-C2'	-5.95	101.14	105.90
1	AA	1301	DT	C4'-C3'-C2'	-5.94	97.75	103.10
1	AA	1575	DG	C1'-O4'-C4'	-5.94	104.16	110.10
52	Az	31	DA	O4'-C1'-C2'	-5.94	101.15	105.90
1	AA	1385	DG	O4'-C1'-C2'	-5.94	101.15	105.90
36	Aj	4	DG	O4'-C1'-C2'	-5.94	101.15	105.90
1	AA	1538	DC	C4'-C3'-C2'	-5.93	97.76	103.10
35	Ai	8	DG	N1-C6-O6	5.93	123.46	119.90
1	AA	821	DT	O4'-C4'-C3'	-5.93	102.13	104.50
1	AA	1524	DA	N1-C6-N6	-5.93	115.04	118.60
1	AA	2845	DT	O4'-C4'-C3'	-5.93	102.13	104.50
4	AD	10	DT	C4'-C3'-C2'	-5.93	97.77	103.10
1	AA	200	DC	O4'-C1'-C2'	-5.92	101.16	105.90
1	AA	1313	DA	O4'-C1'-C2'	-5.92	101.16	105.90
35	Ai	22	DC	P-O5'-C5'	5.92	130.38	120.90
1	AA	1804	DA	C1'-O4'-C4'	-5.92	104.18	110.10
1	AA	518	DC	O4'-C1'-C2'	-5.92	101.17	105.90
1	AA	539	DG	O4'-C1'-C2'	-5.92	101.17	105.90
1	AA	1585	DA	P-O3'-C3'	5.92	126.80	119.70
1	AA	2585	DG	O4'-C1'-C2'	-5.92	101.17	105.90
15	AO	1	DC	C1'-O4'-C4'	-5.92	104.18	110.10
45	As	39	DG	C4'-C3'-C2'	-5.92	97.78	103.10
78	BP	19	DT	O4'-C1'-C2'	-5.92	101.17	105.90
1	AA	2641	DG	O4'-C1'-C2'	-5.92	101.17	105.90
34	Ah	12	DT	C1'-O4'-C4'	-5.92	104.19	110.10
1	AA	1719	DT	O4'-C4'-C3'	-5.91	102.14	104.50
1	AA	1934	DC	O4'-C4'-C3'	-5.91	102.14	104.50
1	AA	2459	DT	C4'-C3'-C2'	-5.91	97.78	103.10
30	Ad	19	DG	O4'-C1'-C2'	-5.91	101.17	105.90
1	AA	361	DT	O4'-C4'-C3'	-5.91	102.14	104.50
27	Aa	6	DT	P-O3'-C3'	5.91	126.79	119.70
40	An	9	DA	P-O3'-C3'	5.91	126.79	119.70
6	AF	11	DT	C1'-O4'-C4'	-5.91	104.19	110.10
56	A3	39	DT	C4'-C3'-C2'	-5.91	97.79	103.10
62	A9	39	DG	P-O3'-C3'	5.90	126.78	119.70
1	AA	1134	DC	O4'-C1'-C2'	-5.90	101.18	105.90
15	AO	17	DT	C4'-C3'-C2'	-5.90	97.79	103.10
56	A3	4	DT	O4'-C1'-C2'	-5.90	101.18	105.90
1	AA	188	DT	C4'-C3'-C2'	-5.90	97.79	103.10
23	AW	9	DG	C1'-O4'-C4'	-5.90	104.20	110.10
52	Az	30	DG	O4'-C1'-N9	5.89	112.12	108.00
1	AA	445	DT	C4'-C3'-C2'	-5.89	97.80	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1258	DT	O4'-C1'-C2'	-5.89	101.19	105.90
28	Ab	9	DA	C1'-O4'-C4'	-5.89	104.21	110.10
9	AI	18	DG	O4'-C1'-C2'	-5.89	101.19	105.90
1	AA	2619	DA	O4'-C1'-C2'	-5.89	101.19	105.90
1	AA	2856	DT	C4'-C3'-C2'	-5.89	97.80	103.10
35	Ai	49	DG	C5-C6-O6	-5.89	125.07	128.60
1	AA	1626	DG	C1'-O4'-C4'	-5.89	104.21	110.10
6	AF	6	DC	P-O5'-C5'	5.88	130.32	120.90
16	AP	9	DG	P-O3'-C3'	5.88	126.76	119.70
1	AA	879	DG	C1'-O4'-C4'	-5.88	104.22	110.10
1	AA	1302	DA	C4'-C3'-C2'	-5.88	97.81	103.10
1	AA	2263	DC	O4'-C4'-C3'	-5.88	102.15	104.50
76	BN	29	DG	O4'-C4'-C3'	-5.88	102.15	104.50
26	AZ	41	DT	P-O3'-C3'	5.87	126.75	119.70
58	A5	15	DA	C4'-C3'-C2'	-5.87	97.81	103.10
1	AA	1057	DT	C4-C5-C7	5.87	122.52	119.00
29	Ac	33	DG	O4'-C1'-C2'	-5.87	101.20	105.90
63	BA	5	DG	C5-C6-O6	-5.87	125.08	128.60
1	AA	109	DA	N1-C6-N6	-5.87	115.08	118.60
1	AA	1104	DC	C4'-C3'-C2'	-5.87	97.82	103.10
1	AA	1804	DA	O4'-C1'-N9	5.87	112.11	108.00
67	BE	22	DG	O4'-C4'-C3'	-5.87	102.15	104.50
1	AA	1330	DG	N1-C6-O6	5.87	123.42	119.90
68	BF	34	DG	O4'-C1'-C2'	-5.87	101.21	105.90
1	AA	1376	DG	O4'-C1'-C2'	-5.86	101.21	105.90
1	AA	311	DA	O4'-C1'-C2'	-5.86	101.21	105.90
37	Ak	10	DT	C4'-C3'-C2'	-5.86	97.83	103.10
1	AA	539	DG	O4'-C1'-N9	5.86	112.10	108.00
1	AA	2322	DG	O4'-C1'-C2'	-5.86	101.21	105.90
33	Ag	17	DG	O4'-C1'-C2'	-5.86	101.21	105.90
34	Ah	9	DT	O4'-C1'-C2'	-5.86	101.22	105.90
1	AA	1825	DC	C6-N1-C2	-5.85	117.96	120.30
1	AA	2387	DA	C5-C6-N6	-5.85	119.02	123.70
16	AP	19	DT	C4'-C3'-C2'	-5.85	97.83	103.10
1	AA	2261	DG	P-O3'-C3'	5.85	126.72	119.70
50	Ax	27	DG	N1-C6-O6	5.85	123.41	119.90
1	AA	1947	DC	O4'-C1'-C2'	-5.85	101.22	105.90
1	AA	1900	DG	C4'-C3'-C2'	-5.84	97.84	103.10
1	AA	2696	DG	C4'-C3'-C2'	-5.84	97.84	103.10
34	Ah	12	DT	O4'-C1'-N1	5.84	112.09	108.00
1	AA	1501	DC	C4'-C3'-C2'	-5.84	97.84	103.10
37	Ak	16	DG	O4'-C1'-N9	5.84	112.09	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1047	DT	O4'-C4'-C3'	-5.84	102.17	104.50
1	AA	398	DT	O4'-C4'-C3'	-5.83	102.17	104.50
72	BJ	1	DT	C1'-O4'-C4'	-5.83	104.27	110.10
70	BH	6	DC	C4'-C3'-C2'	-5.83	97.85	103.10
1	AA	539	DG	C1'-O4'-C4'	-5.83	104.27	110.10
1	AA	2534	DC	O4'-C1'-C2'	-5.83	101.24	105.90
2	AB	7	DA	N1-C6-N6	5.83	122.10	118.60
8	AH	18	DG	P-O3'-C3'	5.83	126.69	119.70
63	BA	9	DG	C1'-O4'-C4'	-5.83	104.27	110.10
45	As	23	DA	P-O3'-C3'	5.83	126.69	119.70
1	AA	1888	DG	C1'-O4'-C4'	-5.82	104.28	110.10
14	AN	9	DA	C1'-O4'-C4'	-5.82	104.28	110.10
28	Ab	28	DC	P-O3'-C3'	5.82	126.69	119.70
1	AA	522	DG	C4'-C3'-C2'	-5.82	97.86	103.10
3	AC	47	DC	O4'-C4'-C3'	-5.82	102.17	104.50
55	A2	23	DA	C1'-O4'-C4'	-5.82	104.28	110.10
53	A0	15	DA	P-O3'-C3'	5.82	126.68	119.70
50	Ax	37	DA	O4'-C1'-C2'	-5.82	101.25	105.90
1	AA	589	DG	C1'-O4'-C4'	-5.81	104.29	110.10
1	AA	1782	DG	O4'-C1'-C2'	-5.81	101.25	105.90
44	Ar	16	DT	P-O3'-C3'	5.81	126.67	119.70
65	BC	16	DT	C4'-C3'-C2'	-5.81	97.88	103.10
33	Ag	22	DG	O4'-C1'-C2'	-5.80	101.26	105.90
75	BM	31	DG	O4'-C1'-C2'	-5.80	101.26	105.90
17	AQ	9	DC	O4'-C1'-C2'	-5.80	101.26	105.90
56	A3	12	DT	O4'-C1'-C2'	-5.80	101.26	105.90
1	AA	344	DT	C4'-C3'-C2'	-5.80	97.88	103.10
1	AA	972	DC	P-O3'-C3'	5.80	126.66	119.70
1	AA	2448	DG	O4'-C1'-C2'	-5.80	101.26	105.90
25	AY	19	DT	C4'-C3'-C2'	-5.80	97.88	103.10
69	BG	3	DC	C4'-C3'-C2'	-5.80	97.88	103.10
1	AA	1147	DT	C4'-C3'-C2'	-5.79	97.89	103.10
1	AA	2427	DA	P-O3'-C3'	5.79	126.65	119.70
1	AA	1446	DT	C4'-C3'-C2'	-5.79	97.89	103.10
64	BB	15	DC	C4'-C3'-C2'	-5.79	97.89	103.10
1	AA	117	DA	P-O3'-C3'	5.79	126.64	119.70
1	AA	887	DC	P-O3'-C3'	5.79	126.64	119.70
1	AA	323	DA	O4'-C1'-C2'	-5.78	101.27	105.90
52	Az	9	DG	C4'-C3'-C2'	-5.78	97.90	103.10
1	AA	370	DG	C5-C6-O6	-5.78	125.14	128.60
1	AA	1366	DA	N1-C6-N6	-5.77	115.14	118.60
1	AA	1710	DT	C1'-O4'-C4'	-5.77	104.33	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	AH	23	DT	O4'-C1'-C2'	-5.77	101.28	105.90
1	AA	1950	DC	O4'-C1'-N1	5.77	112.04	108.00
13	AM	11	DG	O4'-C1'-C2'	-5.77	101.29	105.90
1	AA	980	DG	C5-C6-O6	-5.77	125.14	128.60
1	AA	2242	DG	O4'-C1'-N9	5.76	112.03	108.00
72	BJ	40	DG	C5-C6-O6	-5.76	125.14	128.60
1	AA	291	DC	O4'-C1'-C2'	-5.76	101.29	105.90
48	Av	25	DC	C4'-C3'-C2'	-5.76	97.92	103.10
63	BA	10	DC	C4'-C3'-C2'	-5.76	97.92	103.10
72	BJ	2	DT	O4'-C1'-C2'	-5.76	101.29	105.90
1	AA	1391	DA	C1'-O4'-C4'	-5.76	104.34	110.10
78	BP	7	DC	O4'-C1'-C2'	-5.76	101.29	105.90
32	Af	5	DA	N1-C6-N6	-5.76	115.15	118.60
1	AA	2577	DC	O4'-C1'-C2'	-5.75	101.30	105.90
74	BL	3	DG	P-O3'-C3'	5.75	126.60	119.70
1	AA	2381	DT	O4'-C1'-C2'	-5.75	101.30	105.90
16	AP	3	DG	N1-C6-O6	5.75	123.35	119.90
1	AA	1920	DG	P-O3'-C3'	5.75	126.60	119.70
39	Am	12	DC	C6-N1-C1'	-5.75	113.90	120.80
1	AA	1208	DA	O4'-C1'-C2'	-5.75	101.30	105.90
1	AA	1786	DT	C4'-C3'-C2'	-5.75	97.93	103.10
26	AZ	39	DA	O4'-C1'-C2'	-5.75	101.30	105.90
50	Ax	16	DT	C4'-C3'-C2'	-5.75	97.93	103.10
1	AA	2334	DC	O4'-C1'-N1	-5.75	103.98	108.00
10	AJ	26	DC	C1'-O4'-C4'	-5.74	104.36	110.10
41	Ao	4	DG	C4'-C3'-C2'	-5.74	97.93	103.10
15	AO	10	DT	C4'-C3'-C2'	-5.74	97.93	103.10
23	AW	9	DG	O4'-C4'-C3'	-5.74	102.20	104.50
1	AA	335	DT	P-O3'-C3'	5.74	126.58	119.70
18	AR	13	DG	N1-C6-O6	5.74	123.34	119.90
65	BC	14	DG	P-O3'-C3'	5.74	126.58	119.70
1	AA	240	DT	O4'-C4'-C3'	-5.73	102.21	104.50
1	AA	2561	DT	C6-C5-C7	5.73	126.34	122.90
51	Ay	30	DC	O4'-C1'-C2'	-5.73	101.31	105.90
1	AA	333	DA	O4'-C1'-C2'	-5.73	101.31	105.90
1	AA	1704	DC	C4'-C3'-C2'	-5.73	97.94	103.10
78	BP	17	DG	O4'-C1'-C2'	-5.73	101.31	105.90
1	AA	631	DA	O4'-C4'-C3'	-5.73	102.21	104.50
1	AA	2798	DC	C1'-O4'-C4'	-5.73	104.37	110.10
1	AA	1801	DC	P-O5'-C5'	5.73	130.06	120.90
54	A1	14	DG	P-O3'-C3'	5.73	126.57	119.70
67	BE	17	DG	C1'-O4'-C4'	-5.73	104.37	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2845	DT	C4'-C3'-C2'	-5.73	97.95	103.10
1	AA	2837	DC	O4'-C1'-C2'	-5.72	101.32	105.90
63	BA	28	DG	C4'-C3'-C2'	-5.72	97.95	103.10
21	AU	15	DG	O4'-C1'-N9	5.72	112.01	108.00
65	BC	34	DA	P-O3'-C3'	5.72	126.57	119.70
76	BN	6	DC	P-O5'-C5'	5.72	130.06	120.90
76	BN	29	DG	C1'-O4'-C4'	-5.72	104.38	110.10
1	AA	828	DG	O4'-C1'-N9	5.72	112.00	108.00
1	AA	2605	DG	O4'-C1'-N9	5.72	112.00	108.00
1	AA	665	DG	P-O3'-C3'	5.72	126.56	119.70
1	AA	2532	DG	C1'-O4'-C4'	-5.72	104.38	110.10
1	AA	2006	DC	C4'-C3'-C2'	-5.71	97.96	103.10
28	Ab	42	DG	O4'-C4'-C3'	-5.71	102.22	104.50
29	Ac	30	DG	O4'-C4'-C3'	-5.71	102.22	104.50
1	AA	2074	DT	O4'-C4'-C3'	-5.71	102.22	104.50
1	AA	1388	DA	O4'-C1'-C2'	-5.70	101.34	105.90
1	AA	2693	DG	C1'-O4'-C4'	-5.70	104.40	110.10
19	AS	5	DT	O4'-C1'-N1	5.70	111.99	108.00
1	AA	127	DG	O4'-C1'-C2'	-5.70	101.34	105.90
1	AA	245	DT	C4'-C3'-C2'	-5.70	97.97	103.10
1	AA	1954	DT	C4'-C3'-C2'	-5.70	97.97	103.10
1	AA	2806	DT	C4'-C3'-C2'	-5.70	97.97	103.10
1	AA	2347	DG	O4'-C1'-C2'	-5.70	101.34	105.90
48	Av	16	DC	C1'-O4'-C4'	-5.69	104.41	110.10
1	AA	261	DA	O4'-C1'-C2'	-5.69	101.35	105.90
45	As	16	DA	O4'-C1'-C2'	-5.69	101.35	105.90
68	BF	1	DT	O4'-C4'-C3'	-5.69	102.22	104.50
55	A2	23	DA	P-O3'-C3'	5.69	126.53	119.70
1	AA	2672	DG	C5-C6-O6	-5.69	125.19	128.60
1	AA	227	DT	O4'-C1'-C2'	-5.69	101.35	105.90
1	AA	839	DG	O4'-C4'-C3'	-5.68	102.23	104.50
1	AA	2831	DA	O4'-C4'-C3'	-5.68	102.23	104.50
20	AT	9	DC	P-O3'-C3'	5.68	126.52	119.70
1	AA	145	DT	O4'-C4'-C3'	-5.68	102.23	104.50
1	AA	785	DG	O4'-C1'-C2'	-5.68	101.35	105.90
1	AA	2363	DG	C4'-C3'-C2'	-5.68	97.98	103.10
64	BB	11	DA	N1-C6-N6	-5.68	115.19	118.60
1	AA	1629	DC	C1'-O4'-C4'	-5.67	104.42	110.10
73	BK	24	DC	C2-N1-C1'	5.67	125.04	118.80
1	AA	441	DC	O4'-C4'-C3'	-5.67	102.23	104.50
1	AA	1688	DC	P-O3'-C3'	5.67	126.51	119.70
1	AA	2532	DG	N1-C6-O6	5.67	123.30	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
71	BI	35	DC	O4'-C1'-C2'	-5.67	101.36	105.90
1	AA	37	DT	C4'-C3'-C2'	-5.67	98.00	103.10
10	AJ	2	DT	O4'-C1'-C2'	-5.67	101.37	105.90
1	AA	2354	DT	O4'-C1'-C2'	-5.67	101.37	105.90
22	AV	33	DA	O4'-C1'-C2'	-5.67	101.37	105.90
1	AA	768	DG	C4'-C3'-C2'	-5.66	98.00	103.10
1	AA	885	DC	C2-N1-C1'	5.66	125.03	118.80
1	AA	1966	DG	O4'-C1'-C2'	-5.66	101.37	105.90
61	A8	20	DT	O4'-C4'-C3'	-5.66	102.23	104.50
26	AZ	16	DG	O4'-C1'-C2'	-5.66	101.37	105.90
28	Ab	37	DT	C1'-O4'-C4'	-5.66	104.44	110.10
20	AT	44	DA	O4'-C1'-C2'	-5.66	101.37	105.90
46	At	21	DG	C1'-O4'-C4'	-5.66	104.44	110.10
1	AA	1069	DT	C4'-C3'-C2'	-5.66	98.01	103.10
77	BO	30	DA	C1'-O4'-C4'	-5.66	104.44	110.10
1	AA	749	DC	O4'-C1'-C2'	-5.65	101.38	105.90
45	As	14	DC	C2-N1-C1'	5.65	125.02	118.80
12	AL	34	DT	C4'-C3'-C2'	-5.65	98.01	103.10
31	Ae	12	DT	C4'-C3'-C2'	-5.65	98.01	103.10
23	AW	24	DA	P-O3'-C3'	5.65	126.48	119.70
39	Am	30	DG	P-O3'-C3'	5.65	126.48	119.70
61	A8	23	DA	C4'-C3'-C2'	-5.65	98.02	103.10
1	AA	1719	DT	C4'-C3'-C2'	-5.64	98.02	103.10
1	AA	2413	DG	O4'-C1'-C2'	-5.64	101.38	105.90
69	BG	3	DC	O4'-C4'-C3'	-5.64	102.24	104.50
1	AA	1012	DA	C4'-C3'-C2'	-5.63	98.03	103.10
1	AA	2507	DT	C1'-O4'-C4'	-5.63	104.47	110.10
1	AA	106	DA	O4'-C1'-C2'	-5.63	101.39	105.90
21	AU	7	DA	O4'-C1'-C2'	-5.63	101.40	105.90
44	Ar	23	DA	O4'-C1'-C2'	-5.63	101.39	105.90
1	AA	733	DG	C1'-O4'-C4'	-5.63	104.47	110.10
1	AA	370	DG	N1-C6-O6	5.63	123.28	119.90
1	AA	1070	DC	P-O3'-C3'	5.62	126.45	119.70
1	AA	2326	DC	P-O3'-C3'	5.62	126.45	119.70
1	AA	1799	DT	O4'-C4'-C3'	-5.62	102.25	104.50
39	Am	5	DG	C4'-C3'-C2'	-5.62	98.04	103.10
1	AA	219	DG	O4'-C1'-C2'	-5.62	101.40	105.90
1	AA	441	DC	C4'-C3'-C2'	-5.62	98.04	103.10
1	AA	203	DA	P-O3'-C3'	5.62	126.44	119.70
1	AA	819	DG	P-O3'-C3'	5.62	126.44	119.70
13	AM	9	DT	C4'-C3'-C2'	-5.62	98.04	103.10
1	AA	372	DA	C1'-O4'-C4'	-5.62	104.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2623	DA	P-O3'-C3'	5.62	126.44	119.70
56	A3	7	DA	O4'-C1'-C2'	-5.62	101.41	105.90
1	AA	79	DT	O4'-C1'-C2'	-5.62	101.41	105.90
1	AA	2016	DG	P-O3'-C3'	5.61	126.44	119.70
12	AL	7	DA	O4'-C1'-N9	-5.61	104.07	108.00
24	AX	26	DT	P-O3'-C3'	5.61	126.43	119.70
28	Ab	21	DC	P-O3'-C3'	5.61	126.43	119.70
1	AA	1166	DT	O4'-C4'-C3'	-5.61	102.26	104.50
1	AA	2605	DG	C1'-O4'-C4'	-5.61	104.49	110.10
71	BI	7	DA	P-O3'-C3'	5.61	126.43	119.70
1	AA	613	DG	O4'-C1'-C2'	-5.61	101.42	105.90
16	AP	3	DG	C5-C6-O6	-5.61	125.24	128.60
1	AA	533	DA	O4'-C1'-C2'	-5.60	101.42	105.90
10	AJ	11	DT	C1'-O4'-C4'	-5.60	104.50	110.10
1	AA	149	DT	O4'-C4'-C3'	-5.60	102.26	104.50
15	AO	13	DC	P-O3'-C3'	5.60	126.42	119.70
1	AA	1884	DA	N1-C6-N6	-5.60	115.24	118.60
1	AA	2175	DT	O4'-C1'-C2'	-5.60	101.42	105.90
36	Aj	9	DC	P-O3'-C3'	5.60	126.42	119.70
64	BB	11	DA	P-O3'-C3'	5.60	126.42	119.70
21	AU	15	DG	P-O3'-C3'	5.59	126.41	119.70
21	AU	16	DC	O4'-C1'-C2'	-5.59	101.43	105.90
1	AA	2387	DA	N1-C6-N6	5.59	121.95	118.60
1	AA	2534	DC	P-O3'-C3'	5.59	126.41	119.70
32	Af	2	DG	O4'-C1'-C2'	-5.59	101.43	105.90
79	BQ	7	DG	O4'-C1'-C2'	-5.59	101.43	105.90
18	AR	28	DT	O4'-C4'-C3'	-5.59	102.27	104.50
26	AZ	7	DG	O4'-C1'-C2'	-5.59	101.43	105.90
1	AA	616	DG	C1'-O4'-C4'	-5.58	104.52	110.10
1	AA	1381	DT	C4'-C3'-C2'	-5.58	98.08	103.10
1	AA	1397	DT	C1'-O4'-C4'	-5.58	104.52	110.10
72	BJ	33	DT	O4'-C1'-C2'	-5.58	101.43	105.90
1	AA	975	DA	O4'-C1'-C2'	-5.58	101.44	105.90
1	AA	1248	DC	O4'-C1'-C2'	-5.58	101.44	105.90
8	AH	24	DT	C4'-C3'-C2'	-5.58	98.08	103.10
1	AA	972	DC	O4'-C1'-C2'	-5.57	101.44	105.90
51	Ay	37	DG	O4'-C1'-C2'	-5.57	101.44	105.90
6	AF	24	DG	O4'-C1'-C2'	-5.57	101.44	105.90
25	AY	30	DA	P-O3'-C3'	5.57	126.38	119.70
