Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 06:33 pm GMT

PDB ID	:	7ARQ
EMDB ID	:	EMD-11367
Title	:	Cryo EM of 3D DNA origami 16 helix bundle
Authors	:	Feigl, E.; Kube, M.; Kohler, F.
Deposited on	:	2020-10-26
Resolution	:	10.00 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 ⓘ 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 ⓘ) 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 10.00 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	1317	8% 61% 33% 6%
2	AB	49	59% 39% .
3	AC	42	60% 40%
4	AD	33	. 55% 33% 12%
5	AE	27	56% 30% 15%
6	AF	35	54% 37% 9%
7	AG	49	61% 37% .
8	AH	34	65% 26% 9%
9	AI	34	24% 50% 44% 6%
10	AJ	30	30% 70% 23% 7%
11	AK	46	17% 48% 39% 13%
12	AL	46	. 59% 39% .
13	AM	44	59% 61% 39%
14	AN	29	14% 69% 17% 14%
15	AO	40	65% 30% 5%
16	AP	43	47% 47% 7%
17	AQ	40	48% 52% 40% 8%

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Mol	Chain	Length	Quality of chain
18	AR	30	27% 57% 33% 10%
19	AS	34	15% 50% 44% 6%
20	AT	40	60% 35% 5%
21	AU	42	67% 31%
22	AV	37	65% 24% 11%
23	AW	41	49% 49%
24	AX	33	64% 30% 6%
25	AY	35	60% 34% 6%
26	AZ	31	71% 29%
27	Aa	49	63% 27% 10%
28	Ab	38	32% 63% 32% 5%
29	Ac	48	19% 52% 44%
30	Ad	38	42% 71% 26%
31	Ae	27	22% 56% 37% 7%
32	Af	36	36% 61% 31% 8%
33	Ag	42	50% 45% 5%
34	Ah	35	74% 20% 6%
35	Ai	48	71% 21% 8%
36	Aj	27	63% 37%
37	Ak	40	5% 52% 48%

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 54985 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	1317	26988	12825	4971	7876	1316	0	0

- Molecule 2 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	49	1008	478	191	291	48	0	0

- Molecule 3 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	AC	42	863	412	152	258	41	0	0

- Molecule 4 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	AD	33	676	322	128	194	32	0	0

- Molecule 5 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	AE	27	546	262	95	163	26	0	0

- Molecule 6 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	AF	35	710	340	131	205	34	0	0

- Molecule 7 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	49	Total	C	N	O	P	0	0
			1006	480	189	289	48		

- Molecule 8 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	34	Total	C	N	O	P	0	0
			698	334	125	206	33		

- Molecule 9 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	34	Total	C	N	O	P	0	0
			698	332	130	203	33		

- Molecule 10 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	30	Total	C	N	O	P	0	0
			611	292	110	180	29		

- Molecule 11 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	46	Total	C	N	O	P	0	0
			936	447	165	279	45		

- Molecule 12 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	46	Total	C	N	O	P	0	0
			940	451	167	277	45		

- Molecule 13 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	44	Total	C	N	O	P	0	0
			893	430	143	277	43		

- Molecule 14 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	29	Total	C	N	O	P	0	0
			584	282	96	178	28		

- Molecule 15 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	40	Total	C	N	O	P	0	0
			826	391	161	235	39		

- Molecule 16 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	43	Total	C	N	O	P	0	0
			877	417	156	262	42		

- Molecule 17 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	40	Total	C	N	O	P	0	0
			810	387	144	240	39		

- Molecule 18 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	30	Total	C	N	O	P	0	0
			610	294	108	179	29		

- Molecule 19 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	34	Total	C	N	O	P	0	0
			694	334	119	208	33		

- Molecule 20 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	40	Total	C	N	O	P	0	0
			831	396	150	246	39		

- Molecule 21 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	42	Total	C	N	O	P	0	0
			871	414	168	248	41		

- Molecule 22 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	37	Total	C	N	O	P	0	0
			749	360	129	224	36		

- Molecule 23 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	41	Total	C	N	O	P	0	0
			844	403	158	243	40		

- Molecule 24 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	33	Total	C	N	O	P	0	0
			668	321	114	201	32		

- Molecule 25 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	35	Total	C	N	O	P	0	0
			725	343	143	205	34		

- Molecule 26 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	31	Total	C	N	O	P	0	0
			636	302	124	180	30		

- Molecule 27 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aa	49	Total	C	N	O	P	0	0
			985	473	172	292	48		

- Molecule 28 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	38	Total 776	C 373	N 131	O 235	P 37	0	0

- Molecule 29 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	48	Total 975	C 469	N 164	O 295	P 47	0	0

- Molecule 30 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	38	Total 774	C 370	N 140	O 227	P 37	0	0

- Molecule 31 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	27	Total 547	C 265	N 92	O 164	P 26	0	0

- Molecule 32 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	36	Total 727	C 348	N 132	O 212	P 35	0	0

- Molecule 33 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	42	Total 854	C 411	N 147	O 255	P 41	0	0

- Molecule 34 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ah	35	Total 713	C 340	N 134	O 205	P 34	0	0

- Molecule 35 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ai	48	Total	C	N	O	P	0	0
			966	468	153	298	47		

- Molecule 36 is a DNA chain called STAPLE STRAND.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Aj	27	Total	C	N	O	P	0	0
			551	263	103	159	26		

- Molecule 37 is a DNA chain called STAPLE STRAND.