5	AE	23	DG	O4'-C1'-C2'	-5.56	101.45	105.90
64	BB	28	DT	C4'-C3'-C2'	-5.56	98.09	103.10
1	AA	210	DC	O4'-C4'-C3'	-5.56	102.28	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Au	16	DA	O4'-C1'-C2'	-5.56	101.45	105.90
75	BM	10	DA	C4'-C3'-C2'	-5.56	98.10	103.10
1	AA	495	DG	O4'-C1'-N9	5.56	111.89	108.00
1	AA	2373	DG	N1-C6-O6	5.56	123.23	119.90
35	Ai	47	DC	O4'-C1'-C2'	-5.56	101.45	105.90
23	AW	2	DG	C5-C6-O6	-5.56	125.27	128.60
47	Au	23	DG	O4'-C1'-C2'	-5.56	101.45	105.90
42	Ap	5	DT	O4'-C1'-N1	5.55	111.89	108.00
71	BI	40	DA	P-O3'-C3'	5.55	126.37	119.70
1	AA	1879	DG	C1'-O4'-C4'	-5.55	104.55	110.10
1	AA	161	DT	O4'-C4'-C3'	-5.55	102.28	104.50
1	AA	1405	DG	O4'-C4'-C3'	-5.55	102.28	104.50
1	AA	946	DG	O4'-C4'-C3'	-5.54	102.28	104.50
1	AA	1674	DC	P-O5'-C5'	5.54	129.77	120.90
38	Al	38	DA	O4'-C4'-C3'	-5.54	102.28	104.50
1	AA	708	DG	O4'-C1'-C2'	-5.54	101.47	105.90
1	AA	1949	DG	N1-C6-O6	5.54	123.22	119.90
1	AA	2031	DG	N1-C6-O6	5.54	123.22	119.90
12	AL	12	DG	O4'-C1'-C2'	-5.54	101.47	105.90
1	AA	1207	DA	C4'-C3'-C2'	-5.53	98.12	103.10
7	AG	6	DG	C5-C6-O6	-5.53	125.28	128.60
1	AA	2305	DC	C4'-C3'-C2'	-5.53	98.12	103.10
37	Ak	29	DC	P-O3'-C3'	5.53	126.34	119.70
45	As	34	DG	C1'-O4'-C4'	-5.53	104.57	110.10
1	AA	247	DC	P-O3'-C3'	5.53	126.33	119.70
1	AA	1765	DC	O4'-C1'-C2'	-5.53	101.48	105.90
8	AH	1	DA	C1'-O4'-C4'	-5.53	104.57	110.10
18	AR	14	DC	O4'-C1'-N1	5.53	111.87	108.00
3	AC	44	DC	P-O3'-C3'	5.52	126.33	119.70
40	An	38	DT	C4'-C3'-C2'	-5.52	98.13	103.10
1	AA	1694	DC	P-O5'-C5'	5.52	129.73	120.90
1	AA	2308	DA	O4'-C1'-C2'	-5.52	101.48	105.90
1	AA	2522	DT	C4'-C3'-C2'	-5.52	98.13	103.10
17	AQ	10	DT	C4'-C3'-C2'	-5.52	98.13	103.10
18	AR	13	DG	C5-C6-O6	-5.52	125.29	128.60
3	AC	40	DT	O4'-C4'-C3'	-5.52	102.29	104.50
19	AS	21	DG	O4'-C1'-C2'	-5.52	101.49	105.90
1	AA	2585	DG	O4'-C1'-N9	5.52	111.86	108.00
45	As	23	DA	O4'-C1'-N9	5.52	111.86	108.00
1	AA	815	DT	C4'-C3'-C2'	-5.51	98.14	103.10
70	BH	7	DC	C2-N1-C1'	5.51	124.86	118.80
77	BO	39	DT	C4'-C3'-C2'	-5.51	98.14	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1543	DA	O4'-C1'-C2'	-5.51	101.49	105.90
3	AC	44	DC	O4'-C1'-C2'	-5.51	101.49	105.90
44	Ar	37	DA	O4'-C1'-C2'	-5.51	101.49	105.90
75	BM	44	DA	N1-C6-N6	-5.51	115.30	118.60
1	AA	1866	DG	O4'-C1'-C2'	-5.51	101.50	105.90
38	Al	28	DC	C4'-C3'-C2'	-5.51	98.14	103.10
1	AA	313	DA	P-O3'-C3'	5.50	126.31	119.70
1	AA	2639	DT	O4'-C1'-C2'	-5.50	101.50	105.90
44	Ar	33	DT	C4'-C3'-C2'	-5.50	98.15	103.10
1	AA	2294	DC	O4'-C4'-C3'	-5.50	102.30	104.50
1	AA	55	DT	P-O3'-C3'	-5.50	113.10	119.70
1	AA	252	DG	O4'-C4'-C3'	-5.50	102.30	104.50
1	AA	1588	DC	O4'-C1'-C2'	-5.50	101.50	105.90
1	AA	2081	DT	C4'-C3'-C2'	-5.50	98.15	103.10
1	AA	1362	DA	O4'-C1'-C2'	-5.49	101.50	105.90
37	Ak	57	DT	P-O3'-C3'	5.49	126.29	119.70
1	AA	2251	DT	O4'-C1'-C2'	-5.49	101.51	105.90
1	AA	1343	DG	C5-C6-O6	-5.49	125.31	128.60
1	AA	1810	DT	O4'-C4'-C3'	-5.49	102.30	104.50
1	AA	2377	DG	C4'-C3'-C2'	-5.49	98.16	103.10
31	Ae	33	DA	C1'-O4'-C4'	-5.49	104.61	110.10
1	AA	1832	DT	C4'-C3'-C2'	-5.49	98.16	103.10
1	AA	1825	DC	C4'-C3'-C2'	-5.49	98.16	103.10
1	AA	2753	DC	P-O5'-C5'	5.49	129.68	120.90
66	BD	10	DG	O4'-C1'-C2'	-5.49	101.51	105.90
1	AA	2849	DC	C4'-C3'-C2'	-5.48	98.17	103.10
1	AA	30	DA	O4'-C1'-C2'	-5.48	101.51	105.90
1	AA	1779	DC	O4'-C1'-N1	5.48	111.84	108.00
1	AA	2387	DA	O4'-C1'-C2'	-5.48	101.51	105.90
32	Af	31	DC	C2-N1-C1'	5.48	124.83	118.80
5	AE	26	DA	C4'-C3'-C2'	-5.48	98.17	103.10
71	BI	13	DT	O4'-C4'-C3'	-5.48	102.31	104.50
51	Ay	30	DC	P-O3'-C3'	5.48	126.27	119.70
1	AA	435	DT	O4'-C1'-C2'	-5.48	101.52	105.90
8	AH	23	DT	C1'-O4'-C4'	-5.47	104.62	110.10
35	Ai	49	DG	N1-C6-O6	5.47	123.19	119.90
1	AA	1286	DA	O4'-C1'-C2'	-5.47	101.52	105.90
1	AA	982	DA	O4'-C1'-C2'	-5.47	101.52	105.90
1	AA	667	DT	P-O3'-C3'	5.47	126.26	119.70
1	AA	68	DG	O4'-C1'-C2'	-5.47	101.53	105.90
1	AA	839	DG	C4'-C3'-C2'	-5.46	98.18	103.10
1	AA	1824	DT	P-O3'-C3'	5.46	126.26	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2560	DC	O4'-C1'-N1	5.46	111.82	108.00
1	AA	1751	DC	P-O3'-C3'	5.46	126.25	119.70
1	AA	892	DG	O4'-C1'-C2'	-5.46	101.53	105.90
1	AA	1058	DC	C4'-C3'-C2'	-5.46	98.19	103.10
1	AA	1484	DG	C1'-O4'-C4'	-5.45	104.65	110.10
48	Av	10	DC	C4'-C3'-C2'	-5.45	98.19	103.10
1	AA	2781	DA	O4'-C4'-C3'	-5.45	102.32	104.50
58	A5	26	DG	C4'-C3'-C2'	-5.45	98.20	103.10
1	AA	1689	DC	P-O3'-C3'	5.45	126.23	119.70
76	BN	14	DA	O4'-C1'-N9	-5.45	104.19	108.00
14	AN	7	DT	O4'-C4'-C3'	-5.44	102.32	104.50
10	AJ	7	DT	C1'-O4'-C4'	-5.44	104.66	110.10
58	A5	4	DA	O4'-C1'-C2'	-5.44	101.55	105.90
3	AC	42	DC	C4'-C3'-C2'	-5.44	98.20	103.10
52	Az	28	DC	O4'-C1'-C2'	-5.44	101.55	105.90
1	AA	2539	DT	C4'-C3'-C2'	-5.44	98.20	103.10
1	AA	2633	DG	O4'-C1'-C2'	-5.44	101.55	105.90
1	AA	808	DG	O4'-C1'-C2'	-5.44	101.55	105.90
32	Af	14	DT	C4'-C3'-C2'	-5.44	98.21	103.10
46	At	17	DT	C4'-C3'-C2'	-5.44	98.21	103.10
46	At	40	DG	O4'-C1'-N9	5.44	111.81	108.00
78	BP	11	DG	O4'-C1'-C2'	-5.44	101.55	105.90
1	AA	307	DC	O4'-C1'-N1	-5.43	104.20	108.00
1	AA	834	DG	O4'-C1'-C2'	-5.43	101.55	105.90
6	AF	8	DT	C4'-C3'-C2'	-5.43	98.21	103.10
38	Al	25	DT	C1'-O4'-C4'	-5.43	104.67	110.10
1	AA	11	DT	C4'-C3'-C2'	-5.43	98.21	103.10
7	AG	29	DG	P-O3'-C3'	5.43	126.22	119.70
21	AU	10	DG	P-O3'-C3'	5.43	126.22	119.70
76	BN	10	DT	C4'-C3'-C2'	-5.43	98.21	103.10
56	A3	10	DG	C4'-C3'-C2'	-5.43	98.21	103.10
1	AA	1426	DC	P-O5'-C5'	5.43	129.59	120.90
12	AL	5	DC	C4'-C3'-C2'	-5.43	98.21	103.10
28	Ab	10	DG	O4'-C1'-C2'	-5.43	101.56	105.90
40	An	9	DA	O4'-C1'-C2'	-5.43	101.56	105.90
1	AA	1012	DA	O4'-C4'-C3'	-5.43	102.33	104.50
22	AV	23	DC	O4'-C1'-C2'	-5.43	101.56	105.90
1	AA	409	DA	C1'-O4'-C4'	-5.43	104.67	110.10
1	AA	2445	DG	N1-C6-O6	5.43	123.16	119.90
46	At	26	DA	P-O3'-C3'	5.43	126.21	119.70
1	AA	2355	DA	C1'-O4'-C4'	-5.42	104.67	110.10
13	AM	34	DT	C4'-C3'-C2'	-5.42	98.22	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	AV	39	DG	C1'-O4'-C4'	-5.42	104.67	110.10
1	AA	1175	DT	O4'-C4'-C3'	-5.42	102.33	104.50
10	AJ	29	DC	O4'-C4'-C3'	-5.42	102.33	104.50
39	Am	25	DG	O4'-C1'-C2'	-5.42	101.56	105.90
1	AA	500	DC	O4'-C1'-C2'	-5.42	101.56	105.90
1	AA	700	DT	O4'-C1'-C2'	-5.42	101.56	105.90
1	AA	2779	DG	C5-C6-O6	-5.42	125.35	128.60
24	AX	18	DG	O4'-C1'-C2'	-5.42	101.56	105.90
1	AA	1518	DA	O4'-C1'-C2'	-5.42	101.56	105.90
22	AV	47	DC	O4'-C1'-C2'	-5.42	101.57	105.90
1	AA	907	DA	C4'-C3'-C2'	-5.42	98.22	103.10
1	AA	2578	DC	C6-N1-C2	-5.42	118.13	120.30
14	AN	4	DC	P-O5'-C5'	5.42	129.57	120.90
1	AA	2546	DC	O4'-C1'-C2'	-5.41	101.57	105.90
1	AA	3	DG	C1'-O4'-C4'	-5.41	104.69	110.10
1	AA	2707	DT	C4'-C3'-C2'	-5.41	98.23	103.10
22	AV	25	DC	P-O5'-C5'	5.41	129.55	120.90
22	AV	39	DG	O4'-C4'-C3'	-5.41	102.34	104.50
1	AA	2448	DG	C1'-O4'-C4'	-5.40	104.70	110.10
29	Ac	27	DG	O4'-C1'-C2'	-5.40	101.58	105.90
64	BB	22	DT	C4'-C3'-C2'	-5.40	98.24	103.10
1	AA	2608	DA	P-O3'-C3'	5.40	126.18	119.70
19	AS	13	DC	P-O3'-C3'	5.40	126.18	119.70
37	Ak	2	DA	N1-C6-N6	-5.40	115.36	118.60
1	AA	457	DA	O4'-C1'-C2'	-5.40	101.58	105.90
42	Ap	4	DT	O4'-C1'-C2'	-5.40	101.58	105.90
51	Ay	20	DT	C4'-C3'-C2'	-5.40	98.24	103.10
1	AA	1286	DA	C1'-O4'-C4'	-5.40	104.70	110.10
52	Az	25	DA	C4'-C3'-C2'	-5.40	98.24	103.10
50	Ax	37	DA	P-O3'-C3'	5.40	126.17	119.70
68	BF	22	DC	O4'-C1'-C2'	-5.40	101.58	105.90
13	AM	42	DC	C2-N1-C1'	5.39	124.73	118.80
37	Ak	24	DG	O4'-C1'-C2'	-5.39	101.59	105.90
1	AA	1430	DG	C1'-O4'-C4'	-5.39	104.71	110.10
1	AA	559	DA	C4'-C3'-C2'	-5.39	98.25	103.10
41	Ao	20	DG	O4'-C1'-C2'	-5.39	101.59	105.90
63	BA	22	DA	P-O3'-C3'	5.38	126.16	119.70
54	A1	40	DT	C6-C5-C7	-5.38	119.67	122.90
1	AA	1268	DG	O4'-C1'-C2'	-5.38	101.59	105.90
52	Az	11	DT	P-O3'-C3'	5.38	126.16	119.70
1	AA	931	DT	C1'-O4'-C4'	-5.38	104.72	110.10
1	AA	1179	DC	C4'-C3'-C2'	-5.38	98.26	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	AU	37	DG	O4'-C1'-C2'	-5.38	101.60	105.90
1	AA	2004	DG	N1-C6-O6	5.38	123.13	119.90
1	AA	252	DG	C1'-O4'-C4'	-5.37	104.73	110.10
1	AA	1771	DT	C4'-C3'-C2'	-5.37	98.26	103.10
46	At	15	DG	O4'-C1'-C2'	-5.37	101.60	105.90
68	BF	36	DC	O4'-C1'-C2'	-5.37	101.60	105.90
1	AA	1161	DT	O4'-C1'-C2'	-5.37	101.61	105.90
1	AA	2083	DT	P-O3'-C3'	5.37	126.14	119.70
1	AA	472	DT	C1'-O4'-C4'	-5.37	104.73	110.10
45	As	47	DG	O4'-C1'-C2'	-5.37	101.61	105.90
1	AA	1019	DT	O4'-C4'-C3'	-5.36	102.35	104.50
40	An	30	DG	O4'-C1'-C2'	-5.36	101.61	105.90
74	BL	37	DG	O4'-C1'-C2'	-5.36	101.61	105.90
65	BC	14	DG	O4'-C1'-N9	5.36	111.75	108.00
1	AA	2004	DG	C5-C6-O6	-5.36	125.39	128.60
24	AX	13	DT	C4'-C3'-C2'	-5.36	98.28	103.10
1	AA	293	DT	C4'-C3'-C2'	-5.36	98.28	103.10
1	AA	2254	DG	P-O3'-C3'	5.36	126.13	119.70
1	AA	2856	DT	O4'-C4'-C3'	-5.35	102.36	104.50
1	AA	2618	DC	C6-N1-C2	-5.35	118.16	120.30
1	AA	2779	DG	N1-C6-O6	5.35	123.11	119.90
10	AJ	14	DC	C4'-C3'-C2'	-5.35	98.28	103.10
78	BP	30	DT	C1'-O4'-C4'	-5.35	104.75	110.10
1	AA	104	DT	P-O3'-C3'	5.35	126.12	119.70
74	BL	18	DG	O4'-C1'-C2'	-5.35	101.62	105.90
1	AA	959	DG	O4'-C1'-N9	5.34	111.74	108.00
1	AA	1950	DC	P-O3'-C3'	5.34	126.11	119.70
59	A6	23	DG	C1'-O4'-C4'	-5.34	104.76	110.10
1	AA	1382	DC	C6-N1-C2	-5.34	118.16	120.30
1	AA	1830	DG	P-O3'-C3'	5.34	126.11	119.70
1	AA	2771	DT	P-O3'-C3'	5.34	126.11	119.70
1	AA	1651	DG	O4'-C4'-C3'	-5.34	102.36	104.50
21	AU	31	DG	C4'-C3'-C2'	-5.34	98.30	103.10
22	AV	44	DT	C1'-O4'-C4'	-5.33	104.77	110.10
1	AA	366	DT	C4'-C3'-C2'	-5.33	98.30	103.10
1	AA	1214	DG	C5-C6-O6	-5.33	125.40	128.60
1	AA	2102	DG	O4'-C1'-C2'	-5.33	101.63	105.90
1	AA	270	DG	C5-C6-O6	-5.33	125.40	128.60
19	AS	36	DT	C1'-O4'-C4'	-5.33	104.77	110.10
40	An	30	DG	C1'-O4'-C4'	-5.33	104.77	110.10
56	A3	37	DT	C4'-C3'-C2'	-5.33	98.30	103.10
63	BA	9	DG	O4'-C1'-N9	5.33	111.73	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	739	DA	O4'-C1'-N9	5.32	111.73	108.00
1	AA	1472	DG	O4'-C1'-C2'	-5.32	101.64	105.90
10	AJ	1	DT	C1'-O4'-C4'	-5.32	104.78	110.10
1	AA	448	DC	P-O3'-C3'	5.32	126.09	119.70
1	AA	1882	DG	N3-C2-N2	5.32	123.62	119.90
1	AA	2133	DA	C4'-C3'-C2'	-5.32	98.31	103.10
1	AA	2689	DC	O4'-C1'-C2'	-5.32	101.64	105.90
11	AK	37	DC	O4'-C1'-C2'	-5.32	101.64	105.90
1	AA	520	DC	O4'-C1'-C2'	-5.32	101.64	105.90
21	AU	35	DC	C2-N1-C1'	5.32	124.65	118.80
39	Am	41	DC	P-O3'-C3'	5.32	126.08	119.70
49	Aw	30	DG	O4'-C1'-C2'	-5.32	101.65	105.90
1	AA	31	DC	O4'-C1'-C2'	-5.32	101.65	105.90
1	AA	1265	DG	C1'-O4'-C4'	-5.32	104.78	110.10
30	Ad	19	DG	O4'-C1'-N9	5.31	111.72	108.00
52	Az	20	DC	C4'-C3'-C2'	-5.31	98.32	103.10
38	Al	2	DG	C4'-C3'-C2'	-5.31	98.32	103.10
39	Am	14	DC	O4'-C1'-C2'	-5.31	101.65	105.90
71	BI	16	DT	C4'-C3'-C2'	-5.31	98.32	103.10
1	AA	2488	DG	O4'-C1'-N9	5.31	111.72	108.00
65	BC	9	DT	C4'-C3'-C2'	-5.31	98.32	103.10
72	BJ	26	DC	O4'-C4'-C3'	-5.31	102.38	104.50
55	A2	5	DT	C4'-C3'-C2'	-5.31	98.32	103.10
60	A7	13	DT	C4'-C3'-C2'	-5.31	98.32	103.10
1	AA	961	DT	C4'-C3'-C2'	-5.31	98.32	103.10
6	AF	11	DT	O4'-C1'-N1	5.31	111.72	108.00
1	AA	1410	DG	C5-C6-O6	-5.30	125.42	128.60
1	AA	2154	DG	N1-C6-O6	5.30	123.08	119.90
67	BE	22	DG	C1'-O4'-C4'	-5.30	104.80	110.10
1	AA	1873	DC	O4'-C1'-C2'	-5.30	101.66	105.90
1	AA	689	DG	C4'-C3'-C2'	-5.30	98.33	103.10
50	Ax	19	DC	C4'-C3'-C2'	-5.30	98.33	103.10
1	AA	2077	DA	O4'-C1'-C2'	-5.30	101.66	105.90
10	AJ	10	DC	P-O5'-C5'	5.30	129.38	120.90
39	Am	12	DC	O4'-C1'-C2'	-5.30	101.66	105.90
1	AA	1330	DG	C5-C6-O6	-5.29	125.42	128.60
3	AC	1	DT	C4'-C3'-C2'	-5.29	98.33	103.10
55	A2	12	DG	O4'-C1'-C2'	-5.29	101.67	105.90
1	AA	2615	DC	C4'-C3'-C2'	-5.29	98.34	103.10
29	Ac	16	DC	O4'-C1'-C2'	-5.29	101.67	105.90
1	AA	2854	DT	C4'-C3'-C2'	-5.29	98.34	103.10
25	AY	22	DT	C4'-C3'-C2'	-5.28	98.34	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
76	BN	31	DT	O4'-C1'-C2'	-5.28	101.67	105.90
1	AA	288	DA	O4'-C1'-N9	5.28	111.70	108.00
1	AA	2136	DG	C1'-O4'-C4'	-5.28	104.82	110.10
1	AA	410	DC	P-O5'-C5'	5.28	129.35	120.90
1	AA	389	DG	C5-C6-O6	-5.28	125.43	128.60
41	Ao	1	DA	O4'-C4'-C3'	-5.28	102.39	104.50
56	A3	26	DG	O4'-C1'-C2'	-5.28	101.68	105.90
14	AN	3	DG	C4'-C3'-C2'	-5.27	98.35	103.10
1	AA	779	DA	N1-C6-N6	-5.27	115.44	118.60
1	AA	2373	DG	C5-C6-O6	-5.27	125.44	128.60
54	A1	26	DG	C1'-O4'-C4'	-5.27	104.83	110.10
1	AA	2164	DA	O4'-C1'-C2'	-5.27	101.68	105.90
40	An	14	DG	C4'-C3'-C2'	-5.27	98.36	103.10
1	AA	1325	DG	O4'-C1'-C2'	-5.27	101.68	105.90
1	AA	1371	DG	C1'-O4'-C4'	-5.27	104.83	110.10
1	AA	547	DT	C1'-O4'-C4'	-5.27	104.83	110.10
1	AA	1271	DA	O4'-C1'-C2'	-5.27	101.69	105.90
1	AA	1428	DG	C3'-C2'-C1'	-5.27	96.18	102.50
1	AA	2498	DG	C5-C6-O6	-5.27	125.44	128.60
13	AM	13	DT	C4'-C3'-C2'	-5.27	98.36	103.10
22	AV	16	DG	O4'-C1'-C2'	-5.27	101.69	105.90
79	BQ	6	DG	N3-C2-N2	5.27	123.59	119.90
1	AA	1739	DC	O4'-C1'-C2'	-5.27	101.69	105.90
1	AA	391	DA	N1-C6-N6	-5.26	115.44	118.60
49	Aw	10	DG	O4'-C1'-C2'	-5.26	101.69	105.90
1	AA	2466	DA	O4'-C1'-C2'	-5.26	101.69	105.90
59	A6	3	DT	P-O3'-C3'	5.26	126.01	119.70
32	Af	22	DT	C6-C5-C7	-5.26	119.75	122.90
57	A4	23	DT	C1'-O4'-C4'	-5.26	104.84	110.10
1	AA	2408	DC	O4'-C1'-C2'	-5.25	101.70	105.90
1	AA	1298	DA	N1-C6-N6	-5.25	115.45	118.60
3	AC	47	DC	C1'-O4'-C4'	-5.25	104.85	110.10
76	BN	15	DG	O4'-C1'-C2'	-5.25	101.70	105.90
76	BN	26	DA	N1-C6-N6	-5.25	115.45	118.60
1	AA	1298	DA	O4'-C1'-C2'	-5.25	101.70	105.90
1	AA	1612	DG	O4'-C1'-C2'	-5.25	101.70	105.90
15	AO	2	DA	O4'-C1'-C2'	-5.25	101.70	105.90
1	AA	309	DG	O4'-C1'-C2'	-5.25	101.70	105.90
1	AA	1963	DG	C1'-O4'-C4'	-5.25	104.85	110.10
25	AY	3	DT	P-O3'-C3'	5.25	126.00	119.70
32	Af	14	DT	O4'-C4'-C3'	-5.25	102.40	104.50
36	Aj	9	DC	O4'-C1'-C2'	-5.25	101.70	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2052	DA	N1-C6-N6	-5.25	115.45	118.60
1	AA	1628	DG	C1'-O4'-C4'	-5.24	104.86	110.10
1	AA	1454	DG	C1'-O4'-C4'	-5.24	104.86	110.10
1	AA	2702	DG	N1-C6-O6	5.24	123.05	119.90
4	AD	14	DT	P-O3'-C3'	5.24	125.99	119.70
47	Au	33	DC	C1'-O4'-C4'	-5.24	104.86	110.10
1	AA	2433	DG	O4'-C1'-C2'	-5.24	101.71	105.90
63	BA	17	DA	O4'-C1'-C2'	-5.24	101.71	105.90
72	BJ	33	DT	C1'-O4'-C4'	-5.24	104.86	110.10
1	AA	887	DC	O4'-C1'-N1	5.23	111.66	108.00
1	AA	2565	DA	N1-C6-N6	-5.23	115.46	118.60
49	Aw	32	DC	C4'-C3'-C2'	-5.23	98.39	103.10
1	AA	4	DG	C5-C6-O6	-5.23	125.46	128.60
1	AA	1316	DG	O4'-C1'-C2'	-5.23	101.72	105.90
78	BP	8	DA	C1'-O4'-C4'	-5.23	104.87	110.10
1	AA	479	DA	C1'-O4'-C4'	-5.23	104.87	110.10
63	BA	5	DG	C4'-C3'-C2'	-5.22	98.40	103.10
1	AA	2448	DG	P-O3'-C3'	5.22	125.97	119.70
1	AA	2203	DT	C6-C5-C7	5.22	126.03	122.90
11	AK	9	DT	O4'-C1'-C2'	-5.22	101.72	105.90
48	Av	37	DG	P-O3'-C3'	5.22	125.96	119.70
1	AA	2544	DG	P-O3'-C3'	5.22	125.96	119.70
65	BC	1	DA	N1-C6-N6	-5.22	115.47	118.60
74	BL	37	DG	C1'-O4'-C4'	-5.22	104.88	110.10
1	AA	2650	DG	O4'-C1'-C2'	-5.21	101.73	105.90
16	AP	34	DT	O4'-C1'-C2'	-5.21	101.73	105.90
51	Ay	2	DG	C4'-C3'-C2'	-5.21	98.41	103.10
48	Av	20	DC	C4'-C3'-C2'	-5.21	98.41	103.10
54	A1	45	DT	C2-N1-C1'	5.21	126.54	118.20
1	AA	1660	DG	O4'-C1'-C2'	-5.21	101.73	105.90
1	AA	1884	DA	P-O3'-C3'	5.21	125.95	119.70
1	AA	2420	DG	C4'-C3'-C2'	-5.21	98.41	103.10
42	Ap	11	DG	O4'-C1'-C2'	-5.21	101.73	105.90
1	AA	582	DA	O4'-C1'-C2'	-5.21	101.74	105.90
1	AA	639	DA	O4'-C4'-C3'	-5.21	102.42	104.50
1	AA	2330	DT	C4'-C3'-C2'	-5.21	98.41	103.10
52	Az	32	DG	O4'-C1'-C2'	-5.21	101.73	105.90
1	AA	149	DT	C1'-O4'-C4'	-5.21	104.89	110.10
35	Ai	8	DG	C5-C6-O6	-5.20	125.48	128.60
1	AA	507	DA	O4'-C1'-C2'	-5.20	101.74	105.90
1	AA	1333	DA	O4'-C1'-C2'	-5.20	101.74	105.90
1	AA	2644	DC	P-O5'-C5'	5.20	129.22	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2397	DA	P-O3'-C3'	5.20	125.94	119.70
1	AA	2431	DG	C4'-C3'-C2'	-5.20	98.42	103.10
2	AB	11	DC	C6-N1-C2	-5.20	118.22	120.30
34	Ah	8	DA	O4'-C1'-C2'	-5.20	101.74	105.90
1	AA	1550	DG	O4'-C1'-N9	5.20	111.64	108.00
75	BM	26	DG	O4'-C1'-C2'	-5.20	101.74	105.90
8	AH	29	DG	O4'-C1'-N9	5.20	111.64	108.00
52	Az	32	DG	O4'-C1'-N9	5.20	111.64	108.00
1	AA	687	DA	N1-C6-N6	5.19	121.72	118.60
1	AA	747	DG	O4'-C1'-N9	5.19	111.64	108.00
1	AA	1214	DG	N1-C6-O6	5.19	123.02	119.90
1	AA	1286	DA	O4'-C1'-N9	5.19	111.64	108.00
15	AO	8	DG	O4'-C1'-C2'	-5.19	101.75	105.90
63	BA	30	DA	O4'-C1'-N9	5.19	111.64	108.00
1	AA	1142	DA	P-O3'-C3'	5.19	125.93	119.70
1	AA	1356	DC	P-O3'-C3'	5.19	125.93	119.70
1	AA	2725	DT	C4'-C3'-C2'	-5.19	98.43	103.10
1	AA	318	DT	C4'-C3'-C2'	-5.18	98.43	103.10
15	AO	16	DA	C4'-C3'-C2'	-5.18	98.43	103.10
29	Ac	19	DG	O4'-C1'-N9	5.18	111.63	108.00
75	BM	4	DT	C4'-C3'-C2'	-5.18	98.44	103.10
1	AA	600	DA	C4'-C3'-C2'	-5.18	98.44	103.10
18	AR	4	DT	C6-C5-C7	-5.18	119.79	122.90
22	AV	28	DC	O4'-C1'-C2'	-5.18	101.75	105.90
34	Ah	12	DT	O4'-C4'-C3'	-5.18	102.43	104.50
1	AA	103	DT	C4'-C3'-C2'	-5.18	98.44	103.10
1	AA	2374	DA	O4'-C1'-C2'	-5.18	101.76	105.90
37	Ak	9	DT	C1'-O4'-C4'	-5.18	104.92	110.10
64	BB	41	DT	P-O3'-C3'	5.18	125.91	119.70
1	AA	156	DC	O4'-C1'-C2'	-5.18	101.76	105.90
1	AA	597	DG	C1'-O4'-C4'	-5.17	104.93	110.10
1	AA	1244	DA	N1-C6-N6	5.17	121.70	118.60
1	AA	117	DA	O4'-C1'-C2'	-5.17	101.76	105.90
1	AA	2852	DA	O4'-C4'-C3'	-5.17	102.43	104.50
10	AJ	13	DC	C2-N1-C1'	5.17	124.49	118.80
1	AA	2435	DA	N1-C6-N6	-5.17	115.50	118.60
35	Ai	6	DG	N1-C6-O6	5.17	123.00	119.90
1	AA	2672	DG	N1-C6-O6	5.17	123.00	119.90
1	AA	1851	DA	C1'-O4'-C4'	-5.16	104.94	110.10
7	AG	29	DG	C1'-O4'-C4'	-5.16	104.94	110.10
28	Ab	29	DG	N1-C6-O6	5.16	123.00	119.90
74	BL	3	DG	O4'-C1'-C2'	-5.16	101.77	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	897	DG	O4'-C1'-C2'	-5.16	101.77	105.90
10	AJ	13	DC	C6-N1-C2	-5.16	118.24	120.30
1	AA	371	DT	P-O3'-C3'	5.16	125.89	119.70
1	AA	1547	DT	O4'-C4'-C3'	-5.16	102.44	104.50
1	AA	1968	DC	O4'-C1'-C2'	-5.16	101.77	105.90
1	AA	804	DG	O4'-C1'-C2'	-5.16	101.77	105.90
26	AZ	26	DT	O4'-C1'-C2'	-5.16	101.77	105.90
1	AA	1829	DT	C4'-C3'-C2'	-5.16	98.46	103.10
40	An	23	DG	O4'-C1'-C2'	-5.15	101.78	105.90
76	BN	30	DT	P-O3'-C3'	5.15	125.89	119.70
1	AA	1458	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	2122	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	1997	DG	O4'-C1'-C2'	-5.15	101.78	105.90
22	AV	31	DG	O4'-C4'-C3'	-5.15	102.44	104.50
1	AA	604	DG	P-O3'-C3'	5.15	125.88	119.70
1	AA	282	DG	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	1375	DT	O4'-C1'-C2'	-5.15	101.78	105.90
21	AU	17	DT	C4'-C3'-C2'	-5.15	98.47	103.10
78	BP	12	DT	C4'-C3'-C2'	-5.15	98.47	103.10
1	AA	1601	DG	O4'-C1'-C2'	-5.15	101.78	105.90
11	AK	10	DT	C4'-C3'-C2'	-5.15	98.47	103.10
1	AA	506	DC	C2-N1-C1'	5.14	124.46	118.80
78	BP	6	DC	C1'-O4'-C4'	-5.14	104.96	110.10
79	BQ	20	DA	P-O3'-C3'	5.14	125.87	119.70
1	AA	679	DT	O4'-C1'-C2'	-5.14	101.79	105.90
1	AA	1385	DG	O4'-C1'-N9	5.14	111.60	108.00
1	AA	2665	DG	C1'-O4'-C4'	-5.14	104.96	110.10
18	AR	23	DC	C1'-O4'-C4'	-5.13	104.97	110.10
41	Ao	9	DA	O4'-C1'-C2'	-5.13	101.79	105.90
1	AA	1673	DT	C4'-C3'-C2'	-5.13	98.48	103.10
36	Aj	29	DG	O4'-C1'-C2'	-5.13	101.79	105.90
1	AA	1749	DA	N1-C6-N6	-5.13	115.52	118.60
30	Ad	24	DA	C4'-C3'-C2'	-5.13	98.48	103.10
1	AA	511	DG	C1'-O4'-C4'	-5.13	104.97	110.10
14	AN	7	DT	C4'-C3'-C2'	-5.13	98.48	103.10
1	AA	1698	DC	C4'-C3'-C2'	-5.13	98.48	103.10
1	AA	1786	DT	O4'-C4'-C3'	-5.13	102.45	104.50
1	AA	2204	DC	P-O3'-C3'	5.13	125.85	119.70
56	A3	16	DG	C1'-O4'-C4'	-5.13	104.97	110.10
73	BK	6	DG	C1'-O4'-C4'	-5.13	104.97	110.10
1	AA	2040	DG	C1'-O4'-C4'	-5.13	104.97	110.10
1	AA	2145	DT	C4'-C3'-C2'	-5.13	98.49	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	128	DT	C4'-C3'-C2'	-5.12	98.49	103.10
1	AA	1790	DC	C4'-C3'-C2'	-5.12	98.49	103.10
11	AK	40	DA	P-O3'-C3'	5.12	125.85	119.70
12	AL	13	DG	C5-C6-O6	-5.12	125.53	128.60
34	Ah	21	DG	O4'-C1'-C2'	-5.12	101.80	105.90
43	Aq	12	DG	C5-C6-O6	-5.12	125.53	128.60
1	AA	260	DC	O4'-C1'-C2'	-5.12	101.80	105.90
78	BP	30	DT	C4-C5-C7	-5.12	115.93	119.00
1	AA	520	DC	C1'-O4'-C4'	-5.12	104.98	110.10
13	AM	42	DC	O4'-C1'-N1	-5.12	104.42	108.00
38	Al	9	DC	O4'-C1'-C2'	-5.12	101.81	105.90
1	AA	1586	DG	O4'-C1'-C2'	-5.12	101.81	105.90
8	AH	15	DT	C4'-C3'-C2'	-5.11	98.50	103.10
11	AK	35	DT	O4'-C1'-C2'	-5.11	101.81	105.90
1	AA	855	DA	O4'-C1'-C2'	-5.11	101.81	105.90
1	AA	886	DC	O4'-C1'-N1	5.11	111.58	108.00
1	AA	900	DG	C1'-O4'-C4'	-5.11	104.99	110.10
1	AA	1240	DA	O4'-C1'-C2'	-5.11	101.81	105.90
1	AA	1566	DA	P-O3'-C3'	5.11	125.83	119.70
16	AP	47	DA	C4'-C3'-C2'	-5.11	98.50	103.10
22	AV	21	DA	P-O3'-C3'	5.11	125.83	119.70
59	A6	23	DG	C5-C6-O6	-5.11	125.53	128.60
77	BO	25	DA	O4'-C4'-C3'	-5.11	102.46	104.50
1	AA	74	DG	C4'-C3'-C2'	-5.11	98.50	103.10
1	AA	359	DG	O4'-C1'-C2'	-5.11	101.81	105.90
1	AA	1343	DG	N1-C6-O6	5.11	122.96	119.90
11	AK	36	DT	C6-C5-C7	-5.11	119.84	122.90
45	As	34	DG	O4'-C4'-C3'	-5.11	102.46	104.50
27	Aa	12	DA	O4'-C1'-C2'	-5.10	101.82	105.90
1	AA	1605	DA	C1'-O4'-C4'	-5.10	105.00	110.10
1	AA	2444	DG	C1'-O4'-C4'	-5.10	105.00	110.10
41	Ao	10	DT	O4'-C1'-C2'	-5.10	101.82	105.90
1	AA	1882	DG	C5-C6-O6	-5.10	125.54	128.60
1	AA	1325	DG	P-O3'-C3'	5.10	125.82	119.70
44	Ar	47	DG	O4'-C1'-C2'	-5.10	101.82	105.90
1	AA	2307	DC	C6-N1-C2	-5.10	118.26	120.30
1	AA	2693	DG	O4'-C1'-C2'	-5.10	101.82	105.90
1	AA	1307	DT	C4'-C3'-C2'	-5.09	98.52	103.10
1	AA	1910	DA	P-O3'-C3'	5.09	125.81	119.70
7	AG	10	DG	C1'-O4'-C4'	-5.09	105.01	110.10
11	AK	41	DA	O4'-C1'-C2'	-5.09	101.83	105.90
35	Ai	27	DG	C5-C6-O6	-5.09	125.55	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	524	DG	O4'-C1'-N9	5.09	111.56	108.00
1	AA	2498	DG	N1-C6-O6	5.09	122.95	119.90
75	BM	30	DG	C1'-O4'-C4'	-5.09	105.01	110.10
3	AC	21	DT	O4'-C4'-C3'	-5.09	102.47	104.50
75	BM	37	DG	O4'-C1'-C2'	-5.09	101.83	105.90
1	AA	1043	DT	P-O3'-C3'	5.09	125.80	119.70
1	AA	1622	DA	P-O5'-C5'	5.08	129.03	120.90
22	AV	9	DC	C1'-O4'-C4'	-5.08	105.02	110.10
51	Ay	23	DG	O4'-C1'-C2'	-5.08	101.83	105.90
1	AA	1529	DA	O4'-C1'-C2'	-5.08	101.83	105.90
32	Af	30	DT	P-O3'-C3'	5.08	125.80	119.70
52	Az	31	DA	C1'-O4'-C4'	-5.08	105.02	110.10
1	AA	121	DG	C1'-O4'-C4'	-5.08	105.02	110.10
47	Au	42	DA	O4'-C1'-C2'	-5.08	101.84	105.90
1	AA	2700	DA	O4'-C1'-C2'	-5.08	101.84	105.90
1	AA	561	DG	C1'-O4'-C4'	-5.08	105.02	110.10
1	AA	1678	DT	C1'-O4'-C4'	-5.08	105.02	110.10
1	AA	2213	DC	O4'-C1'-N1	5.08	111.55	108.00
50	Ax	18	DA	C5-C6-N6	5.08	127.76	123.70
50	Ax	28	DC	C6-N1-C2	-5.08	118.27	120.30
33	Ag	24	DT	C4'-C3'-C2'	-5.07	98.53	103.10
1	AA	1937	DA	N1-C6-N6	5.07	121.64	118.60
49	Aw	31	DG	C5-C6-O6	-5.07	125.56	128.60
1	AA	959	DG	O4'-C1'-C2'	-5.07	101.85	105.90
1	AA	2427	DA	C1'-O4'-C4'	-5.07	105.03	110.10
32	Af	8	DA	O4'-C1'-C2'	-5.07	101.85	105.90
1	AA	727	DC	P-O5'-C5'	5.07	129.00	120.90
1	AA	1145	DG	O4'-C1'-C2'	-5.07	101.85	105.90
1	AA	1313	DA	C1'-O4'-C4'	-5.06	105.04	110.10
54	A1	27	DG	P-O3'-C3'	5.06	125.78	119.70
1	AA	1553	DA	C4'-C3'-C2'	-5.06	98.54	103.10
1	AA	2507	DT	O4'-C1'-C2'	-5.06	101.85	105.90
42	Ap	5	DT	O4'-C1'-C2'	-5.06	101.85	105.90
74	BL	12	DG	O4'-C1'-C2'	-5.06	101.85	105.90
1	AA	1454	DG	O4'-C1'-N9	5.06	111.54	108.00
1	AA	1505	DC	O4'-C1'-N1	5.06	111.54	108.00
1	AA	1647	DG	O4'-C1'-C2'	-5.06	101.85	105.90
1	AA	2421	DC	P-O5'-C5'	5.06	129.00	120.90
8	AH	1	DA	O4'-C4'-C3'	-5.06	102.48	104.50
44	Ar	23	DA	C3'-C2'-C1'	-5.06	96.43	102.50
1	AA	2209	DT	C4'-C3'-C2'	-5.06	98.55	103.10
1	AA	2511	DG	C5-C6-O6	-5.06	125.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	Ay	27	DT	O4'-C1'-N1	-5.06	104.46	108.00
1	AA	22	DT	C1'-O4'-C4'	-5.05	105.05	110.10
1	AA	2488	DG	C1'-O4'-C4'	-5.05	105.05	110.10
1	AA	2838	DG	C4'-C3'-C2'	-5.05	98.55	103.10
72	BJ	40	DG	N1-C6-O6	5.05	122.93	119.90
79	BQ	33	DT	C4'-C3'-C2'	-5.05	98.55	103.10
1	AA	1483	DG	N3-C2-N2	5.05	123.44	119.90
18	AR	4	DT	C4-C5-C7	5.05	122.03	119.00
1	AA	1107	DG	O4'-C1'-C2'	-5.05	101.86	105.90
1	AA	1405	DG	C4'-C3'-C2'	-5.05	98.56	103.10
1	AA	539	DG	P-O3'-C3'	5.05	125.75	119.70
1	AA	1250	DA	P-O3'-C3'	5.05	125.76	119.70
37	Ak	13	DT	O4'-C4'-C3'	-5.04	102.48	104.50
65	BC	10	DA	P-O3'-C3'	5.04	125.75	119.70
46	At	46	DG	O4'-C1'-C2'	-5.04	101.86	105.90
1	AA	111	DT	O4'-C1'-C2'	-5.04	101.87	105.90
1	AA	1708	DG	O4'-C1'-C2'	-5.04	101.87	105.90
1	AA	2475	DG	N1-C6-O6	5.04	122.92	119.90
54	A1	45	DT	C6-N1-C1'	-5.04	112.84	120.40
79	BQ	1	DT	O4'-C4'-C3'	-5.04	102.48	104.50
1	AA	1538	DC	P-O3'-C3'	-5.04	113.65	119.70
33	Ag	20	DG	O4'-C1'-C2'	-5.04	101.87	105.90
1	AA	286	DA	N1-C6-N6	-5.04	115.58	118.60
1	AA	2031	DG	C5-C6-O6	-5.04	125.58	128.60
1	AA	2698	DC	P-O3'-C3'	5.04	125.75	119.70
1	AA	2822	DT	O4'-C4'-C3'	-5.04	102.48	104.50
76	BN	1	DT	C1'-O4'-C4'	-5.04	105.06	110.10
1	AA	1547	DT	C4'-C3'-C2'	-5.04	98.57	103.10
50	Ax	37	DA	C3'-C2'-C1'	-5.04	96.46	102.50
23	AW	41	DA	P-O3'-C3'	5.04	125.74	119.70
73	BK	1	DT	C4'-C3'-C2'	-5.03	98.57	103.10
35	Ai	21	DA	C4'-C3'-C2'	-5.03	98.57	103.10
1	AA	372	DA	P-O3'-C3'	5.03	125.74	119.70
1	AA	401	DC	O4'-C1'-N1	5.03	111.52	108.00
1	AA	605	DC	C6-N1-C2	-5.03	118.29	120.30
1	AA	1755	DA	O4'-C1'-C2'	-5.03	101.88	105.90
1	AA	1997	DG	O4'-C1'-N9	5.03	111.52	108.00
1	AA	2657	DA	O4'-C4'-C3'	-5.03	102.49	104.50
1	AA	1225	DT	C4'-C3'-C2'	-5.03	98.57	103.10
1	AA	876	DG	O4'-C1'-C2'	-5.03	101.88	105.90
1	AA	2794	DC	C4'-C3'-C2'	-5.03	98.58	103.10
20	AT	30	DA	C1'-O4'-C4'	-5.03	105.07	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	Ar	20	DT	C4'-C3'-C2'	-5.03	98.58	103.10
70	BH	9	DG	O4'-C1'-C2'	-5.03	101.88	105.90
1	AA	1026	DG	O4'-C1'-C2'	-5.02	101.88	105.90
1	AA	1937	DA	C5-C6-N6	-5.02	119.68	123.70
1	AA	1758	DA	N1-C6-N6	-5.02	115.59	118.60
22	AV	16	DG	P-O3'-C3'	5.02	125.72	119.70
67	BE	9	DG	P-O3'-C3'	5.02	125.72	119.70
71	BI	40	DA	O4'-C1'-C2'	-5.02	101.89	105.90
1	AA	6	DA	P-O5'-C5'	5.02	128.93	120.90
1	AA	1941	DC	C1'-O4'-C4'	-5.02	105.08	110.10
1	AA	2763	DT	C4'-C3'-C2'	-5.02	98.58	103.10
68	BF	30	DG	C4'-C3'-C2'	-5.02	98.58	103.10
56	A3	16	DG	O4'-C1'-C2'	-5.02	101.89	105.90
1	AA	1173	DT	C4'-C3'-C2'	-5.01	98.59	103.10
50	Ax	27	DG	C5-C6-O6	-5.01	125.59	128.60
1	AA	570	DG	O4'-C1'-C2'	-5.01	101.89	105.90
23	AW	40	DC	C2-N1-C1'	5.01	124.31	118.80
1	AA	2219	DT	C6-C5-C7	-5.01	119.89	122.90
32	Af	5	DA	C1'-O4'-C4'	-5.01	105.09	110.10
49	Aw	30	DG	C1'-O4'-C4'	-5.01	105.09	110.10
1	AA	881	DT	O4'-C1'-C2'	-5.01	101.89	105.90
24	AX	24	DC	C2-N1-C1'	5.01	124.31	118.80
1	AA	1187	DC	C2-N1-C1'	5.00	124.31	118.80
48	Av	12	DA	P-O3'-C3'	5.00	125.70	119.70
1	AA	1818	DG	O4'-C1'-N9	5.00	111.50	108.00
43	Aq	8	DC	C4'-C3'-C2'	-5.00	98.60	103.10
45	As	23	DA	C1'-O4'-C4'	-5.00	105.10	110.10
45	As	37	DC	O4'-C1'-C2'	-5.00	101.90	105.90
66	BD	5	DG	O4'-C1'-C2'	-5.00	101.90	105.90