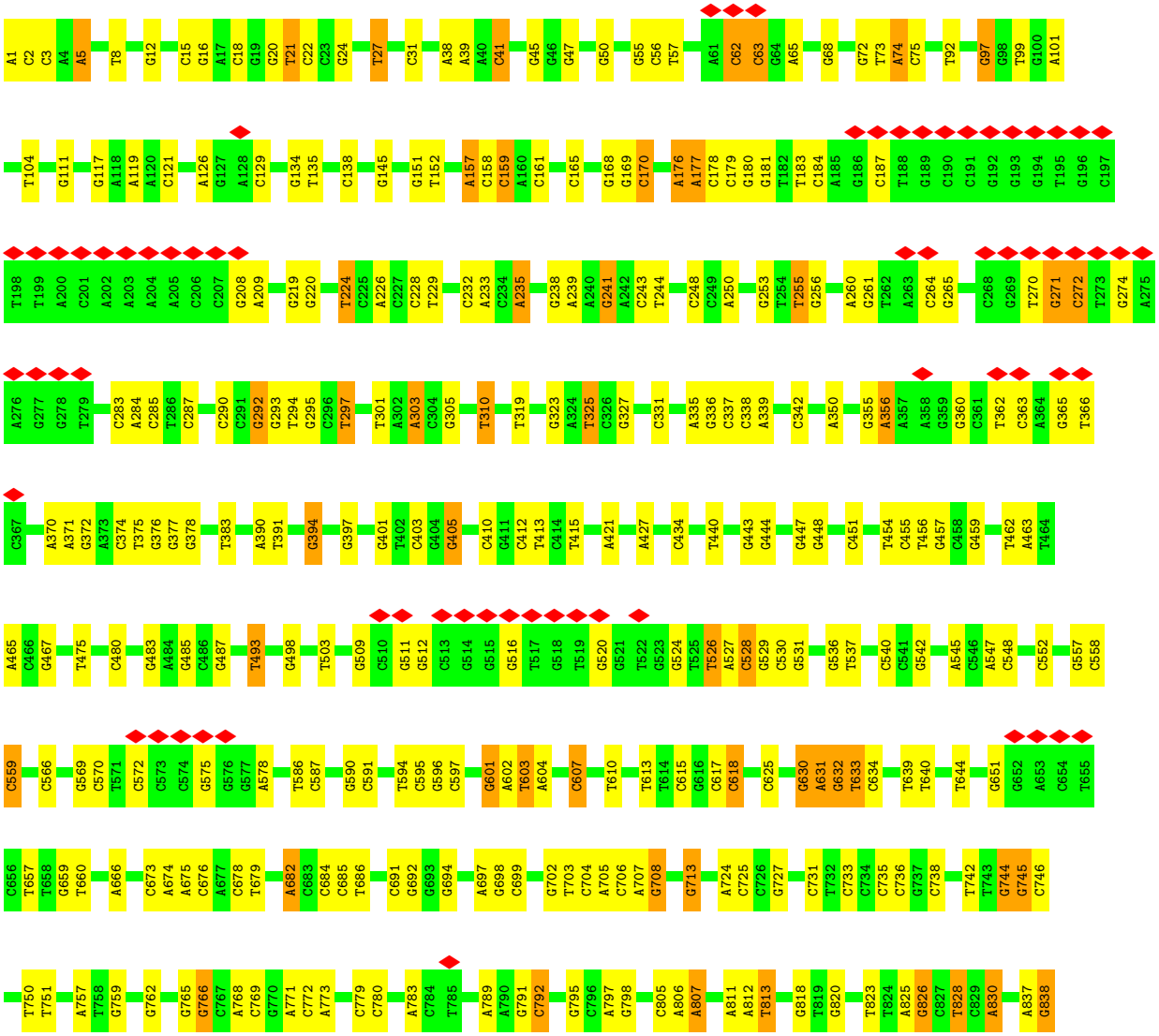
Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ak	40	Total	C	N	O	P	0	0
			819	386	163	231	39		

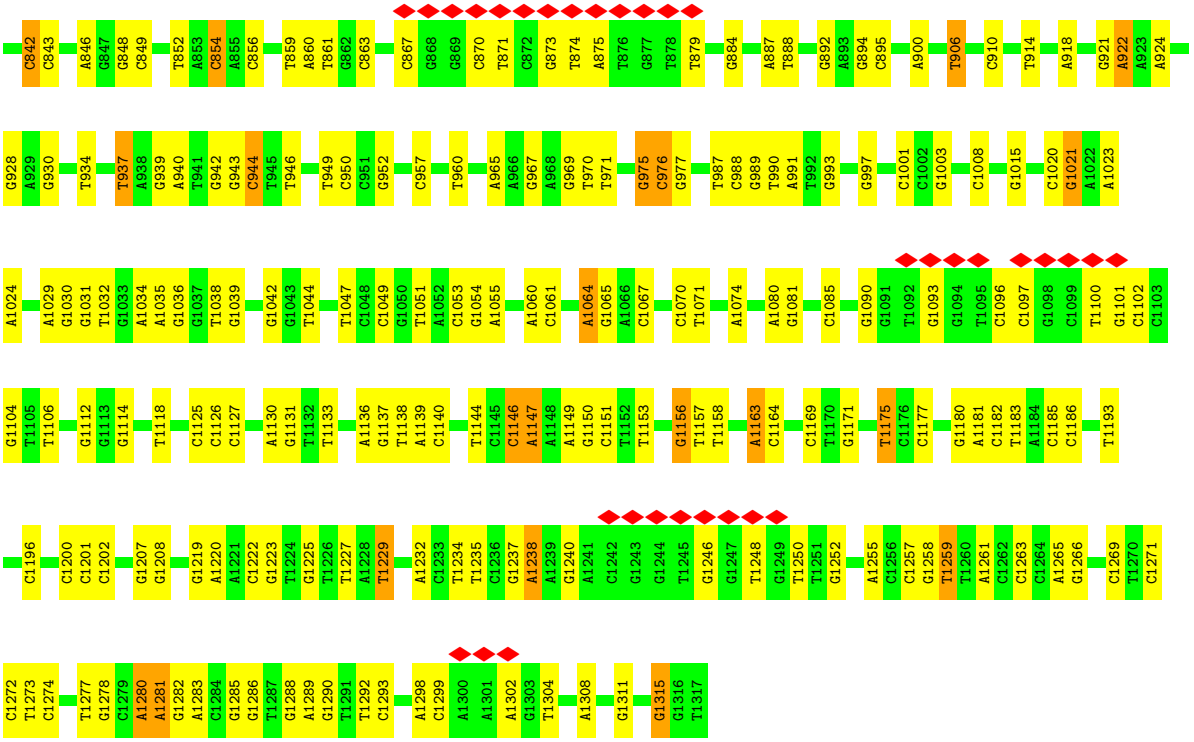
3 Residue-property plots (i)

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

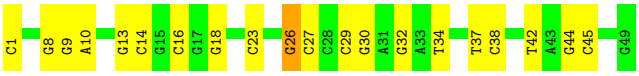
Chain AA: 





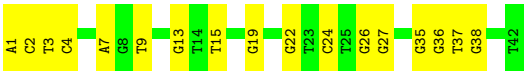
• Molecule 2: STAPLE STRAND

Chain AB:



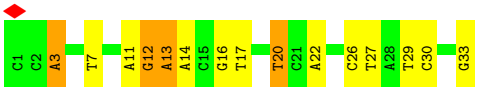
• Molecule 3: STAPLE STRAND

Chain AC:



• Molecule 4: STAPLE STRAND

Chain AD:



• Molecule 5: STAPLE STRAND

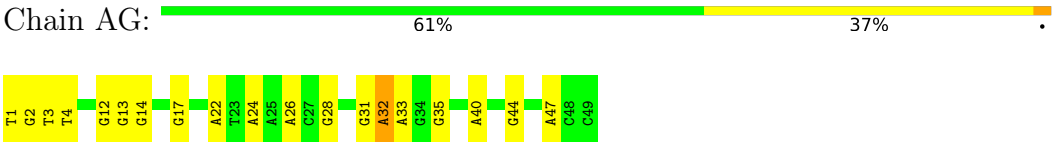
Chain AE:

• Molecule 6: STAPLE STRAND

Chain AF:

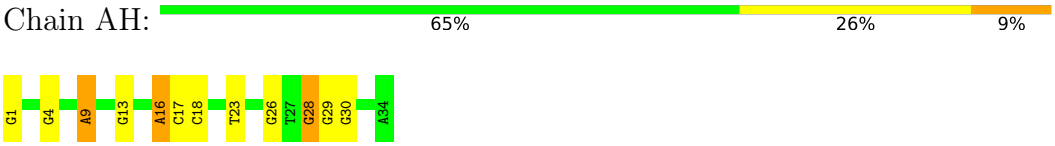
• Molecule 7: STAPLE STRAND

Chain AG:



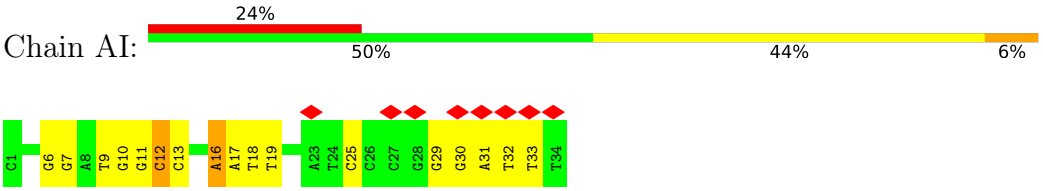
• Molecule 8: STAPLE STRAND

Chain AH:



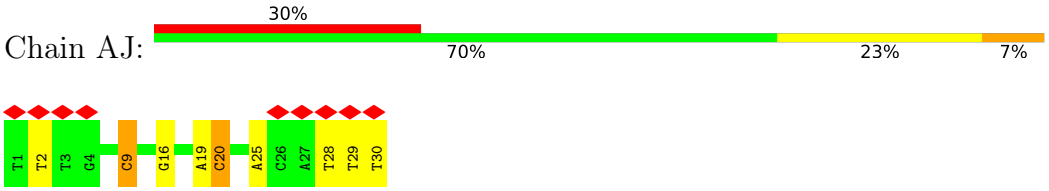
• Molecule 9: STAPLE STRAND

Chain AI:



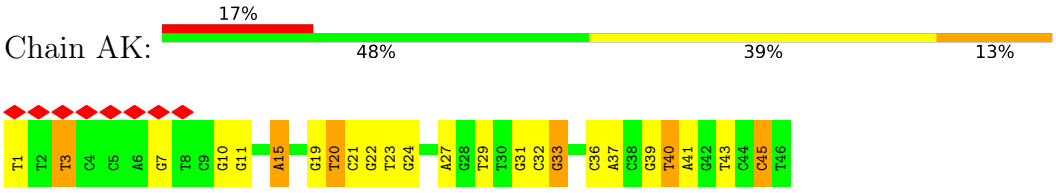
• Molecule 10: STAPLE STRAND

Chain AJ:



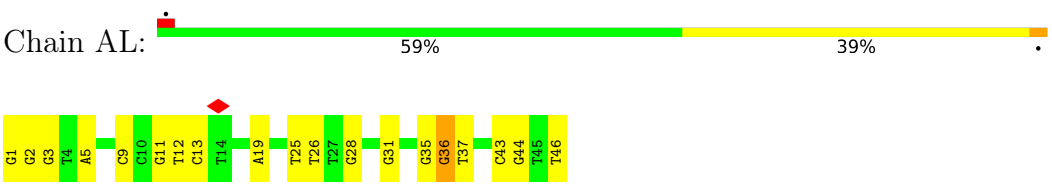
• Molecule 11: STAPLE STRAND

Chain AK:



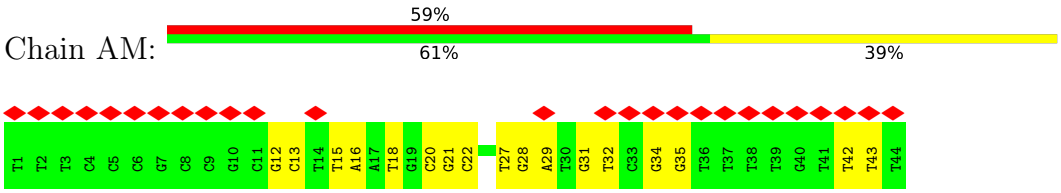
• Molecule 12: STAPLE STRAND

Chain AL:



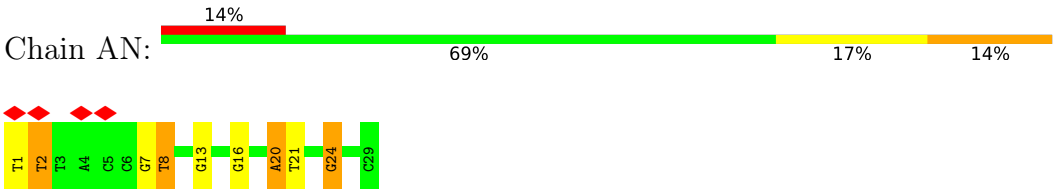
• Molecule 13: STAPLE STRAND

Chain AM:



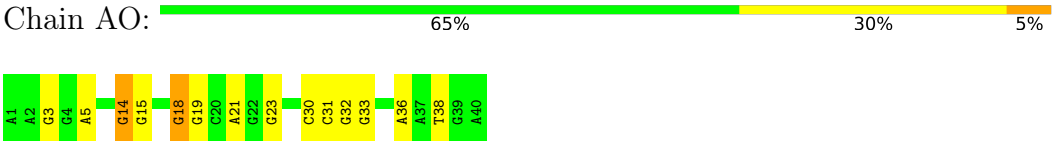
• Molecule 14: STAPLE STRAND

Chain AN:



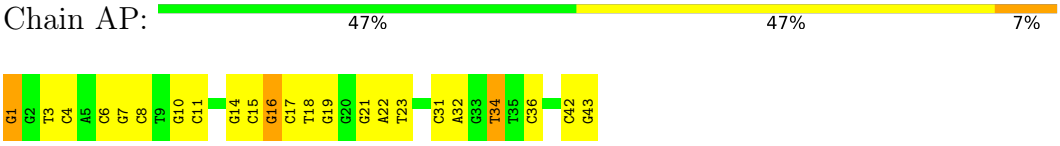
• Molecule 15: STAPLE STRAND

Chain AO:



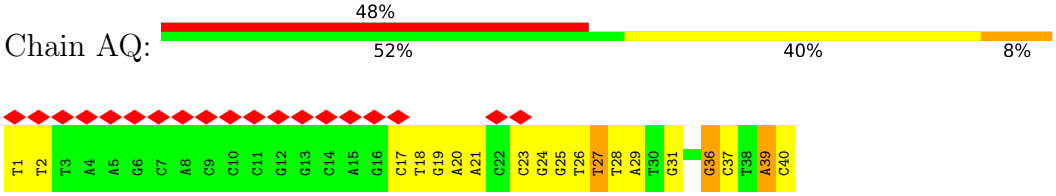
• Molecule 16: STAPLE STRAND

Chain AP:



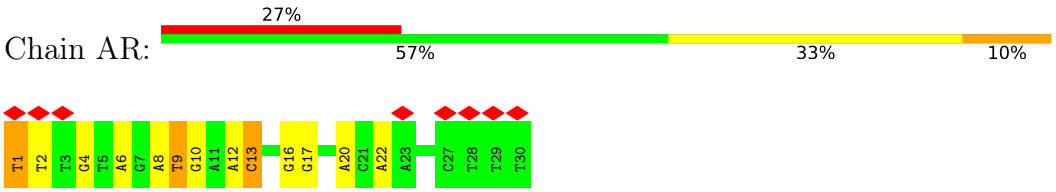
• Molecule 17: STAPLE STRAND

Chain AQ:



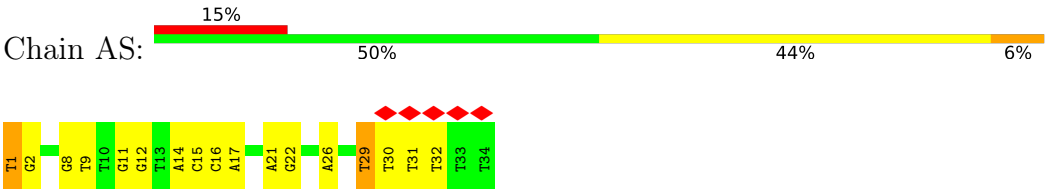
• Molecule 18: STAPLE STRAND

Chain AR:



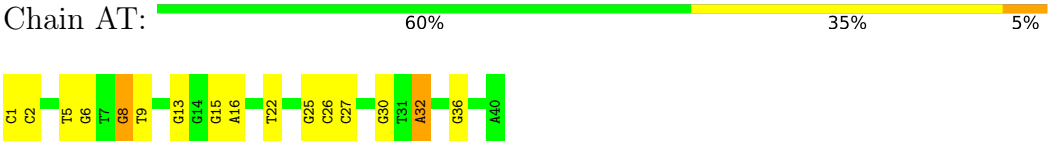
• Molecule 19: STAPLE STRAND

Chain AS:



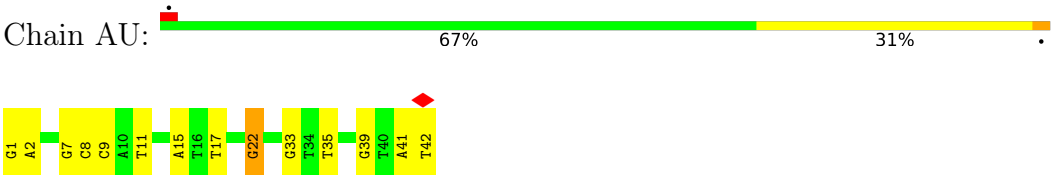
• Molecule 20: STAPLE STRAND

Chain AT:



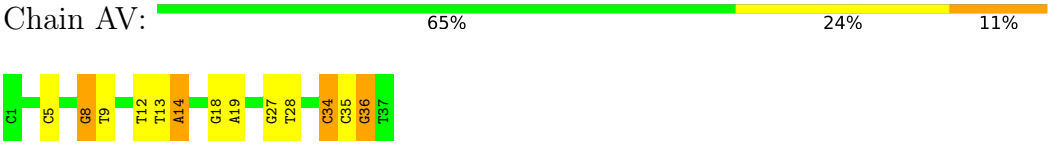
• Molecule 21: STAPLE STRAND

Chain AU:



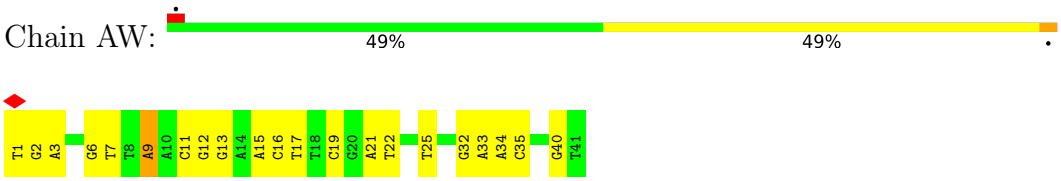
• Molecule 22: STAPLE STRAND

Chain AV:



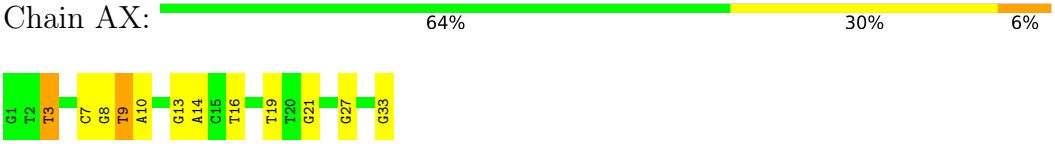
• Molecule 23: STAPLE STRAND

Chain AW:



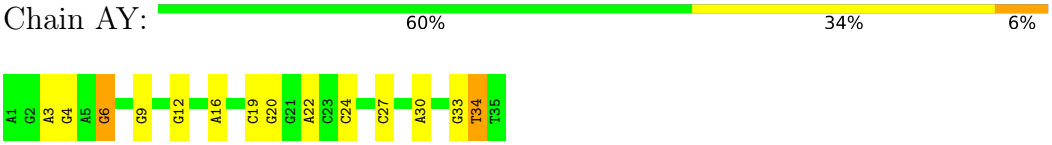
• Molecule 24: STAPLE STRAND

Chain AX:



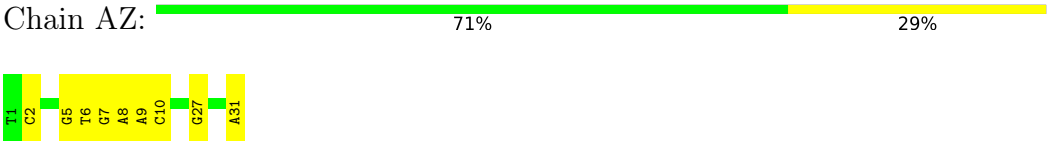
• Molecule 25: STAPLE STRAND

Chain AY:



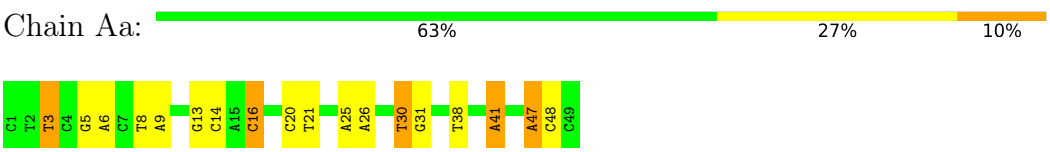
• Molecule 26: STAPLE STRAND

Chain AZ:



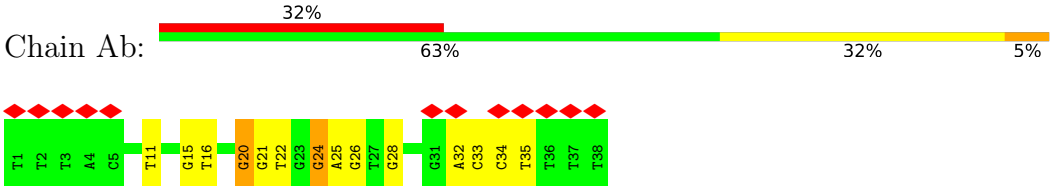
• Molecule 27: STAPLE STRAND

Chain Aa:



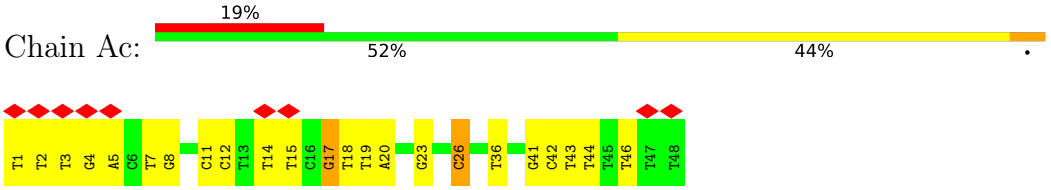
• Molecule 28: STAPLE STRAND

Chain Ab:



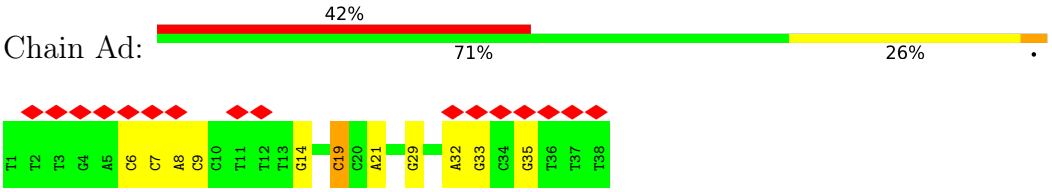
• Molecule 29: STAPLE STRAND

Chain Ac:



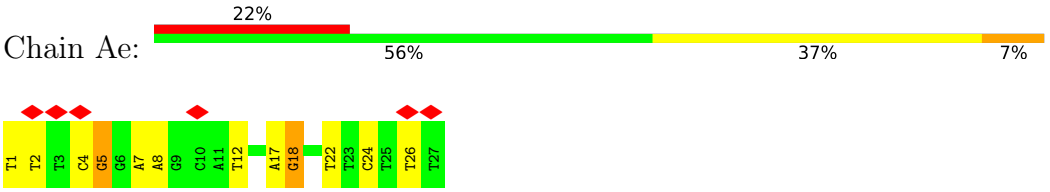
• Molecule 30: STAPLE STRAND

Chain Ad:



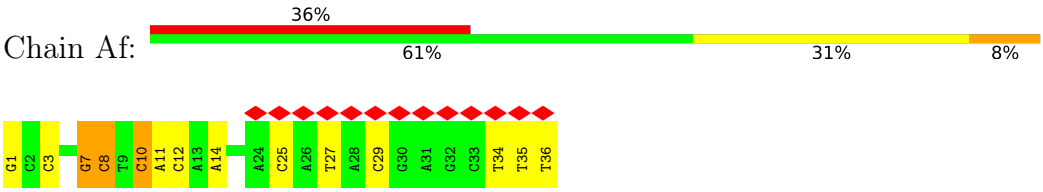
• Molecule 31: STAPLE STRAND

Chain Ae:



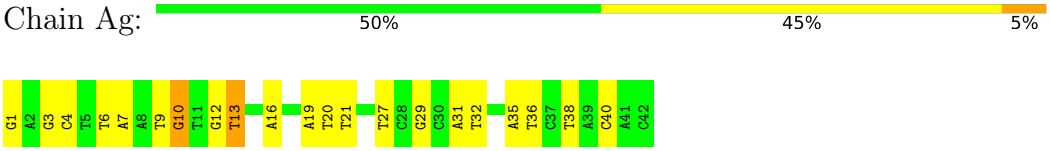
• Molecule 32: STAPLE STRAND

Chain Af:



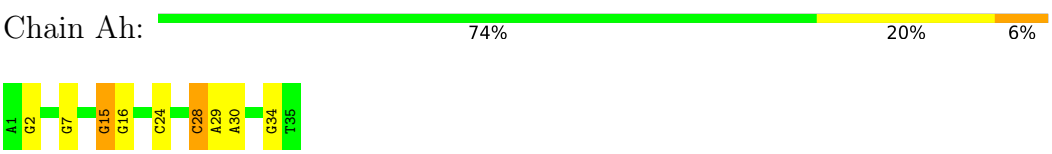
• Molecule 33: STAPLE STRAND

Chain Ag:



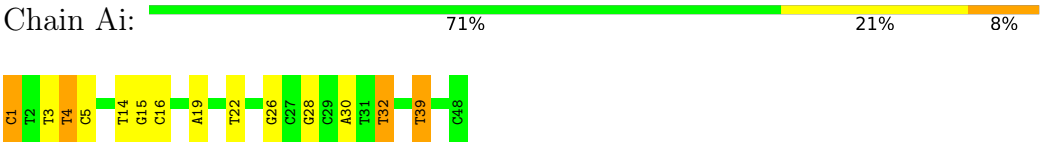
• Molecule 34: STAPLE STRAND

Chain Ah:



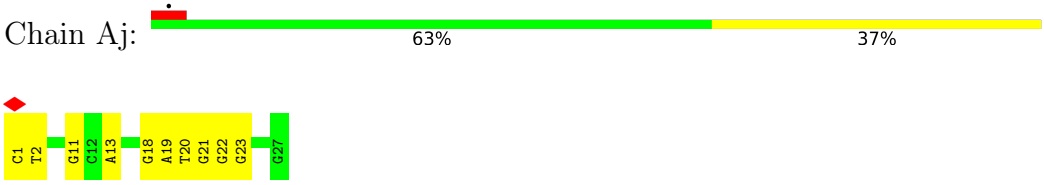
• Molecule 35: STAPLE STRAND

Chain Ai:



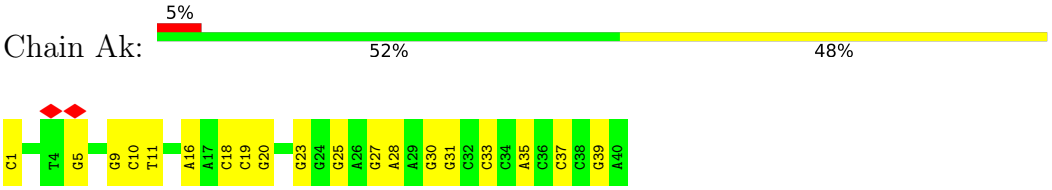
• Molecule 36: STAPLE STRAND

Chain Aj:



• Molecule 37: STAPLE STRAND

Chain Ak:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44605	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	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	0.551	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.17	Depositor
Map size (Å)	828.0, 828.0, 828.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.3, 2.3, 2.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	AA	1.24	1/30285 (0.0%)	1.41	410/46736 (0.9%)
2	AB	1.29	0/1132	1.44	15/1747 (0.9%)
3	AC	1.30	1/966 (0.1%)	1.39	11/1492 (0.7%)
4	AD	1.31	0/759	1.45	13/1170 (1.1%)
5	AE	1.28	1/610 (0.2%)	1.51	16/939 (1.7%)
6	AF	1.23	0/796	1.44	14/1225 (1.1%)
7	AG	1.24	0/1130	1.33	14/1743 (0.8%)
8	AH	1.29	0/782	1.43	13/1207 (1.1%)
9	AI	1.25	0/783	1.39	8/1208 (0.7%)
10	AJ	1.29	0/684	1.49	8/1054 (0.8%)
11	AK	1.27	1/1047 (0.1%)	1.49	19/1614 (1.2%)
12	AL	1.27	0/1053	1.51	18/1624 (1.1%)
13	AM	1.20	0/995	1.33	11/1535 (0.7%)
14	AN	1.19	0/651	1.38	7/1002 (0.7%)
15	AO	1.26	0/929	1.47	12/1434 (0.8%)
16	AP	1.28	0/981	1.49	16/1513 (1.1%)
17	AQ	1.27	0/906	1.43	11/1395 (0.8%)
18	AR	1.23	0/683	1.56	14/1052 (1.3%)
19	AS	1.23	0/776	1.33	9/1197 (0.8%)
20	AT	1.32	1/932 (0.1%)	1.45	14/1442 (1.0%)
21	AU	1.26	0/980	1.36	13/1514 (0.9%)
22	AV	1.24	0/837	1.38	8/1289 (0.6%)
23	AW	1.23	0/948	1.54	21/1463 (1.4%)
24	AX	1.21	0/746	1.36	9/1149 (0.8%)
25	AY	1.30	0/816	1.46	15/1260 (1.2%)
26	AZ	1.28	0/715	1.31	5/1102 (0.5%)
27	Aa	1.21	0/1101	1.51	15/1693 (0.9%)
28	Ab	1.22	0/867	1.45	12/1338 (0.9%)
29	Ac	1.22	0/1089	1.50	19/1679 (1.1%)
30	Ad	1.18	0/867	1.29	9/1336 (0.7%)
31	Ae	1.18	0/611	1.43	10/941 (1.1%)
32	Af	1.19	0/814	1.34	6/1252 (0.5%)
33	Ag	1.28	0/955	1.48	20/1472 (1.4%)
34	Ah	1.26	0/800	1.40	10/1232 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
35	Ai	1.18	0/1076	1.36	14/1657 (0.8%)
36	Aj	1.27	0/618	1.48	11/952 (1.2%)
37	Ak	1.28	0/921	1.41	13/1419 (0.9%)
All	All	1.24	5/61641 (0.0%)	1.42	863/95077 (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	3	313
2	AB	0	12
3	AC	0	11
4	AD	0	12
5	AE	0	8
6	AF	0	11
7	AG	0	10
8	AH	0	8
9	AI	0	13
10	AJ	0	6
11	AK	0	15
12	AL	0	11
13	AM	0	9
14	AN	0	7
15	AO	0	8
16	AP	0	17
17	AQ	0	13
18	AR	0	10
19	AS	0	12
20	AT	0	11
21	AU	0	8
22	AV	0	11
23	AW	0	10
24	AX	0	7
25	AY	0	7
26	AZ	0	5
27	Aa	0	14
28	Ab	1	5
29	Ac	0	14
30	Ad	0	5
31	Ae	0	7

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	Af	0	12
33	Ag	0	11
34	Ah	0	5
35	Ai	0	9
36	Aj	0	5
37	Ak	0	10
All	All	4	662

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AK	33	DG	C2-N2	-5.78	1.28	1.34
1	AA	1285	DG	C2-N2	-5.74	1.28	1.34
20	AT	8	DG	C4'-C3'	5.44	1.58	1.53
3	AC	1	DA	C4'-C3'	5.12	1.58	1.53
5	AE	10	DT	C4'-C3'	5.02	1.58	1.53

All (863) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	129	DC	O4'-C4'-C3'	-15.74	96.55	106.00
28	Ab	20	DG	P-O3'-C3'	15.70	138.54	119.70
29	Ac	17	DG	P-O3'-C3'	14.63	137.26	119.70
27	Aa	41	DA	P-O3'-C3'	14.36	136.93	119.70
16	AP	16	DG	P-O3'-C3'	14.30	136.85	119.70
31	Ae	26	DT	P-O3'-C3'	14.27	136.83	119.70
1	AA	870	DC	P-O3'-C3'	14.27	136.82	119.70
1	AA	1101	DG	O4'-C4'-C3'	-13.81	97.71	106.00
1	AA	806	DA	P-O3'-C3'	13.50	135.90	119.70
1	AA	181	DG	O4'-C4'-C3'	-13.46	97.92	106.00
1	AA	1156	DG	P-O3'-C3'	13.46	135.86	119.70
22	AV	8	DG	P-O3'-C3'	13.41	135.79	119.70
14	AN	24	DG	P-O3'-C3'	13.34	135.71	119.70
22	AV	9	DT	P-O3'-C3'	13.20	135.54	119.70
1	AA	16	DG	P-O3'-C3'	13.16	135.49	119.70
3	AC	36	DG	P-O3'-C3'	12.98	135.28	119.70
1	AA	493	DT	P-O3'-C3'	12.96	135.25	119.70
1	AA	1246	DG	O4'-C4'-C3'	-12.55	98.47	106.00
1	AA	572	DC	O4'-C4'-C3'	-12.52	98.49	106.00
1	AA	220	DG	P-O3'-C3'	12.51	134.71	119.70
1	AA	1049	DC	O4'-C4'-C3'	-12.51	98.50	106.00
1	AA	1039	DG	P-O3'-C3'	12.24	134.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AW	2	DG	O4'-C4'-C3'	-12.23	98.66	106.00
12	AL	13	DC	P-O3'-C3'	12.22	134.36	119.70
1	AA	271	DG	P-O3'-C3'	12.12	134.24	119.70
1	AA	75	DC	P-O3'-C3'	12.06	134.17	119.70
18	AR	16	DG	P-O3'-C3'	11.99	134.09	119.70
23	AW	40	DG	P-O3'-C3'	11.94	134.02	119.70
29	Ac	11	DC	O4'-C4'-C3'	-11.93	98.84	106.00
9	AI	9	DT	O4'-C4'-C3'	-11.90	98.86	106.00
2	AB	10	DA	P-O3'-C3'	11.84	133.91	119.70
28	Ab	22	DT	O4'-C4'-C3'	-11.76	98.94	106.00
28	Ab	24	DG	P-O3'-C3'	11.63	133.66	119.70
1	AA	63	DC	P-O3'-C3'	11.58	133.59	119.70
1	AA	1112	DG	O4'-C4'-C3'	-11.52	99.09	106.00
18	AR	10	DG	O4'-C4'-C3'	-11.51	99.10	106.00
1	AA	922	DA	P-O3'-C3'	11.42	133.40	119.70
2	AB	30	DG	P-O3'-C3'	11.41	133.39	119.70
11	AK	32	DC	P-O3'-C3'	11.41	133.39	119.70
1	AA	45	DG	O4'-C4'-C3'	-11.39	99.17	106.00
21	AU	1	DG	O4'-C4'-C3'	-11.36	99.18	106.00
1	AA	1140	DC	P-O3'-C3'	11.35	133.31	119.70
1	AA	467	DG	O4'-C4'-C3'	-11.29	99.23	106.00
1	AA	1280	DA	P-O3'-C3'	11.24	133.19	119.70
22	AV	34	DC	O4'-C4'-C3'	-11.23	99.26	106.00
1	AA	863	DC	P-O3'-C3'	11.22	133.17	119.70
1	AA	16	DG	O4'-C4'-C3'	-11.20	99.28	106.00
36	Aj	18	DG	P-O3'-C3'	11.16	133.09	119.70
15	AO	32	DG	O4'-C4'-C3'	-10.99	99.41	106.00
12	AL	12	DT	O4'-C4'-C3'	-10.89	99.47	106.00
15	AO	38	DT	O4'-C4'-C3'	-10.87	99.48	106.00
23	AW	12	DG	P-O3'-C3'	10.79	132.65	119.70
27	Aa	26	DA	O4'-C4'-C3'	-10.78	99.53	106.00
20	AT	13	DG	O4'-C4'-C3'	-10.73	99.56	106.00
33	Ag	40	DC	P-O3'-C3'	10.64	132.47	119.70
1	AA	820	DG	P-O3'-C3'	10.62	132.45	119.70
8	AH	26	DG	P-O3'-C3'	10.61	132.43	119.70
33	Ag	40	DC	O4'-C4'-C3'	-10.59	99.65	106.00
12	AL	3	DG	P-O3'-C3'	10.56	132.38	119.70
27	Aa	31	DG	O4'-C4'-C3'	-10.54	99.68	106.00
1	AA	331	DC	P-O3'-C3'	10.48	132.27	119.70
16	AP	1	DG	P-O3'-C3'	10.37	132.14	119.70
1	AA	1104	DG	O4'-C4'-C3'	-10.36	99.79	106.00
1	AA	1219	DG	P-O3'-C3'	10.31	132.08	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	894	DG	P-O3'-C3'	10.31	132.07	119.70
1	AA	618	DC	C6-N1-C2	-10.27	116.19	120.30
1	AA	233	DA	P-O3'-C3'	10.17	131.90	119.70
10	AJ	9	DC	O4'-C1'-C2'	-10.12	97.81	105.90
17	AQ	27	DT	P-O3'-C3'	10.09	131.81	119.70
1	AA	570	DC	P-O3'-C3'	10.06	131.77	119.70
15	AO	23	DG	O4'-C4'-C3'	-10.04	99.98	106.00
11	AK	15	DA	P-O3'-C3'	10.02	131.72	119.70
36	Aj	1	DC	O4'-C4'-C3'	-10.02	99.99	106.00
1	AA	861	DT	P-O3'-C3'	9.89	131.56	119.70
33	Ag	16	DA	P-O3'-C3'	9.84	131.51	119.70
18	AR	1	DT	O4'-C4'-C3'	-9.82	100.11	106.00
25	AY	12	DG	O4'-C4'-C3'	-9.81	100.11	106.00
10	AJ	20	DC	P-O3'-C3'	9.70	131.33	119.70
1	AA	177	DA	O4'-C4'-C3'	-9.56	100.26	106.00
1	AA	41	DC	O4'-C4'-C3'	-9.52	100.29	106.00
18	AR	1	DT	O4'-C1'-C2'	-9.52	98.29	105.90
7	AG	1	DT	O4'-C1'-C2'	-9.51	98.29	105.90
1	AA	233	DA	O4'-C4'-C3'	-9.47	100.32	106.00
1	AA	1003	DG	N1-C6-O6	9.40	125.54	119.90
33	Ag	1	DG	P-O3'-C3'	9.38	130.96	119.70
1	AA	697	DA	O4'-C4'-C3'	-9.37	100.38	106.00
1	AA	1003	DG	C5-C6-O6	-9.29	123.03	128.60
1	AA	863	DC	O4'-C1'-C2'	-9.29	98.47	105.90
3	AC	1	DA	O4'-C1'-C2'	-9.25	98.50	105.90
1	AA	540	DC	O4'-C4'-C3'	-9.24	100.46	106.00
29	Ac	1	DT	O4'-C4'-C3'	-9.22	100.47	106.00
1	AA	512	DG	P-O3'-C3'	9.19	130.73	119.70
20	AT	8	DG	O4'-C1'-N9	9.16	114.41	108.00
1	AA	1208	DG	P-O3'-C3'	9.16	130.69	119.70
14	AN	1	DT	O4'-C4'-C3'	-9.14	100.52	106.00
1	AA	397	DG	O4'-C4'-C3'	-9.02	100.59	106.00
31	Ae	18	DG	O4'-C4'-C3'	-8.95	100.63	106.00
1	AA	261	DG	O4'-C4'-C3'	-8.88	100.67	106.00
1	AA	820	DG	O4'-C4'-C3'	-8.87	100.67	106.00
16	AP	16	DG	O4'-C1'-N9	8.85	114.19	108.00
1	AA	1039	DG	O4'-C1'-C2'	-8.81	98.85	105.90
1	AA	797	DA	O4'-C1'-C2'	-8.79	98.87	105.90
15	AO	18	DG	O4'-C1'-C2'	-8.73	98.91	105.90
1	AA	233	DA	O4'-C1'-C2'	-8.69	98.95	105.90
1	AA	976	DC	O4'-C1'-C2'	-8.66	98.97	105.90
18	AR	16	DG	O4'-C4'-C3'	-8.64	100.81	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	AL	25	DT	O4'-C1'-C2'	-8.62	99.01	105.90
1	AA	780	DC	P-O3'-C3'	8.61	130.03	119.70
1	AA	807	DA	N1-C6-N6	-8.58	113.45	118.60
4	AD	20	DT	P-O3'-C3'	8.56	129.98	119.70
29	Ac	11	DC	C1'-O4'-C4'	-8.55	101.55	110.10
3	AC	19	DG	O4'-C1'-C2'	-8.54	99.07	105.90