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	342	DG	C3'
1	AA	738	DC	C3'
1	AA	1302	DA	C3'
1	AA	1360	DC	C3'
1	AA	1774	DG	C3'
1	AA	1908	DT	C3'
1	AA	2278	DG	C3'
1	AA	2390	DG	C3'
1	AA	2740	DC	C3'

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Mol	Chain	Res	Type	Atom
1	AA	2852	DA	C3'
19	AS	37	DG	C3'
25	AY	5	DT	C3'

All (1459) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	A0	18	DA	Sidechain
53	A0	2	DC	Sidechain
53	A0	22	DC	Sidechain
53	A0	6	DG	Sidechain
53	A0	8	DG	Sidechain
53	A0	9	DT	Sidechain
54	A1	10	DC	Sidechain
54	A1	17	DA	Sidechain
54	A1	22	DG	Sidechain
54	A1	26	DG	Sidechain
54	A1	30	DA	Sidechain
54	A1	32	DT	Sidechain
54	A1	37	DG	Sidechain
54	A1	4	DG	Sidechain
54	A1	41	DT	Sidechain
54	A1	6	DG	Sidechain
55	A2	13	DG	Sidechain
55	A2	14	DG	Sidechain
55	A2	15	DG	Sidechain
55	A2	18	DA	Sidechain
55	A2	20	DG	Sidechain
55	A2	22	DA	Sidechain
55	A2	24	DG	Sidechain
55	A2	29	DA	Sidechain
55	A2	31	DT	Sidechain
55	A2	32	DT	Sidechain
55	A2	5	DT	Sidechain
55	A2	7	DT	Sidechain
55	A2	9	DT	Sidechain
56	A3	10	DG	Sidechain
56	A3	11	DT	Sidechain
56	A3	13	DT	Sidechain
56	A3	15	DC	Sidechain
56	A3	19	DG	Sidechain
56	A3	20	DA	Sidechain

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Mol	Chain	Res	Type	Group
56	A3	21	DA	Sidechain
56	A3	28	DT	Sidechain
56	A3	4	DT	Sidechain
56	A3	7	DA	Sidechain
56	A3	8	DT	Sidechain
57	A4	1	DC	Sidechain
57	A4	12	DC	Sidechain
57	A4	18	DA	Sidechain
57	A4	23	DT	Sidechain
57	A4	24	DA	Sidechain
57	A4	29	DA	Sidechain
57	A4	31	DT	Sidechain
57	A4	34	DG	Sidechain
57	A4	37	DC	Sidechain
57	A4	38	DC	Sidechain
58	A5	18	DC	Sidechain
58	A5	25	DA	Sidechain
58	A5	26	DG	Sidechain
58	A5	29	DT	Sidechain
58	A5	3	DA	Sidechain
58	A5	6	DA	Sidechain
58	A5	8	DA	Sidechain
59	A6	17	DT	Sidechain
59	A6	18	DT	Sidechain
59	A6	19	DG	Sidechain
59	A6	3	DT	Sidechain
59	A6	9	DG	Sidechain
60	A7	23	DA	Sidechain
60	A7	28	DT	Sidechain
60	A7	31	DT	Sidechain
60	A7	32	DT	Sidechain
60	A7	5	DT	Sidechain
60	A7	9	DG	Sidechain
61	A8	12	DG	Sidechain
61	A8	13	DT	Sidechain
61	A8	19	DT	Sidechain
61	A8	7	DT	Sidechain
62	A9	15	DG	Sidechain
62	A9	19	DT	Sidechain
62	A9	25	DT	Sidechain
62	A9	26	DC	Sidechain
62	A9	28	DA	Sidechain

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Mol	Chain	Res	Type	Group
62	A9	37	DA	Sidechain
62	A9	38	DG	Sidechain
62	A9	40	DG	Sidechain
62	A9	41	DA	Sidechain
62	A9	6	DG	Sidechain
1	AA	1002	DG	Sidechain
1	AA	1014	DA	Sidechain
1	AA	1015	DT	Sidechain
1	AA	1023	DA	Sidechain
1	AA	103	DT	Sidechain
1	AA	1030	DT	Sidechain
1	AA	1033	DA	Sidechain
1	AA	1040	DT	Sidechain
1	AA	1042	DT	Sidechain
1	AA	1048	DT	Sidechain
1	AA	1059	DT	Sidechain
1	AA	1061	DG	Sidechain
1	AA	1063	DT	Sidechain
1	AA	1066	DA	Sidechain
1	AA	1068	DA	Sidechain
1	AA	1069	DT	Sidechain
1	AA	1078	DA	Sidechain
1	AA	1082	DT	Sidechain
1	AA	1084	DT	Sidechain
1	AA	1086	DA	Sidechain
1	AA	1101	DT	Sidechain
1	AA	1106	DT	Sidechain
1	AA	111	DT	Sidechain
1	AA	1110	DT	Sidechain
1	AA	1112	DT	Sidechain
1	AA	1113	DT	Sidechain
1	AA	1121	DC	Sidechain
1	AA	1124	DA	Sidechain
1	AA	1127	DG	Sidechain
1	AA	113	DT	Sidechain
1	AA	1130	DA	Sidechain
1	AA	1135	DC	Sidechain
1	AA	1137	DG	Sidechain
1	AA	1138	DT	Sidechain
1	AA	1149	DA	Sidechain
1	AA	1150	DA	Sidechain
1	AA	1158	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	116	DA	Sidechain
1	AA	1161	DT	Sidechain
1	AA	1162	DG	Sidechain
1	AA	1163	DA	Sidechain
1	AA	1166	DT	Sidechain
1	AA	1167	DC	Sidechain
1	AA	1171	DT	Sidechain
1	AA	1172	DT	Sidechain
1	AA	1173	DT	Sidechain
1	AA	1175	DT	Sidechain
1	AA	1180	DG	Sidechain
1	AA	1185	DA	Sidechain
1	AA	1189	DG	Sidechain
1	AA	1190	DC	Sidechain
1	AA	1192	DG	Sidechain
1	AA	1203	DA	Sidechain
1	AA	1209	DC	Sidechain
1	AA	1213	DC	Sidechain
1	AA	1214	DG	Sidechain
1	AA	1215	DC	Sidechain
1	AA	1217	DA	Sidechain
1	AA	122	DG	Sidechain
1	AA	1221	DG	Sidechain
1	AA	1223	DG	Sidechain
1	AA	1226	DG	Sidechain
1	AA	1227	DG	Sidechain
1	AA	1228	DT	Sidechain
1	AA	1229	DT	Sidechain
1	AA	1234	DT	Sidechain
1	AA	1236	DC	Sidechain
1	AA	1237	DC	Sidechain
1	AA	1239	DG	Sidechain
1	AA	1240	DA	Sidechain
1	AA	1245	DG	Sidechain
1	AA	1246	DA	Sidechain
1	AA	1259	DT	Sidechain
1	AA	1266	DA	Sidechain
1	AA	127	DG	Sidechain
1	AA	1270	DT	Sidechain
1	AA	1273	DC	Sidechain
1	AA	1274	DT	Sidechain
1	AA	1276	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1277	DC	Sidechain
1	AA	1287	DG	Sidechain
1	AA	1289	DG	Sidechain
1	AA	129	DA	Sidechain
1	AA	1290	DC	Sidechain
1	AA	1294	DT	Sidechain
1	AA	1295	DA	Sidechain
1	AA	1299	DA	Sidechain
1	AA	13	DG	Sidechain
1	AA	1302	DA	Sidechain
1	AA	1308	DC	Sidechain
1	AA	131	DG	Sidechain
1	AA	1310	DT	Sidechain
1	AA	132	DA	Sidechain
1	AA	1323	DT	Sidechain
1	AA	1326	DT	Sidechain
1	AA	1327	DT	Sidechain
1	AA	1329	DG	Sidechain
1	AA	133	DG	Sidechain
1	AA	1333	DA	Sidechain
1	AA	1338	DT	Sidechain
1	AA	134	DT	Sidechain
1	AA	1343	DG	Sidechain
1	AA	1346	DC	Sidechain
1	AA	1350	DG	Sidechain
1	AA	1353	DG	Sidechain
1	AA	1357	DC	Sidechain
1	AA	136	DT	Sidechain
1	AA	1361	DT	Sidechain
1	AA	1367	DC	Sidechain
1	AA	1373	DT	Sidechain
1	AA	1377	DC	Sidechain
1	AA	1380	DA	Sidechain
1	AA	1381	DT	Sidechain
1	AA	1382	DC	Sidechain
1	AA	1384	DT	Sidechain
1	AA	1392	DG	Sidechain
1	AA	1398	DG	Sidechain
1	AA	14	DG	Sidechain
1	AA	1403	DC	Sidechain
1	AA	1405	DG	Sidechain
1	AA	1409	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1410	DG	Sidechain
1	AA	1411	DA	Sidechain
1	AA	1412	DT	Sidechain
1	AA	1413	DA	Sidechain
1	AA	1426	DC	Sidechain
1	AA	1428	DG	Sidechain
1	AA	1429	DG	Sidechain
1	AA	1441	DG	Sidechain
1	AA	1443	DC	Sidechain
1	AA	1447	DA	Sidechain
1	AA	1449	DT	Sidechain
1	AA	145	DT	Sidechain
1	AA	1462	DC	Sidechain
1	AA	1467	DC	Sidechain
1	AA	1468	DG	Sidechain
1	AA	1469	DG	Sidechain
1	AA	147	DC	Sidechain
1	AA	1471	DC	Sidechain
1	AA	1476	DT	Sidechain
1	AA	1481	DG	Sidechain
1	AA	1482	DG	Sidechain
1	AA	1484	DG	Sidechain
1	AA	1485	DG	Sidechain
1	AA	149	DT	Sidechain
1	AA	1490	DG	Sidechain
1	AA	1496	DA	Sidechain
1	AA	1505	DC	Sidechain
1	AA	1509	DG	Sidechain
1	AA	1521	DT	Sidechain
1	AA	153	DG	Sidechain
1	AA	1530	DC	Sidechain
1	AA	1534	DG	Sidechain
1	AA	1536	DT	Sidechain
1	AA	1537	DA	Sidechain
1	AA	1539	DC	Sidechain
1	AA	1541	DA	Sidechain
1	AA	1548	DG	Sidechain
1	AA	1550	DG	Sidechain
1	AA	1555	DG	Sidechain
1	AA	156	DC	Sidechain
1	AA	1561	DG	Sidechain
1	AA	1566	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1567	DC	Sidechain
1	AA	1568	DG	Sidechain
1	AA	1570	DT	Sidechain
1	AA	1573	DC	Sidechain
1	AA	1574	DC	Sidechain
1	AA	1579	DG	Sidechain
1	AA	159	DA	Sidechain
1	AA	1605	DA	Sidechain
1	AA	1607	DC	Sidechain
1	AA	161	DT	Sidechain
1	AA	1617	DG	Sidechain
1	AA	162	DC	Sidechain
1	AA	1623	DG	Sidechain
1	AA	1634	DG	Sidechain
1	AA	1637	DG	Sidechain
1	AA	1638	DG	Sidechain
1	AA	1639	DA	Sidechain
1	AA	1640	DG	Sidechain
1	AA	1648	DG	Sidechain
1	AA	165	DT	Sidechain
1	AA	1656	DG	Sidechain
1	AA	1658	DC	Sidechain
1	AA	1668	DT	Sidechain
1	AA	1671	DA	Sidechain
1	AA	1672	DG	Sidechain
1	AA	1676	DT	Sidechain
1	AA	1681	DG	Sidechain
1	AA	1683	DT	Sidechain
1	AA	1685	DT	Sidechain
1	AA	1688	DC	Sidechain
1	AA	1690	DA	Sidechain
1	AA	1691	DC	Sidechain
1	AA	1695	DT	Sidechain
1	AA	1698	DC	Sidechain
1	AA	1701	DG	Sidechain
1	AA	1703	DG	Sidechain
1	AA	1704	DC	Sidechain
1	AA	171	DG	Sidechain
1	AA	1716	DT	Sidechain
1	AA	172	DC	Sidechain
1	AA	1720	DG	Sidechain
1	AA	1721	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1723	DC	Sidechain
1	AA	1728	DG	Sidechain
1	AA	173	DG	Sidechain
1	AA	1731	DG	Sidechain
1	AA	1733	DG	Sidechain
1	AA	1737	DA	Sidechain
1	AA	1738	DG	Sidechain
1	AA	174	DG	Sidechain
1	AA	1746	DA	Sidechain
1	AA	1753	DC	Sidechain
1	AA	1758	DA	Sidechain
1	AA	176	DA	Sidechain
1	AA	1761	DG	Sidechain
1	AA	1762	DC	Sidechain
1	AA	1763	DG	Sidechain
1	AA	1768	DT	Sidechain
1	AA	177	DT	Sidechain
1	AA	1784	DC	Sidechain
1	AA	1786	DT	Sidechain
1	AA	1792	DG	Sidechain
1	AA	1794	DC	Sidechain
1	AA	1796	DT	Sidechain
1	AA	1806	DA	Sidechain
1	AA	1808	DG	Sidechain
1	AA	181	DG	Sidechain
1	AA	1811	DC	Sidechain
1	AA	1812	DT	Sidechain
1	AA	1813	DT	Sidechain
1	AA	1814	DT	Sidechain
1	AA	1818	DG	Sidechain
1	AA	1819	DC	Sidechain
1	AA	1820	DG	Sidechain
1	AA	1824	DT	Sidechain
1	AA	1826	DC	Sidechain
1	AA	1827	DC	Sidechain
1	AA	1828	DC	Sidechain
1	AA	1830	DG	Sidechain
1	AA	1832	DT	Sidechain
1	AA	1835	DT	Sidechain
1	AA	1837	DT	Sidechain
1	AA	1840	DA	Sidechain
1	AA	1846	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1852	DC	Sidechain
1	AA	1854	DG	Sidechain
1	AA	1855	DC	Sidechain
1	AA	1858	DT	Sidechain
1	AA	1863	DT	Sidechain
1	AA	1865	DA	Sidechain
1	AA	1867	DC	Sidechain
1	AA	1871	DT	Sidechain
1	AA	1876	DC	Sidechain
1	AA	1877	DT	Sidechain
1	AA	1879	DG	Sidechain
1	AA	188	DT	Sidechain
1	AA	1882	DG	Sidechain
1	AA	1886	DC	Sidechain
1	AA	1893	DA	Sidechain
1	AA	1894	DC	Sidechain
1	AA	1895	DC	Sidechain
1	AA	1900	DG	Sidechain
1	AA	1907	DG	Sidechain
1	AA	1916	DC	Sidechain
1	AA	1917	DG	Sidechain
1	AA	1918	DA	Sidechain
1	AA	1919	DG	Sidechain
1	AA	1923	DG	Sidechain
1	AA	1924	DC	Sidechain
1	AA	1927	DA	Sidechain
1	AA	1931	DG	Sidechain
1	AA	194	DT	Sidechain
1	AA	1941	DC	Sidechain
1	AA	1942	DG	Sidechain
1	AA	1949	DG	Sidechain
1	AA	195	DG	Sidechain
1	AA	1953	DC	Sidechain
1	AA	1959	DG	Sidechain
1	AA	1960	DC	Sidechain
1	AA	1963	DG	Sidechain
1	AA	1964	DT	Sidechain
1	AA	1967	DG	Sidechain
1	AA	1969	DC	Sidechain
1	AA	1970	DG	Sidechain
1	AA	1972	DT	Sidechain
1	AA	1976	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1977	DT	Sidechain
1	AA	1987	DG	Sidechain
1	AA	1988	DG	Sidechain
1	AA	1989	DC	Sidechain
1	AA	1994	DC	Sidechain
1	AA	1995	DA	Sidechain
1	AA	1997	DG	Sidechain
1	AA	2000	DT	Sidechain
1	AA	2002	DC	Sidechain
1	AA	2005	DA	Sidechain
1	AA	2007	DT	Sidechain
1	AA	2010	DA	Sidechain
1	AA	2013	DG	Sidechain
1	AA	2018	DC	Sidechain
1	AA	202	DC	Sidechain
1	AA	2022	DG	Sidechain
1	AA	2024	DG	Sidechain
1	AA	2027	DC	Sidechain
1	AA	203	DA	Sidechain
1	AA	2030	DC	Sidechain
1	AA	204	DG	Sidechain
1	AA	2043	DA	Sidechain
1	AA	2044	DG	Sidechain
1	AA	2045	DT	Sidechain
1	AA	2055	DC	Sidechain
1	AA	2056	DA	Sidechain
1	AA	2060	DG	Sidechain
1	AA	2063	DA	Sidechain
1	AA	2066	DC	Sidechain
1	AA	2068	DA	Sidechain
1	AA	2069	DG	Sidechain
1	AA	2070	DG	Sidechain
1	AA	2076	DC	Sidechain
1	AA	2083	DT	Sidechain
1	AA	2086	DT	Sidechain
1	AA	2089	DC	Sidechain
1	AA	209	DG	Sidechain
1	AA	2090	DG	Sidechain
1	AA	2094	DC	Sidechain
1	AA	2095	DG	Sidechain
1	AA	21	DG	Sidechain
1	AA	2103	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2109	DA	Sidechain
1	AA	211	DT	Sidechain
1	AA	2111	DT	Sidechain
1	AA	2112	DG	Sidechain
1	AA	2116	DG	Sidechain
1	AA	2117	DC	Sidechain
1	AA	2120	DA	Sidechain
1	AA	2121	DT	Sidechain
1	AA	2123	DA	Sidechain
1	AA	2127	DT	Sidechain
1	AA	2143	DG	Sidechain
1	AA	2145	DT	Sidechain
1	AA	2152	DA	Sidechain
1	AA	216	DA	Sidechain
1	AA	2172	DT	Sidechain
1	AA	2179	DG	Sidechain
1	AA	2186	DA	Sidechain
1	AA	2191	DG	Sidechain
1	AA	2196	DC	Sidechain
1	AA	2198	DG	Sidechain
1	AA	2199	DG	Sidechain
1	AA	22	DT	Sidechain
1	AA	2201	DC	Sidechain
1	AA	2203	DT	Sidechain
1	AA	2206	DT	Sidechain
1	AA	2209	DT	Sidechain
1	AA	2210	DA	Sidechain
1	AA	2217	DG	Sidechain
1	AA	2223	DG	Sidechain
1	AA	2224	DC	Sidechain
1	AA	223	DA	Sidechain
1	AA	2232	DG	Sidechain
1	AA	2235	DT	Sidechain
1	AA	2238	DT	Sidechain
1	AA	224	DA	Sidechain
1	AA	2242	DG	Sidechain
1	AA	2243	DG	Sidechain
1	AA	2245	DT	Sidechain
1	AA	2251	DT	Sidechain
1	AA	2255	DC	Sidechain
1	AA	2261	DG	Sidechain
1	AA	2264	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2265	DG	Sidechain
1	AA	227	DT	Sidechain
1	AA	2277	DC	Sidechain
1	AA	228	DG	Sidechain
1	AA	2281	DG	Sidechain
1	AA	2282	DT	Sidechain
1	AA	2287	DG	Sidechain
1	AA	2289	DG	Sidechain
1	AA	229	DC	Sidechain
1	AA	2291	DA	Sidechain
1	AA	2295	DC	Sidechain
1	AA	2297	DT	Sidechain
1	AA	2299	DG	Sidechain
1	AA	2307	DC	Sidechain
1	AA	2311	DT	Sidechain
1	AA	2316	DC	Sidechain
1	AA	2317	DG	Sidechain
1	AA	2318	DC	Sidechain
1	AA	2325	DG	Sidechain
1	AA	2332	DC	Sidechain
1	AA	2334	DC	Sidechain
1	AA	2336	DT	Sidechain
1	AA	234	DG	Sidechain
1	AA	2344	DG	Sidechain
1	AA	2348	DG	Sidechain
1	AA	2354	DT	Sidechain
1	AA	2357	DC	Sidechain
1	AA	2367	DC	Sidechain
1	AA	2368	DG	Sidechain
1	AA	2372	DC	Sidechain
1	AA	2374	DA	Sidechain
1	AA	2375	DT	Sidechain
1	AA	2380	DC	Sidechain
1	AA	2381	DT	Sidechain
1	AA	2391	DT	Sidechain
1	AA	2396	DC	Sidechain
1	AA	2397	DA	Sidechain
1	AA	2400	DC	Sidechain
1	AA	2402	DG	Sidechain
1	AA	2404	DA	Sidechain
1	AA	2407	DG	Sidechain
1	AA	2411	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2416	DA	Sidechain
1	AA	242	DG	Sidechain
1	AA	2427	DA	Sidechain
1	AA	2428	DG	Sidechain
1	AA	2429	DC	Sidechain
1	AA	2432	DC	Sidechain
1	AA	2433	DG	Sidechain
1	AA	2435	DA	Sidechain
1	AA	2442	DG	Sidechain
1	AA	2443	DC	Sidechain
1	AA	2444	DG	Sidechain
1	AA	2446	DC	Sidechain
1	AA	2448	DG	Sidechain
1	AA	2449	DG	Sidechain
1	AA	2452	DT	Sidechain
1	AA	2453	DG	Sidechain
1	AA	2454	DG	Sidechain
1	AA	2455	DT	Sidechain
1	AA	2458	DT	Sidechain
1	AA	2459	DT	Sidechain
1	AA	2464	DG	Sidechain
1	AA	2466	DA	Sidechain
1	AA	2467	DG	Sidechain
1	AA	2484	DG	Sidechain
1	AA	2488	DG	Sidechain
1	AA	2489	DC	Sidechain
1	AA	249	DC	Sidechain
1	AA	2491	DC	Sidechain
1	AA	2492	DC	Sidechain
1	AA	2493	DC	Sidechain
1	AA	2497	DC	Sidechain
1	AA	2499	DC	Sidechain
1	AA	2503	DC	Sidechain
1	AA	2505	DC	Sidechain
1	AA	2506	DC	Sidechain
1	AA	2507	DT	Sidechain
1	AA	2509	DT	Sidechain
1	AA	2512	DC	Sidechain
1	AA	2523	DT	Sidechain
1	AA	2526	DT	Sidechain
1	AA	253	DT	Sidechain
1	AA	2530	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2531	DC	Sidechain
1	AA	2532	DG	Sidechain
1	AA	2535	DA	Sidechain
1	AA	2538	DT	Sidechain
1	AA	2542	DC	Sidechain
1	AA	2544	DG	Sidechain
1	AA	2547	DT	Sidechain
1	AA	2552	DC	Sidechain
1	AA	2553	DC	Sidechain
1	AA	2554	DG	Sidechain
1	AA	2559	DG	Sidechain
1	AA	2560	DC	Sidechain
1	AA	2561	DT	Sidechain
1	AA	2563	DT	Sidechain
1	AA	2564	DA	Sidechain
1	AA	2565	DA	Sidechain
1	AA	257	DT	Sidechain
1	AA	2571	DG	Sidechain
1	AA	2578	DC	Sidechain
1	AA	258	DT	Sidechain
1	AA	2580	DT	Sidechain
1	AA	2581	DT	Sidechain
1	AA	2583	DG	Sidechain
1	AA	2584	DG	Sidechain
1	AA	2593	DT	Sidechain
1	AA	2594	DT	Sidechain
1	AA	2597	DT	Sidechain
1	AA	2598	DG	Sidechain
1	AA	2600	DT	Sidechain
1	AA	2605	DG	Sidechain
1	AA	2606	DG	Sidechain
1	AA	2609	DC	Sidechain
1	AA	2610	DC	Sidechain
1	AA	2618	DC	Sidechain
1	AA	2629	DA	Sidechain
1	AA	2630	DT	Sidechain
1	AA	2632	DA	Sidechain
1	AA	2638	DA	Sidechain
1	AA	2640	DG	Sidechain
1	AA	2642	DT	Sidechain
1	AA	2654	DG	Sidechain
1	AA	2655	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2656	DC	Sidechain
1	AA	2661	DC	Sidechain
1	AA	2663	DC	Sidechain
1	AA	2666	DA	Sidechain
1	AA	2673	DG	Sidechain
1	AA	2675	DT	Sidechain
1	AA	2676	DT	Sidechain
1	AA	2682	DC	Sidechain
1	AA	2687	DG	Sidechain
1	AA	269	DG	Sidechain
1	AA	2691	DT	Sidechain
1	AA	270	DG	Sidechain
1	AA	2700	DA	Sidechain
1	AA	2704	DT	Sidechain
1	AA	2706	DT	Sidechain
1	AA	2708	DT	Sidechain
1	AA	2710	DA	Sidechain
1	AA	2711	DT	Sidechain
1	AA	2718	DC	Sidechain
1	AA	2723	DG	Sidechain
1	AA	2724	DT	Sidechain
1	AA	2725	DT	Sidechain
1	AA	2727	DC	Sidechain
1	AA	2729	DA	Sidechain
1	AA	273	DC	Sidechain
1	AA	2730	DA	Sidechain
1	AA	2735	DA	Sidechain
1	AA	2742	DC	Sidechain
1	AA	2746	DA	Sidechain
1	AA	2748	DC	Sidechain
1	AA	2755	DC	Sidechain
1	AA	2756	DG	Sidechain
1	AA	2758	DT	Sidechain
1	AA	2762	DT	Sidechain
1	AA	2765	DT	Sidechain
1	AA	2766	DT	Sidechain
1	AA	2771	DT	Sidechain
1	AA	2779	DG	Sidechain
1	AA	2780	DG	Sidechain
1	AA	2784	DT	Sidechain
1	AA	2786	DG	Sidechain
1	AA	2788	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2790	DA	Sidechain
1	AA	2795	DG	Sidechain
1	AA	280	DG	Sidechain
1	AA	2803	DG	Sidechain
1	AA	2804	DG	Sidechain
1	AA	2805	DT	Sidechain
1	AA	2806	DT	Sidechain
1	AA	2811	DA	Sidechain
1	AA	2816	DG	Sidechain
1	AA	2825	DA	Sidechain
1	AA	2835	DA	Sidechain
1	AA	2840	DG	Sidechain
1	AA	2846	DT	Sidechain
1	AA	2847	DA	Sidechain
1	AA	2852	DA	Sidechain
1	AA	2856	DT	Sidechain
1	AA	286	DA	Sidechain
1	AA	2862	DC	Sidechain
1	AA	2869	DT	Sidechain
1	AA	288	DA	Sidechain
1	AA	289	DT	Sidechain
1	AA	292	DT	Sidechain
1	AA	294	DG	Sidechain
1	AA	295	DA	Sidechain
1	AA	296	DG	Sidechain
1	AA	297	DA	Sidechain
1	AA	3	DG	Sidechain
1	AA	30	DA	Sidechain
1	AA	305	DC	Sidechain
1	AA	307	DC	Sidechain
1	AA	31	DC	Sidechain
1	AA	32	DC	Sidechain
1	AA	331	DG	Sidechain
1	AA	333	DA	Sidechain
1	AA	335	DT	Sidechain
1	AA	337	DT	Sidechain
1	AA	342	DG	Sidechain
1	AA	344	DT	Sidechain
1	AA	351	DT	Sidechain
1	AA	352	DG	Sidechain
1	AA	353	DT	Sidechain
1	AA	355	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	356	DC	Sidechain
1	AA	360	DG	Sidechain
1	AA	361	DT	Sidechain
1	AA	370	DG	Sidechain
1	AA	38	DT	Sidechain
1	AA	382	DG	Sidechain
1	AA	389	DG	Sidechain
1	AA	392	DA	Sidechain
1	AA	401	DC	Sidechain
1	AA	402	DC	Sidechain
1	AA	415	DC	Sidechain
1	AA	419	DG	Sidechain
1	AA	420	DA	Sidechain
1	AA	423	DG	Sidechain
1	AA	427	DT	Sidechain
1	AA	43	DT	Sidechain
1	AA	433	DA	Sidechain
1	AA	434	DG	Sidechain
1	AA	435	DT	Sidechain
1	AA	438	DT	Sidechain
1	AA	444	DG	Sidechain
1	AA	447	DA	Sidechain
1	AA	454	DA	Sidechain
1	AA	458	DT	Sidechain
1	AA	469	DG	Sidechain
1	AA	470	DC	Sidechain
1	AA	471	DA	Sidechain
1	AA	481	DG	Sidechain
1	AA	483	DG	Sidechain
1	AA	49	DT	Sidechain
1	AA	490	DG	Sidechain
1	AA	495	DG	Sidechain
1	AA	497	DT	Sidechain
1	AA	5	DC	Sidechain
1	AA	504	DA	Sidechain
1	AA	510	DA	Sidechain
1	AA	515	DT	Sidechain
1	AA	522	DG	Sidechain
1	AA	524	DG	Sidechain
1	AA	529	DA	Sidechain
1	AA	530	DC	Sidechain
1	AA	534	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	535	DT	Sidechain
1	AA	539	DG	Sidechain
1	AA	545	DG	Sidechain
1	AA	55	DT	Sidechain
1	AA	561	DG	Sidechain
1	AA	57	DC	Sidechain
1	AA	579	DC	Sidechain
1	AA	585	DA	Sidechain
1	AA	589	DG	Sidechain
1	AA	59	DT	Sidechain
1	AA	590	DG	Sidechain
1	AA	592	DA	Sidechain
1	AA	593	DT	Sidechain
1	AA	61	DC	Sidechain
1	AA	610	DA	Sidechain
1	AA	621	DC	Sidechain
1	AA	626	DG	Sidechain
1	AA	627	DC	Sidechain
1	AA	628	DT	Sidechain
1	AA	632	DT	Sidechain
1	AA	637	DC	Sidechain
1	AA	641	DA	Sidechain
1	AA	647	DC	Sidechain
1	AA	648	DG	Sidechain
1	AA	65	DT	Sidechain
1	AA	653	DG	Sidechain
1	AA	657	DG	Sidechain
1	AA	664	DC	Sidechain
1	AA	667	DT	Sidechain
1	AA	668	DG	Sidechain
1	AA	67	DT	Sidechain
1	AA	671	DT	Sidechain
1	AA	678	DA	Sidechain
1	AA	681	DG	Sidechain
1	AA	687	DA	Sidechain
1	AA	688	DC	Sidechain
1	AA	691	DT	Sidechain
1	AA	694	DG	Sidechain
1	AA	698	DA	Sidechain
1	AA	702	DT	Sidechain
1	AA	706	DC	Sidechain
1	AA	712	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	718	DT	Sidechain
1	AA	723	DC	Sidechain
1	AA	725	DA	Sidechain
1	AA	726	DG	Sidechain
1	AA	727	DC	Sidechain
1	AA	731	DC	Sidechain
1	AA	732	DC	Sidechain
1	AA	74	DG	Sidechain
1	AA	741	DT	Sidechain
1	AA	747	DG	Sidechain
1	AA	748	DA	Sidechain
1	AA	750	DT	Sidechain
1	AA	76	DT	Sidechain
1	AA	761	DG	Sidechain
1	AA	762	DG	Sidechain
1	AA	77	DC	Sidechain
1	AA	773	DA	Sidechain
1	AA	788	DC	Sidechain
1	AA	79	DT	Sidechain
1	AA	802	DC	Sidechain
1	AA	806	DC	Sidechain
1	AA	813	DA	Sidechain
1	AA	818	DT	Sidechain
1	AA	82	DG	Sidechain
1	AA	828	DG	Sidechain
1	AA	829	DG	Sidechain
1	AA	830	DA	Sidechain
1	AA	834	DG	Sidechain
1	AA	835	DG	Sidechain
1	AA	838	DA	Sidechain
1	AA	842	DT	Sidechain
1	AA	844	DG	Sidechain
1	AA	846	DT	Sidechain
1	AA	853	DG	Sidechain
1	AA	864	DG	Sidechain
1	AA	867	DC	Sidechain
1	AA	868	DT	Sidechain
1	AA	87	DT	Sidechain
1	AA	870	DG	Sidechain
1	AA	871	DG	Sidechain
1	AA	872	DG	Sidechain
1	AA	879	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	880	DG	Sidechain
1	AA	884	DG	Sidechain
1	AA	885	DC	Sidechain
1	AA	887	DC	Sidechain
1	AA	888	DT	Sidechain
1	AA	890	DC	Sidechain
1	AA	892	DG	Sidechain
1	AA	895	DT	Sidechain
1	AA	897	DG	Sidechain
1	AA	901	DT	Sidechain
1	AA	906	DT	Sidechain
1	AA	91	DC	Sidechain
1	AA	926	DA	Sidechain
1	AA	93	DT	Sidechain
1	AA	930	DA	Sidechain
1	AA	932	DG	Sidechain
1	AA	938	DA	Sidechain
1	AA	948	DC	Sidechain
1	AA	957	DG	Sidechain
1	AA	96	DT	Sidechain
1	AA	964	DG	Sidechain
1	AA	970	DC	Sidechain
1	AA	973	DT	Sidechain
1	AA	975	DA	Sidechain
1	AA	977	DT	Sidechain
1	AA	980	DG	Sidechain
1	AA	982	DA	Sidechain
1	AA	99	DA	Sidechain
1	AA	992	DG	Sidechain
1	AA	998	DC	Sidechain
2	AB	1	DT	Sidechain
2	AB	10	DC	Sidechain
2	AB	11	DC	Sidechain
2	AB	25	DG	Sidechain
2	AB	26	DT	Sidechain
2	AB	28	DG	Sidechain
2	AB	3	DC	Sidechain
2	AB	6	DA	Sidechain
3	AC	13	DC	Sidechain
3	AC	19	DG	Sidechain
3	AC	2	DG	Sidechain
3	AC	24	DT	Sidechain

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Mol	Chain	Res	Type	Group
3	AC	25	DT	Sidechain
3	AC	26	DG	Sidechain
3	AC	41	DA	Sidechain
3	AC	43	DG	Sidechain
3	AC	46	DA	Sidechain
4	AD	11	DC	Sidechain
4	AD	12	DC	Sidechain
4	AD	19	DC	Sidechain
4	AD	2	DA	Sidechain
4	AD	21	DA	Sidechain
4	AD	22	DA	Sidechain
4	AD	4	DG	Sidechain
4	AD	6	DA	Sidechain
5	AE	14	DG	Sidechain
5	AE	2	DC	Sidechain
5	AE	20	DA	Sidechain
5	AE	28	DA	Sidechain
5	AE	29	DA	Sidechain
5	AE	30	DG	Sidechain
5	AE	32	DT	Sidechain
5	AE	34	DG	Sidechain
5	AE	36	DT	Sidechain
5	AE	9	DT	Sidechain
6	AF	20	DG	Sidechain
6	AF	25	DT	Sidechain
6	AF	26	DC	Sidechain
6	AF	30	DG	Sidechain
6	AF	31	DT	Sidechain
6	AF	39	DA	Sidechain
6	AF	5	DG	Sidechain
6	AF	6	DC	Sidechain
7	AG	10	DG	Sidechain
7	AG	19	DT	Sidechain
7	AG	24	DT	Sidechain
7	AG	25	DA	Sidechain
7	AG	29	DG	Sidechain
7	AG	30	DC	Sidechain
7	AG	32	DC	Sidechain
7	AG	33	DA	Sidechain
7	AG	8	DG	Sidechain
7	AG	9	DA	Sidechain
8	AH	13	DG	Sidechain

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Mol	Chain	Res	Type	Group
8	AH	14	DT	Sidechain
8	AH	17	DC	Sidechain
8	AH	2	DG	Sidechain
8	AH	27	DC	Sidechain
8	AH	28	DA	Sidechain
8	AH	29	DG	Sidechain
8	AH	30	DG	Sidechain
8	AH	36	DT	Sidechain
8	AH	38	DT	Sidechain
8	AH	5	DG	Sidechain
8	AH	6	DT	Sidechain
9	AI	11	DA	Sidechain
9	AI	12	DA	Sidechain
9	AI	15	DG	Sidechain
9	AI	20	DG	Sidechain
9	AI	21	DT	Sidechain
9	AI	22	DG	Sidechain
9	AI	28	DG	Sidechain
9	AI	3	DT	Sidechain
9	AI	5	DT	Sidechain
10	AJ	13	DC	Sidechain
10	AJ	18	DG	Sidechain
10	AJ	19	DT	Sidechain
10	AJ	21	DC	Sidechain
10	AJ	28	DA	Sidechain
10	AJ	29	DC	Sidechain
10	AJ	3	DT	Sidechain
10	AJ	31	DT	Sidechain
10	AJ	32	DT	Sidechain
10	AJ	33	DT	Sidechain
11	AK	12	DG	Sidechain
11	AK	17	DG	Sidechain
11	AK	2	DA	Sidechain
11	AK	23	DA	Sidechain
11	AK	24	DG	Sidechain
11	AK	3	DG	Sidechain
11	AK	30	DT	Sidechain
11	AK	32	DG	Sidechain
11	AK	34	DG	Sidechain
11	AK	36	DT	Sidechain
11	AK	37	DC	Sidechain
11	AK	4	DT	Sidechain

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Mol	Chain	Res	Type	Group
11	AK	5	DT	Sidechain
12	AL	12	DG	Sidechain
12	AL	13	DG	Sidechain
12	AL	20	DT	Sidechain
12	AL	25	DA	Sidechain
12	AL	29	DG	Sidechain
12	AL	30	DA	Sidechain
12	AL	31	DA	Sidechain
12	AL	33	DA	Sidechain
12	AL	35	DG	Sidechain
12	AL	38	DG	Sidechain
12	AL	4	DG	Sidechain
12	AL	40	DG	Sidechain
12	AL	41	DG	Sidechain
13	AM	10	DC	Sidechain
13	AM	15	DT	Sidechain
13	AM	20	DC	Sidechain
13	AM	28	DC	Sidechain
13	AM	29	DT	Sidechain
13	AM	3	DT	Sidechain
13	AM	31	DT	Sidechain
13	AM	4	DA	Sidechain
13	AM	41	DG	Sidechain
13	AM	9	DT	Sidechain
14	AN	1	DA	Sidechain
14	AN	12	DG	Sidechain
14	AN	15	DC	Sidechain
14	AN	16	DG	Sidechain
14	AN	19	DG	Sidechain
14	AN	20	DA	Sidechain
14	AN	25	DG	Sidechain
14	AN	37	DG	Sidechain
14	AN	42	DC	Sidechain
14	AN	7	DT	Sidechain
14	AN	8	DC	Sidechain
15	AO	11	DA	Sidechain
15	AO	12	DA	Sidechain
15	AO	14	DG	Sidechain
15	AO	15	DT	Sidechain
15	AO	27	DG	Sidechain
15	AO	34	DG	Sidechain
15	AO	35	DC	Sidechain

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Mol	Chain	Res	Type	Group
15	AO	39	DG	Sidechain
15	AO	45	DG	Sidechain
16	AP	11	DG	Sidechain
16	AP	17	DG	Sidechain
16	AP	19	DT	Sidechain
16	AP	29	DG	Sidechain
16	AP	34	DT	Sidechain
16	AP	40	DG	Sidechain
16	AP	42	DC	Sidechain
16	AP	45	DT	Sidechain
17	AQ	11	DT	Sidechain
17	AQ	12	DC	Sidechain
17	AQ	14	DT	Sidechain
17	AQ	15	DC	Sidechain
17	AQ	18	DT	Sidechain
17	AQ	21	DC	Sidechain
17	AQ	23	DG	Sidechain
17	AQ	26	DT	Sidechain
17	AQ	7	DT	Sidechain
17	AQ	8	DG	Sidechain
18	AR	10	DG	Sidechain
18	AR	15	DG	Sidechain
18	AR	16	DC	Sidechain
18	AR	23	DC	Sidechain
18	AR	24	DT	Sidechain
18	AR	5	DT	Sidechain
18	AR	7	DC	Sidechain
19	AS	1	DT	Sidechain
19	AS	2	DT	Sidechain
19	AS	22	DG	Sidechain
19	AS	25	DA	Sidechain
19	AS	26	DG	Sidechain
19	AS	27	DA	Sidechain
19	AS	33	DG	Sidechain
19	AS	37	DG	Sidechain
19	AS	38	DT	Sidechain
19	AS	39	DT	Sidechain
19	AS	5	DT	Sidechain
20	AT	10	DC	Sidechain
20	AT	12	DC	Sidechain
20	AT	14	DG	Sidechain
20	AT	15	DG	Sidechain

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Mol	Chain	Res	Type	Group
20	AT	17	DC	Sidechain
20	AT	2	DC	Sidechain
20	AT	28	DG	Sidechain
20	AT	33	DC	Sidechain
20	AT	44	DA	Sidechain
20	AT	45	DG	Sidechain
20	AT	46	DT	Sidechain
20	AT	48	DT	Sidechain
20	AT	5	DA	Sidechain
20	AT	51	DT	Sidechain
20	AT	7	DC	Sidechain
20	AT	8	DG	Sidechain
21	AU	16	DC	Sidechain
21	AU	23	DC	Sidechain
21	AU	25	DG	Sidechain
21	AU	28	DG	Sidechain
21	AU	29	DG	Sidechain
21	AU	31	DG	Sidechain
21	AU	34	DT	Sidechain
21	AU	35	DC	Sidechain
21	AU	43	DC	Sidechain
21	AU	44	DG	Sidechain
21	AU	6	DT	Sidechain
21	AU	7	DA	Sidechain
21	AU	9	DT	Sidechain
22	AV	1	DG	Sidechain
22	AV	14	DG	Sidechain
22	AV	2	DA	Sidechain
22	AV	30	DG	Sidechain
22	AV	37	DG	Sidechain
22	AV	4	DT	Sidechain
22	AV	6	DG	Sidechain
22	AV	7	DC	Sidechain
23	AW	1	DG	Sidechain
23	AW	2	DG	Sidechain
23	AW	26	DC	Sidechain
23	AW	30	DA	Sidechain
23	AW	31	DG	Sidechain
23	AW	32	DC	Sidechain
23	AW	36	DA	Sidechain
23	AW	38	DG	Sidechain
23	AW	4	DA	Sidechain

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Mol	Chain	Res	Type	Group
24	AX	16	DT	Sidechain
24	AX	21	DT	Sidechain
24	AX	25	DC	Sidechain
24	AX	27	DC	Sidechain
24	AX	32	DC	Sidechain
24	AX	35	DT	Sidechain
24	AX	37	DG	Sidechain
24	AX	38	DG	Sidechain
24	AX	6	DC	Sidechain
24	AX	9	DA	Sidechain
25	AY	14	DC	Sidechain
25	AY	18	DT	Sidechain
25	AY	19	DT	Sidechain
25	AY	4	DT	Sidechain
25	AY	5	DT	Sidechain
26	AZ	12	DT	Sidechain
26	AZ	17	DC	Sidechain
26	AZ	18	DC	Sidechain
26	AZ	2	DT	Sidechain
26	AZ	26	DT	Sidechain
26	AZ	27	DA	Sidechain
26	AZ	3	DA	Sidechain
26	AZ	35	DC	Sidechain
26	AZ	36	DC	Sidechain
26	AZ	39	DA	Sidechain
26	AZ	4	DC	Sidechain
26	AZ	43	DA	Sidechain
26	AZ	46	DC	Sidechain
27	Aa	19	DA	Sidechain
27	Aa	32	DA	Sidechain
27	Aa	33	DA	Sidechain
27	Aa	35	DA	Sidechain
27	Aa	5	DC	Sidechain
27	Aa	6	DT	Sidechain
27	Aa	7	DA	Sidechain
28	Ab	13	DA	Sidechain
28	Ab	19	DC	Sidechain
28	Ab	20	DC	Sidechain
28	Ab	21	DC	Sidechain
28	Ab	23	DC	Sidechain
28	Ab	33	DA	Sidechain
28	Ab	39	DA	Sidechain

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Mol	Chain	Res	Type	Group
28	Ab	41	DG	Sidechain
29	Ac	1	DC	Sidechain
29	Ac	15	DG	Sidechain
29	Ac	16	DC	Sidechain
29	Ac	19	DG	Sidechain
29	Ac	2	DT	Sidechain
29	Ac	28	DT	Sidechain
29	Ac	3	DG	Sidechain
29	Ac	35	DT	Sidechain
29	Ac	41	DC	Sidechain
29	Ac	9	DG	Sidechain
30	Ad	12	DA	Sidechain
30	Ad	13	DT	Sidechain
30	Ad	15	DA	Sidechain
30	Ad	16	DT	Sidechain
30	Ad	17	DG	Sidechain
30	Ad	19	DG	Sidechain
30	Ad	21	DG	Sidechain
30	Ad	3	DT	Sidechain
30	Ad	4	DT	Sidechain
31	Ae	16	DG	Sidechain
31	Ae	2	DT	Sidechain
31	Ae	20	DA	Sidechain
31	Ae	31	DT	Sidechain
31	Ae	34	DC	Sidechain
31	Ae	4	DT	Sidechain
31	Ae	41	DT	Sidechain
31	Ae	5	DT	Sidechain
31	Ae	6	DT	Sidechain
31	Ae	7	DC	Sidechain
32	Af	16	DG	Sidechain
32	Af	18	DT	Sidechain
32	Af	21	DT	Sidechain
32	Af	24	DT	Sidechain
32	Af	30	DT	Sidechain
32	Af	32	DT	Sidechain
32	Af	6	DG	Sidechain
32	Af	7	DC	Sidechain
33	Ag	1	DT	Sidechain
33	Ag	19	DC	Sidechain
33	Ag	27	DC	Sidechain
33	Ag	28	DC	Sidechain

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Mol	Chain	Res	Type	Group
33	Ag	4	DT	Sidechain
33	Ag	9	DT	Sidechain
34	Ah	10	DC	Sidechain
34	Ah	11	DC	Sidechain
34	Ah	12	DT	Sidechain
34	Ah	2	DT	Sidechain
34	Ah	25	DC	Sidechain
34	Ah	28	DG	Sidechain
34	Ah	29	DA	Sidechain
34	Ah	3	DT	Sidechain
34	Ah	33	DT	Sidechain
34	Ah	6	DA	Sidechain
34	Ah	8	DA	Sidechain
35	Ai	1	DA	Sidechain
35	Ai	17	DA	Sidechain
35	Ai	24	DA	Sidechain
35	Ai	30	DT	Sidechain
35	Ai	34	DT	Sidechain
35	Ai	45	DA	Sidechain
35	Ai	46	DA	Sidechain
35	Ai	48	DA	Sidechain
35	Ai	7	DT	Sidechain
36	Aj	14	DG	Sidechain
36	Aj	17	DC	Sidechain
36	Aj	35	DG	Sidechain
36	Aj	36	DC	Sidechain
36	Aj	37	DT	Sidechain
36	Aj	4	DG	Sidechain
37	Ak	1	DT	Sidechain
37	Ak	16	DG	Sidechain
37	Ak	17	DG	Sidechain
37	Ak	3	DT	Sidechain
37	Ak	30	DT	Sidechain
37	Ak	34	DG	Sidechain
37	Ak	36	DT	Sidechain
37	Ak	37	DT	Sidechain
37	Ak	39	DC	Sidechain
37	Ak	46	DC	Sidechain
37	Ak	9	DT	Sidechain
38	Al	10	DC	Sidechain
38	Al	15	DG	Sidechain
38	Al	18	DG	Sidechain

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Mol	Chain	Res	Type	Group
38	Al	23	DG	Sidechain
38	Al	26	DA	Sidechain
38	Al	27	DA	Sidechain
38	Al	35	DG	Sidechain
38	Al	37	DG	Sidechain
38	Al	38	DA	Sidechain
38	Al	4	DG	Sidechain
38	Al	9	DC	Sidechain
39	Am	10	DG	Sidechain
39	Am	12	DC	Sidechain
39	Am	16	DC	Sidechain
39	Am	17	DT	Sidechain
39	Am	18	DT	Sidechain
39	Am	21	DT	Sidechain
39	Am	25	DG	Sidechain
39	Am	29	DG	Sidechain
39	Am	3	DA	Sidechain
39	Am	31	DG	Sidechain
39	Am	37	DT	Sidechain
39	Am	41	DC	Sidechain
40	An	11	DA	Sidechain
40	An	14	DG	Sidechain
40	An	17	DC	Sidechain
40	An	19	DT	Sidechain
40	An	22	DT	Sidechain
40	An	23	DG	Sidechain
40	An	31	DA	Sidechain
40	An	37	DT	Sidechain
40	An	40	DT	Sidechain
40	An	42	DA	Sidechain
40	An	5	DC	Sidechain
40	An	6	DT	Sidechain
41	Ao	10	DT	Sidechain
41	Ao	11	DT	Sidechain
41	Ao	12	DC	Sidechain
41	Ao	15	DG	Sidechain
41	Ao	18	DG	Sidechain
41	Ao	24	DT	Sidechain
41	Ao	25	DT	Sidechain
41	Ao	28	DT	Sidechain
41	Ao	3	DG	Sidechain
41	Ao	5	DC	Sidechain

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Mol	Chain	Res	Type	Group
42	Ap	17	DG	Sidechain
42	Ap	2	DT	Sidechain
42	Ap	22	DG	Sidechain
42	Ap	23	DA	Sidechain
42	Ap	26	DT	Sidechain
42	Ap	9	DT	Sidechain
43	Aq	12	DG	Sidechain
43	Aq	13	DT	Sidechain
43	Aq	25	DG	Sidechain
43	Aq	30	DC	Sidechain
43	Aq	36	DG	Sidechain
43	Aq	37	DT	Sidechain
43	Aq	6	DC	Sidechain
43	Aq	8	DC	Sidechain
44	Ar	10	DA	Sidechain
44	Ar	17	DT	Sidechain
44	Ar	20	DT	Sidechain
44	Ar	27	DT	Sidechain
44	Ar	3	DC	Sidechain
44	Ar	33	DT	Sidechain
44	Ar	38	DA	Sidechain
44	Ar	46	DC	Sidechain
44	Ar	47	DG	Sidechain
44	Ar	48	DT	Sidechain
44	Ar	49	DT	Sidechain
44	Ar	8	DA	Sidechain
45	As	10	DG	Sidechain
45	As	15	DC	Sidechain
45	As	17	DT	Sidechain
45	As	23	DA	Sidechain
45	As	25	DC	Sidechain
45	As	29	DC	Sidechain
45	As	33	DG	Sidechain
45	As	41	DT	Sidechain
45	As	42	DG	Sidechain
45	As	45	DC	Sidechain
45	As	6	DA	Sidechain
46	At	10	DC	Sidechain
46	At	11	DG	Sidechain
46	At	16	DC	Sidechain
46	At	20	DG	Sidechain
46	At	26	DA	Sidechain

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Mol	Chain	Res	Type	Group
46	At	37	DG	Sidechain
46	At	38	DC	Sidechain
46	At	39	DT	Sidechain
46	At	9	DG	Sidechain
47	Au	1	DT	Sidechain
47	Au	21	DT	Sidechain
47	Au	26	DC	Sidechain
47	Au	28	DG	Sidechain
47	Au	39	DT	Sidechain
47	Au	42	DA	Sidechain
47	Au	44	DC	Sidechain
47	Au	48	DA	Sidechain
47	Au	49	DC	Sidechain
48	Av	12	DA	Sidechain
48	Av	17	DC	Sidechain
48	Av	19	DG	Sidechain
48	Av	30	DT	Sidechain
48	Av	33	DT	Sidechain
48	Av	36	DG	Sidechain
48	Av	41	DC	Sidechain
48	Av	6	DA	Sidechain
48	Av	8	DA	Sidechain
49	Aw	1	DG	Sidechain
49	Aw	15	DC	Sidechain
49	Aw	19	DG	Sidechain
49	Aw	20	DC	Sidechain
49	Aw	23	DG	Sidechain
49	Aw	30	DG	Sidechain
49	Aw	31	DG	Sidechain
49	Aw	32	DC	Sidechain
49	Aw	39	DG	Sidechain
50	Ax	1	DA	Sidechain
50	Ax	10	DT	Sidechain
50	Ax	15	DG	Sidechain
50	Ax	19	DC	Sidechain
50	Ax	20	DG	Sidechain
50	Ax	22	DG	Sidechain
50	Ax	23	DC	Sidechain
50	Ax	24	DG	Sidechain
50	Ax	26	DC	Sidechain
50	Ax	27	DG	Sidechain
50	Ax	28	DC	Sidechain

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Mol	Chain	Res	Type	Group
50	Ax	30	DT	Sidechain
50	Ax	31	DA	Sidechain
50	Ax	33	DG	Sidechain
50	Ax	36	DC	Sidechain
50	Ax	38	DT	Sidechain
50	Ax	5	DT	Sidechain
50	Ax	7	DG	Sidechain
50	Ax	8	DT	Sidechain
51	Ay	10	DG	Sidechain
51	Ay	11	DT	Sidechain
51	Ay	13	DT	Sidechain
51	Ay	16	DG	Sidechain
51	Ay	2	DG	Sidechain
51	Ay	21	DC	Sidechain
51	Ay	28	DT	Sidechain
51	Ay	3	DT	Sidechain
51	Ay	30	DC	Sidechain
51	Ay	35	DG	Sidechain
51	Ay	39	DG	Sidechain
51	Ay	40	DC	Sidechain
51	Ay	41	DT	Sidechain
52	Az	2	DG	Sidechain
52	Az	29	DG	Sidechain
52	Az	3	DC	Sidechain
52	Az	30	DG	Sidechain
52	Az	33	DC	Sidechain
63	BA	15	DG	Sidechain
63	BA	17	DA	Sidechain
63	BA	27	DT	Sidechain
63	BA	28	DG	Sidechain
63	BA	3	DC	Sidechain
63	BA	30	DA	Sidechain
63	BA	4	DG	Sidechain
63	BA	5	DG	Sidechain
64	BB	1	DT	Sidechain
64	BB	12	DA	Sidechain
64	BB	13	DC	Sidechain
64	BB	15	DC	Sidechain
64	BB	18	DA	Sidechain
64	BB	19	DT	Sidechain
64	BB	31	DT	Sidechain
64	BB	34	DA	Sidechain

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Mol	Chain	Res	Type	Group
64	BB	42	DT	Sidechain
64	BB	44	DT	Sidechain
64	BB	5	DA	Sidechain
64	BB	7	DG	Sidechain
64	BB	8	DA	Sidechain
65	BC	10	DA	Sidechain
65	BC	13	DG	Sidechain
65	BC	16	DT	Sidechain
65	BC	2	DT	Sidechain
65	BC	20	DC	Sidechain
65	BC	23	DT	Sidechain
65	BC	24	DT	Sidechain
65	BC	35	DA	Sidechain
66	BD	10	DG	Sidechain
66	BD	14	DG	Sidechain
66	BD	22	DA	Sidechain
66	BD	23	DT	Sidechain
66	BD	28	DT	Sidechain
66	BD	8	DT	Sidechain
67	BE	14	DA	Sidechain
67	BE	18	DT	Sidechain
67	BE	20	DG	Sidechain
67	BE	3	DT	Sidechain
67	BE	4	DT	Sidechain
67	BE	6	DT	Sidechain
68	BF	1	DT	Sidechain
68	BF	13	DT	Sidechain
68	BF	14	DT	Sidechain
68	BF	21	DA	Sidechain
68	BF	23	DT	Sidechain
68	BF	27	DC	Sidechain
68	BF	34	DG	Sidechain
68	BF	35	DG	Sidechain
68	BF	37	DT	Sidechain
68	BF	6	DA	Sidechain
69	BG	10	DG	Sidechain
69	BG	11	DT	Sidechain
69	BG	12	DC	Sidechain
69	BG	18	DG	Sidechain
69	BG	21	DA	Sidechain
69	BG	26	DT	Sidechain
69	BG	30	DT	Sidechain

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Mol	Chain	Res	Type	Group
69	BG	31	DT	Sidechain
69	BG	32	DT	Sidechain
69	BG	33	DA	Sidechain
69	BG	5	DA	Sidechain
70	BH	1	DA	Sidechain
70	BH	16	DT	Sidechain
70	BH	18	DT	Sidechain
70	BH	19	DT	Sidechain
70	BH	3	DG	Sidechain
70	BH	41	DA	Sidechain
71	BI	16	DT	Sidechain
71	BI	17	DG	Sidechain
71	BI	18	DT	Sidechain
71	BI	19	DA	Sidechain
71	BI	32	DC	Sidechain
71	BI	37	DC	Sidechain
71	BI	5	DT	Sidechain
72	BJ	11	DG	Sidechain
72	BJ	14	DA	Sidechain
72	BJ	16	DT	Sidechain
72	BJ	18	DT	Sidechain
72	BJ	2	DT	Sidechain
72	BJ	25	DA	Sidechain
72	BJ	27	DC	Sidechain
72	BJ	37	DT	Sidechain
72	BJ	4	DT	Sidechain
72	BJ	6	DT	Sidechain
73	BK	11	DT	Sidechain
73	BK	23	DC	Sidechain
73	BK	26	DA	Sidechain
73	BK	27	DT	Sidechain
74	BL	13	DA	Sidechain
74	BL	21	DG	Sidechain
74	BL	27	DT	Sidechain
74	BL	30	DT	Sidechain
74	BL	31	DT	Sidechain
74	BL	40	DT	Sidechain
74	BL	7	DC	Sidechain
75	BM	10	DA	Sidechain
75	BM	15	DA	Sidechain
75	BM	20	DC	Sidechain
75	BM	22	DA	Sidechain

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Mol	Chain	Res	Type	Group
75	BM	3	DC	Sidechain
75	BM	30	DG	Sidechain
75	BM	37	DG	Sidechain
75	BM	38	DG	Sidechain
75	BM	39	DC	Sidechain
75	BM	4	DT	Sidechain
75	BM	43	DC	Sidechain
75	BM	46	DT	Sidechain
75	BM	48	DA	Sidechain
75	BM	49	DA	Sidechain
76	BN	10	DT	Sidechain
76	BN	11	DA	Sidechain
76	BN	12	DT	Sidechain
76	BN	14	DA	Sidechain
76	BN	23	DG	Sidechain
76	BN	24	DT	Sidechain
76	BN	26	DA	Sidechain
76	BN	29	DG	Sidechain
76	BN	40	DT	Sidechain
76	BN	5	DG	Sidechain
77	BO	10	DT	Sidechain
77	BO	17	DA	Sidechain
77	BO	18	DT	Sidechain
77	BO	24	DA	Sidechain
77	BO	25	DA	Sidechain
77	BO	29	DC	Sidechain
77	BO	34	DT	Sidechain
77	BO	37	DC	Sidechain
77	BO	39	DT	Sidechain
78	BP	17	DG	Sidechain
78	BP	21	DA	Sidechain
78	BP	23	DG	Sidechain
79	BQ	11	DA	Sidechain
79	BQ	2	DT	Sidechain
79	BQ	23	DG	Sidechain
79	BQ	37	DT	Sidechain
79	BQ	5	DT	Sidechain
79	BQ	6	DG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein molecules in this entry.

5.3.2 Protein sidechains

There are no protein molecules in this entry.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

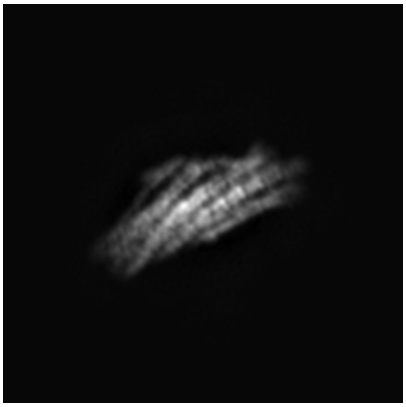
6 Map visualisation

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

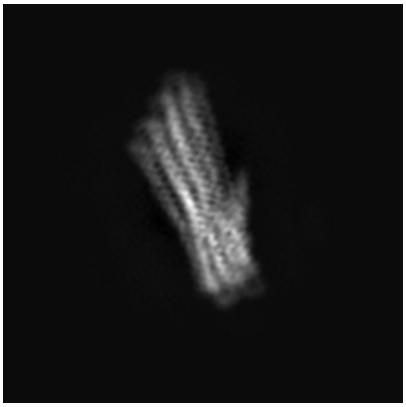
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

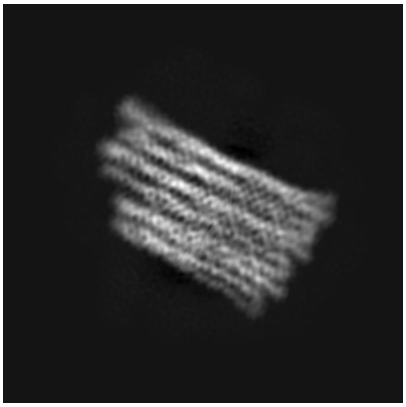
6.1.1 Primary map



X



Y



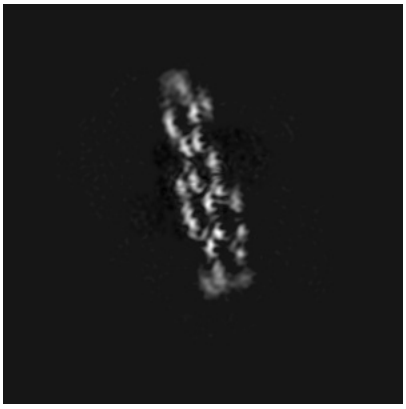
Z

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

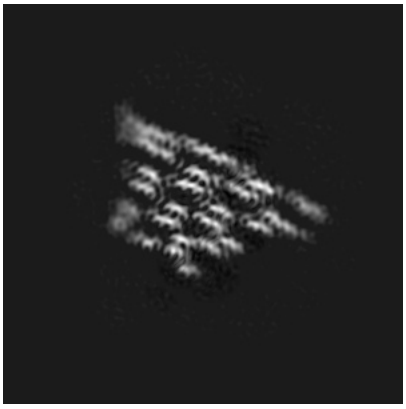
6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150

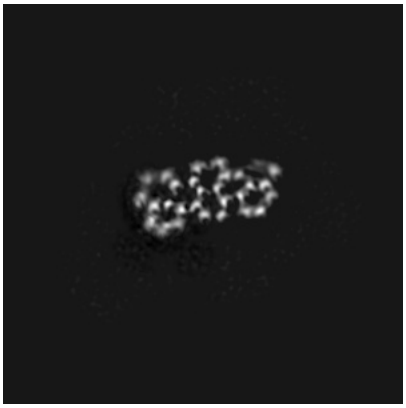


Z Index: 150

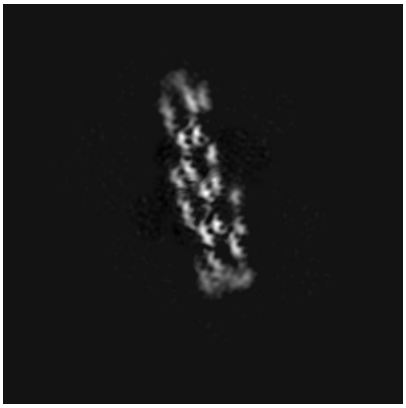
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

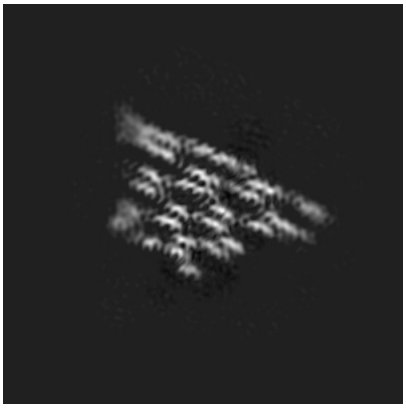
6.3.1 Primary map



X Index: 133



Y Index: 147



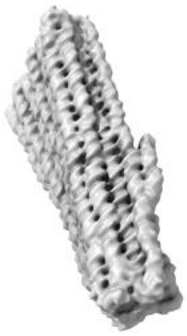
Z Index: 149

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

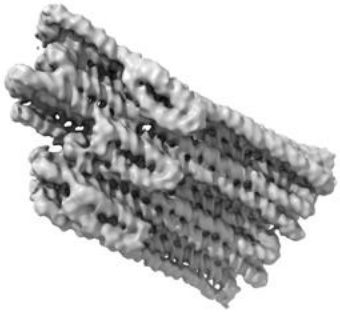
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0628. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

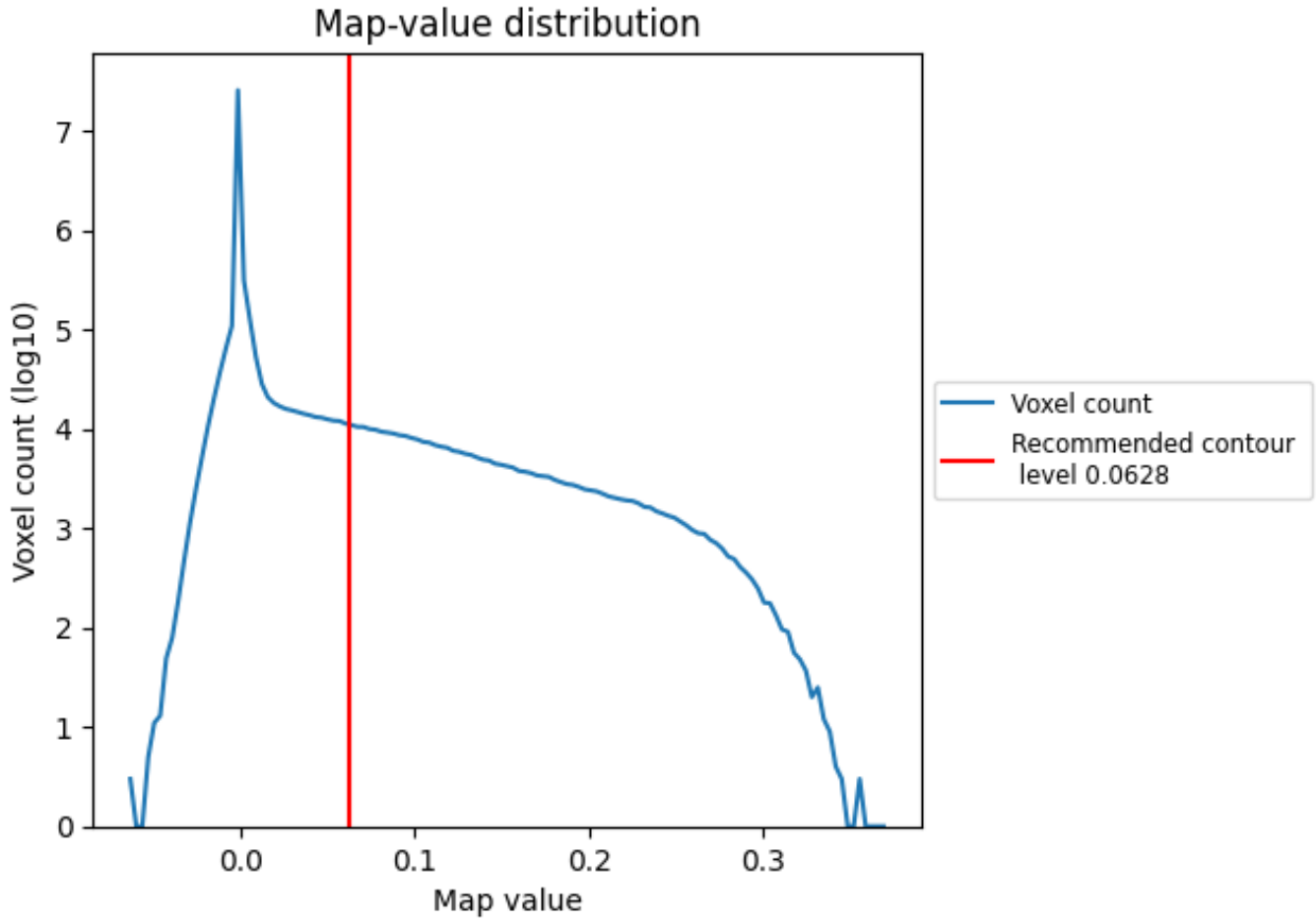
6.5 Mask visualisation (i)

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

7 Map analysis

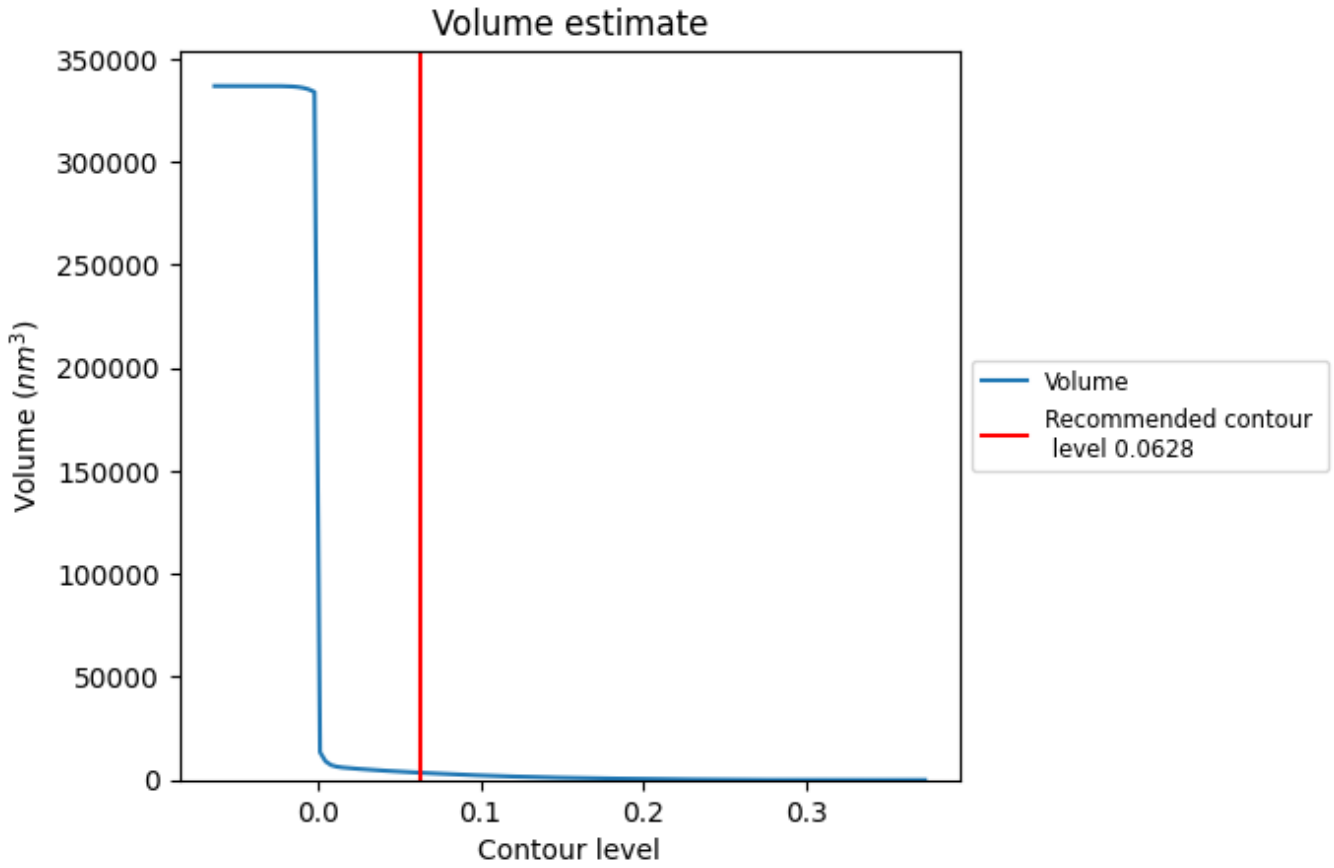
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

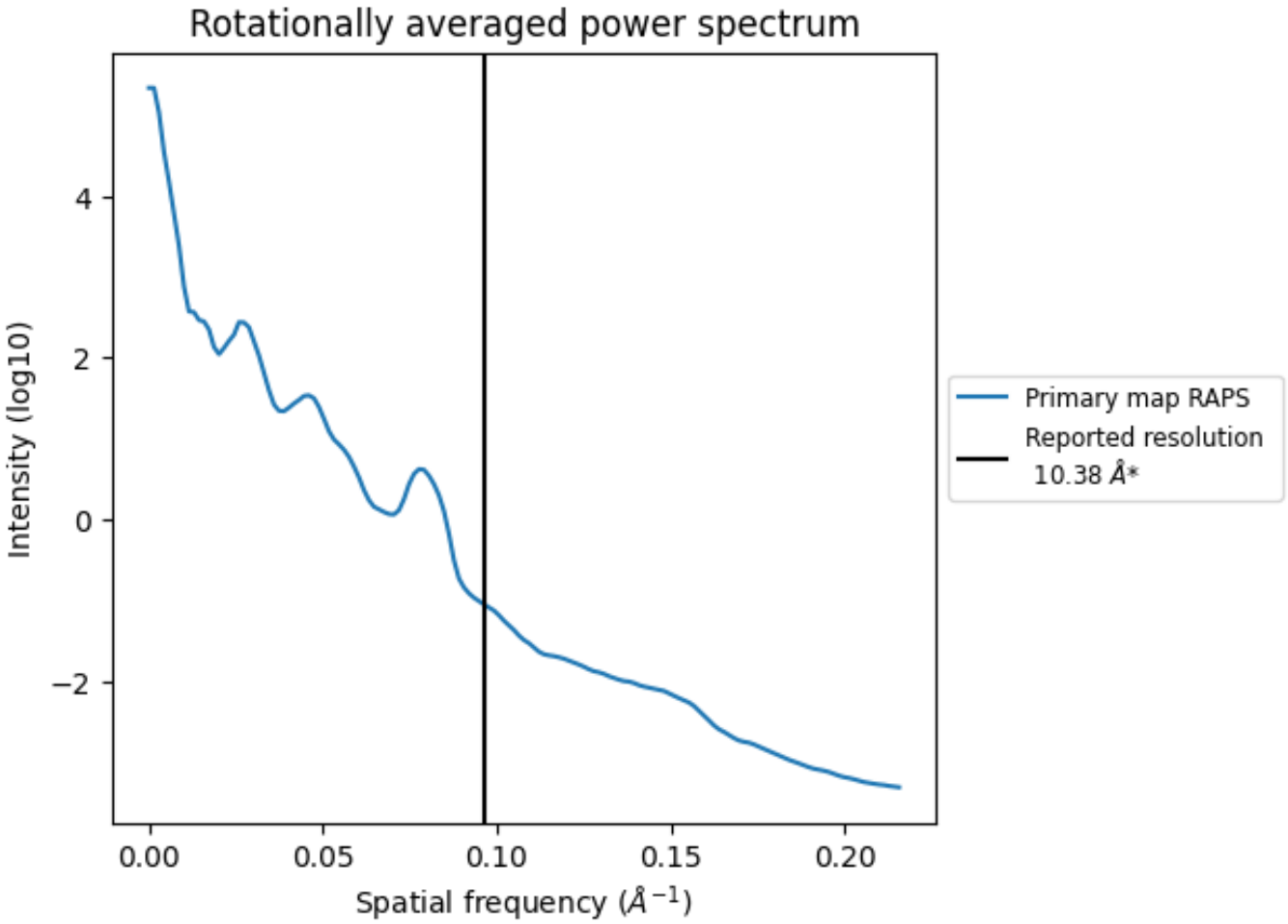
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)

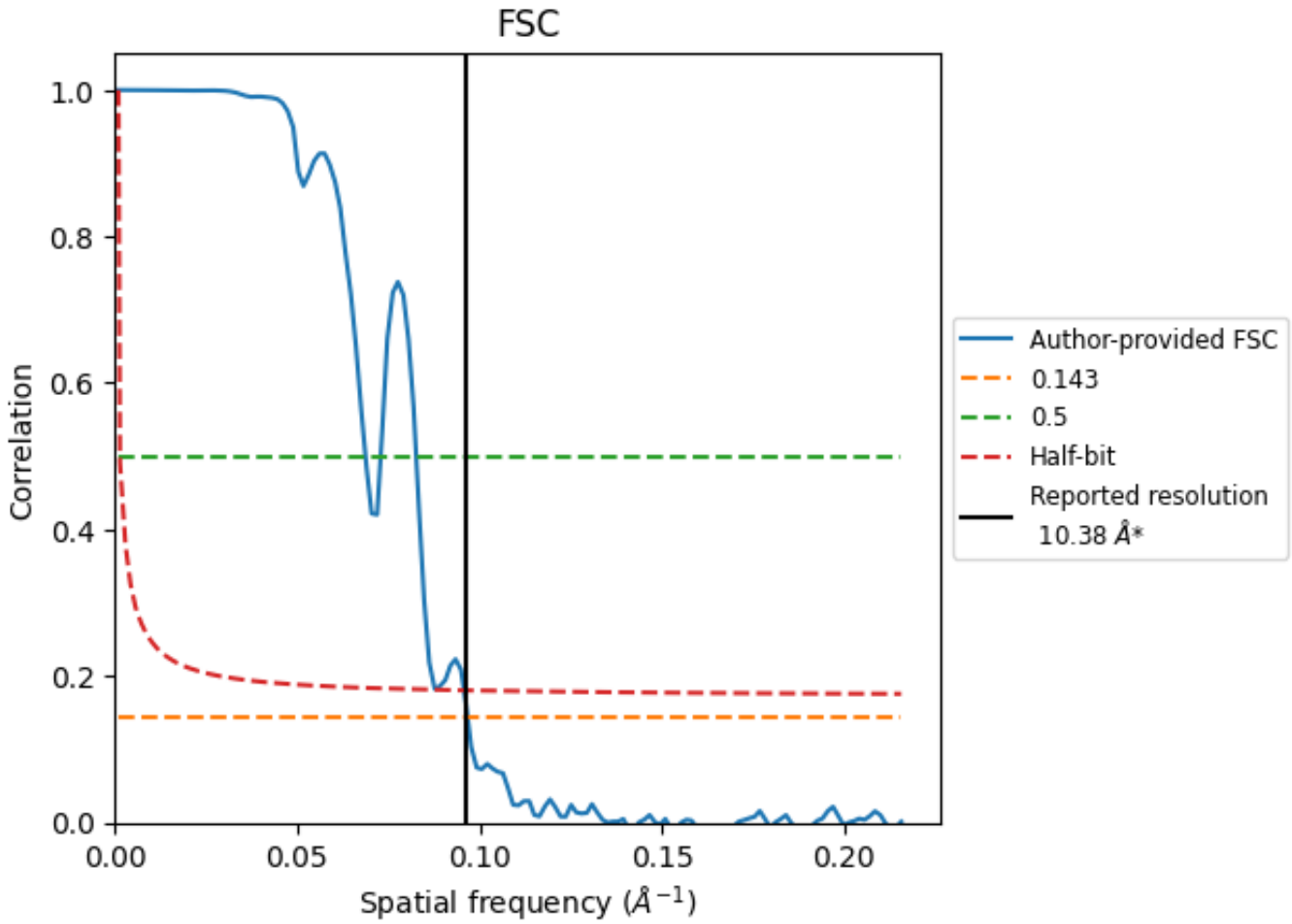


*Reported resolution corresponds to spatial frequency of 0.096 $Å^{-1}$

8 Fourier-Shell correlation

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



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

8.2 Resolution estimates (i)

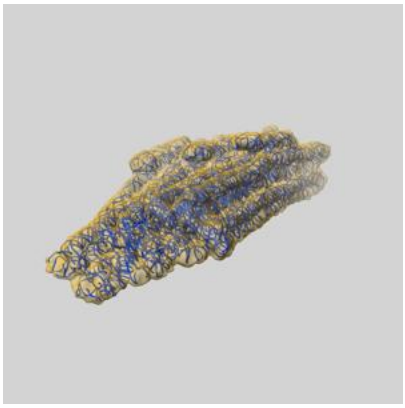
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.38	-	-
Author-provided FSC curve	10.34	14.56	10.45
Unmasked-calculated*	-	-	-

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

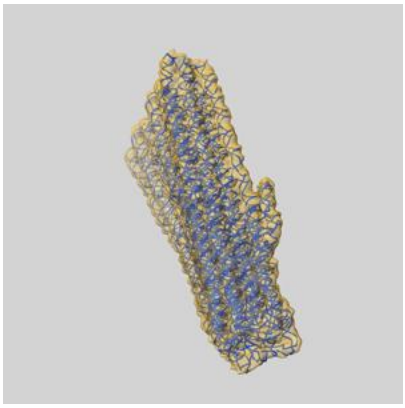
9 Map-model fit

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

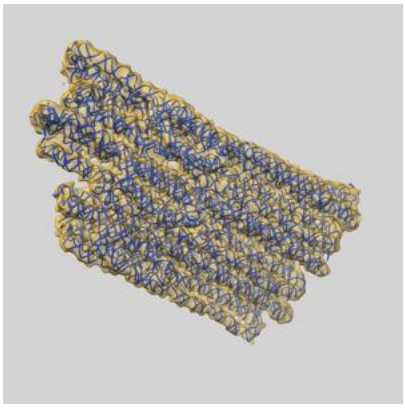
9.1 Map-model overlay



X



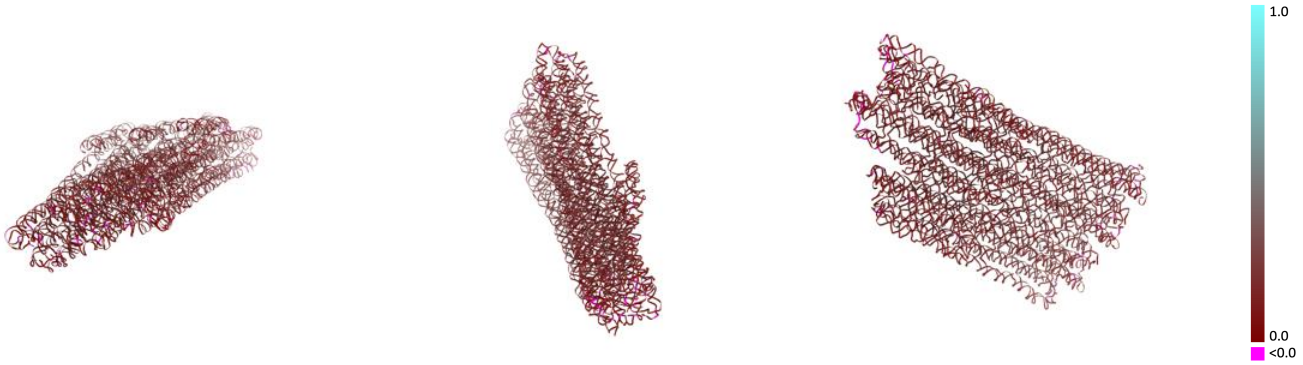
Y



Z

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

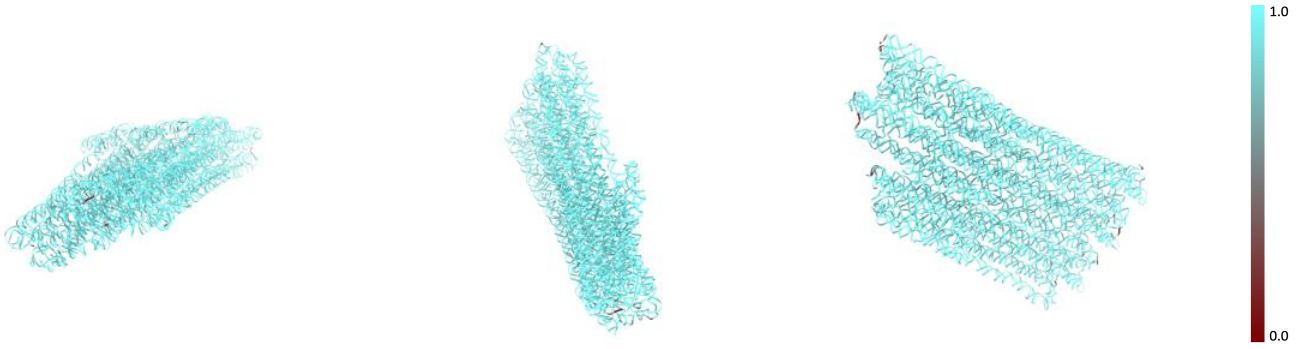
9.2 Q-score mapped to coordinate model



X Y Z

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.

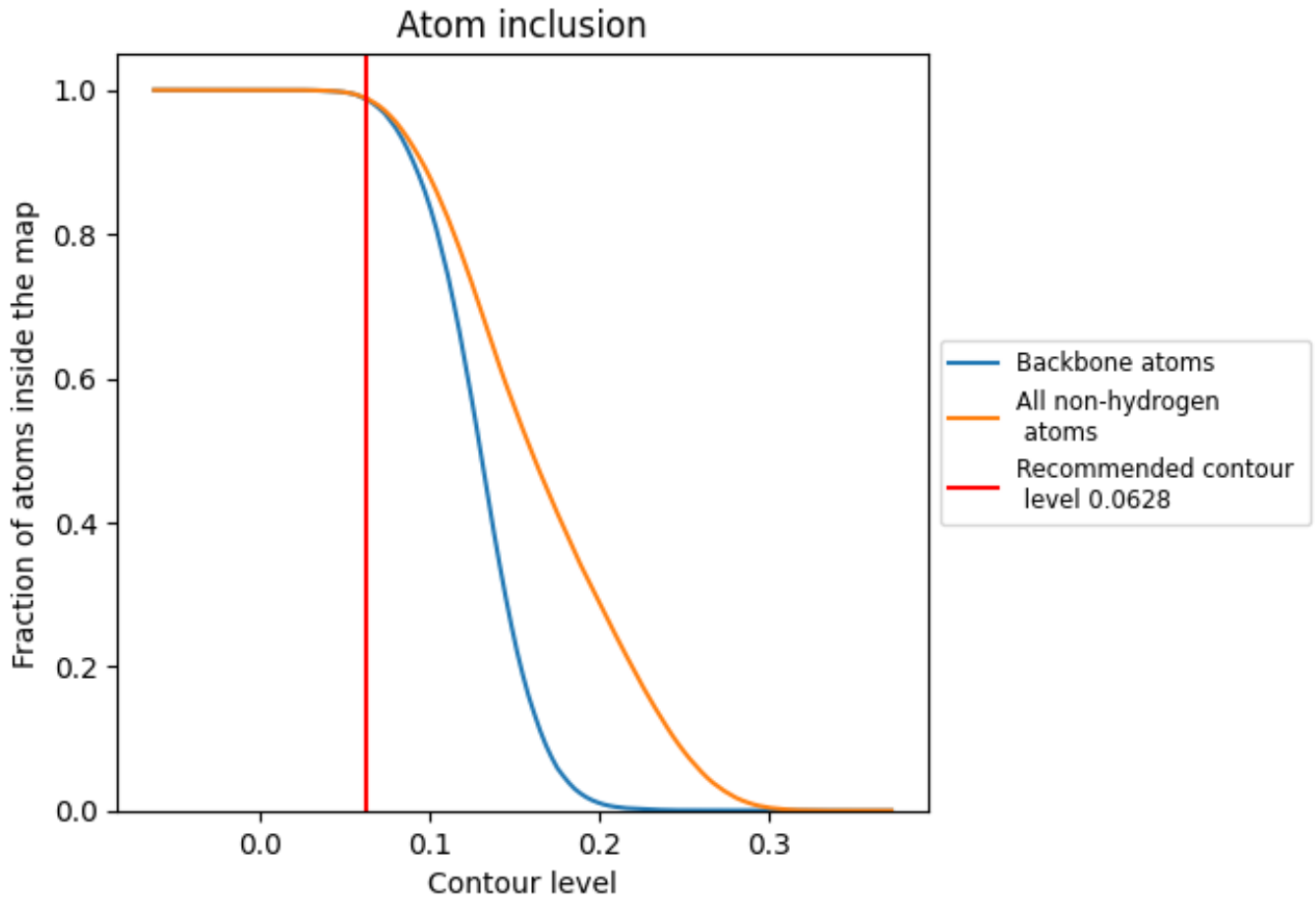
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0628).

9.4 Atom inclusion (i)



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

9.5 Map-model fit summary

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

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

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

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