31	Ae	2	DT	O4'-C1'-C2'	-8.52	99.08	105.90
15	AO	18	DG	P-O3'-C3'	8.52	129.92	119.70
24	AX	14	DA	O4'-C4'-C3'	-8.49	100.90	106.00
1	AA	792	DC	P-O3'-C3'	8.48	129.87	119.70
29	Ac	17	DG	O4'-C1'-C2'	-8.46	99.13	105.90
1	AA	374	DC	O4'-C1'-C2'	-8.44	99.15	105.90
18	AR	16	DG	O4'-C1'-C2'	-8.42	99.16	105.90
1	AA	528	DC	O4'-C4'-C3'	-8.41	100.95	106.00
29	Ac	36	DT	O4'-C1'-C2'	-8.39	99.19	105.90
1	AA	63	DC	O4'-C1'-C2'	-8.36	99.21	105.90
1	AA	119	DA	P-O3'-C3'	8.33	129.70	119.70
1	AA	285	DC	O4'-C4'-C3'	-8.32	101.01	106.00
2	AB	10	DA	O4'-C1'-C2'	-8.27	99.28	105.90
16	AP	21	DG	P-O3'-C3'	8.26	129.62	119.70
34	Ah	15	DG	P-O3'-C3'	8.26	129.61	119.70
35	Ai	1	DC	O4'-C1'-C2'	-8.24	99.31	105.90
1	AA	863	DC	O4'-C4'-C3'	-8.22	101.07	106.00
1	AA	918	DA	O4'-C4'-C3'	-8.18	101.09	106.00
1	AA	20	DG	P-O3'-C3'	8.17	129.51	119.70
1	AA	325	DT	O4'-C4'-C3'	-8.17	101.10	106.00
1	AA	145	DG	O4'-C4'-C3'	-8.17	101.10	106.00
29	Ac	11	DC	O4'-C1'-N1	8.15	113.70	108.00
10	AJ	9	DC	O4'-C4'-C3'	-8.13	101.12	106.00
32	Af	7	DG	P-O3'-C3'	8.07	129.39	119.70
1	AA	1140	DC	O4'-C1'-C2'	-8.05	99.46	105.90
1	AA	1081	DG	O4'-C4'-C3'	-8.05	101.17	106.00
32	Af	25	DC	P-O3'-C3'	8.02	129.33	119.70
13	AM	21	DG	O4'-C4'-C3'	-8.02	101.19	106.00
11	AK	3	DT	P-O3'-C3'	8.00	129.30	119.70
6	AF	31	DG	C5-C6-O6	-7.99	123.81	128.60
21	AU	39	DG	O4'-C1'-C2'	-7.99	99.51	105.90
29	Ac	42	DC	O4'-C1'-C2'	-7.99	99.51	105.90
35	Ai	26	DG	O4'-C4'-C3'	-7.95	101.23	106.00
1	AA	41	DC	P-O3'-C3'	7.95	129.24	119.70
7	AG	28	DG	P-O3'-C3'	7.94	129.22	119.70
23	AW	9	DA	O4'-C1'-C2'	-7.90	99.58	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	272	DC	C2-N1-C1'	7.90	127.49	118.80
1	AA	1140	DC	O4'-C4'-C3'	-7.90	101.26	106.00
20	AT	8	DG	P-O3'-C3'	7.90	129.18	119.70
1	AA	528	DC	C4'-C3'-C2'	-7.88	96.01	103.10
13	AM	21	DG	O4'-C1'-C2'	-7.88	99.60	105.90
16	AP	22	DA	O4'-C4'-C3'	-7.87	101.28	106.00
35	Ai	1	DC	O4'-C4'-C3'	-7.87	101.28	106.00
1	AA	1272	DC	O4'-C4'-C3'	-7.87	101.28	106.00
23	AW	1	DT	O4'-C4'-C3'	-7.87	101.28	106.00
1	AA	220	DG	O4'-C1'-C2'	-7.86	99.61	105.90
1	AA	457	DG	O4'-C1'-C2'	-7.86	99.61	105.90
1	AA	255	DT	C4'-C3'-C2'	-7.85	96.04	103.10
1	AA	1146	DC	C6-N1-C2	-7.84	117.16	120.30
1	AA	791	DG	O4'-C4'-C3'	-7.82	101.31	106.00
23	AW	9	DA	P-O3'-C3'	7.82	129.08	119.70
2	AB	1	DC	O4'-C1'-C2'	-7.81	99.65	105.90
20	AT	30	DG	O4'-C1'-C2'	-7.79	99.67	105.90
1	AA	892	DG	O4'-C1'-C2'	-7.76	99.69	105.90
23	AW	11	DC	P-O3'-C3'	7.75	129.00	119.70
17	AQ	25	DG	O4'-C1'-C2'	-7.73	99.71	105.90
12	AL	3	DG	O4'-C4'-C3'	-7.71	101.37	106.00
12	AL	43	DC	O4'-C1'-C2'	-7.71	99.73	105.90
30	Ad	19	DC	O4'-C4'-C3'	-7.70	101.38	106.00
11	AK	1	DT	O4'-C4'-C3'	-7.70	101.38	106.00
34	Ah	15	DG	O4'-C1'-C2'	-7.69	99.75	105.90
18	AR	16	DG	C1'-O4'-C4'	-7.69	102.41	110.10
1	AA	292	DG	O4'-C1'-C2'	-7.69	99.75	105.90
1	AA	1207	DG	O4'-C1'-C2'	-7.67	99.77	105.90
1	AA	789	DA	O4'-C1'-C2'	-7.66	99.77	105.90
23	AW	40	DG	O4'-C1'-C2'	-7.63	99.79	105.90
20	AT	1	DC	O4'-C1'-C2'	-7.63	99.80	105.90
2	AB	10	DA	O4'-C4'-C3'	-7.62	101.43	106.00
1	AA	1180	DG	P-O3'-C3'	7.61	128.84	119.70
1	AA	493	DT	O4'-C1'-C2'	-7.60	99.82	105.90
32	Af	10	DC	O4'-C1'-C2'	-7.59	99.83	105.90
22	AV	34	DC	C1'-O4'-C4'	-7.58	102.52	110.10
1	AA	791	DG	C4'-C3'-C2'	-7.57	96.28	103.10
18	AR	9	DT	P-O3'-C3'	7.57	128.78	119.70
29	Ac	23	DG	O4'-C1'-C2'	-7.57	99.84	105.90
30	Ad	35	DG	O4'-C1'-C2'	-7.56	99.85	105.90
19	AS	1	DT	O4'-C1'-C2'	-7.55	99.86	105.90
36	Aj	18	DG	O4'-C1'-C2'	-7.55	99.86	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AQ	25	DG	C1'-O4'-C4'	-7.53	102.57	110.10
12	AL	3	DG	C1'-O4'-C4'	-7.51	102.59	110.10
17	AQ	17	DC	P-O3'-C3'	7.51	128.72	119.70
24	AX	27	DG	O4'-C1'-C2'	-7.48	99.92	105.90
1	AA	97	DG	O4'-C1'-C2'	-7.47	99.92	105.90
1	AA	181	DG	C1'-O4'-C4'	-7.47	102.63	110.10
32	Af	8	DC	O4'-C1'-C2'	-7.45	99.94	105.90
20	AT	8	DG	C1'-O4'-C4'	-7.45	102.65	110.10
1	AA	1039	DG	O4'-C4'-C3'	-7.45	101.52	104.50
1	AA	1030	DG	O4'-C1'-C2'	-7.44	99.95	105.90
12	AL	9	DC	O4'-C1'-C2'	-7.44	99.95	105.90
37	Ak	39	DG	O4'-C1'-C2'	-7.41	99.97	105.90
1	AA	1229	DT	O4'-C1'-C2'	-7.40	99.98	105.90
5	AE	10	DT	O4'-C1'-N1	7.40	113.18	108.00
17	AQ	1	DT	O4'-C1'-C2'	-7.40	99.98	105.90
5	AE	18	DG	O4'-C1'-C2'	-7.39	99.98	105.90
21	AU	22	DG	O4'-C1'-C2'	-7.39	99.99	105.90
12	AL	3	DG	O4'-C1'-C2'	-7.38	100.00	105.90
26	AZ	9	DA	C4'-C3'-C2'	-7.37	96.46	103.10
7	AG	17	DG	O4'-C1'-C2'	-7.37	100.01	105.90
1	AA	145	DG	C4'-C3'-C2'	-7.34	96.49	103.10
27	Aa	41	DA	O4'-C1'-N9	7.31	113.12	108.00
23	AW	2	DG	P-O3'-C3'	7.30	128.46	119.70
1	AA	707	DA	O4'-C1'-C2'	-7.29	100.07	105.90
1	AA	566	DC	P-O3'-C3'	7.26	128.41	119.70
33	Ag	6	DT	P-O3'-C3'	7.26	128.41	119.70
5	AE	13	DC	P-O3'-C3'	7.25	128.41	119.70
1	AA	165	DC	P-O3'-C3'	7.25	128.40	119.70
1	AA	297	DT	O4'-C4'-C3'	-7.25	101.60	104.50
1	AA	977	DG	C5-C6-O6	-7.25	124.25	128.60
37	Ak	5	DG	O4'-C1'-C2'	-7.24	100.11	105.90
6	AF	31	DG	N1-C6-O6	7.24	124.25	119.90
1	AA	293	DG	O4'-C1'-C2'	-7.22	100.12	105.90
12	AL	12	DT	C4'-C3'-C2'	-7.21	96.61	103.10
20	AT	1	DC	C1'-O4'-C4'	-7.21	102.89	110.10
1	AA	856	DC	O4'-C4'-C3'	-7.21	101.62	104.50
23	AW	25	DT	C4'-C3'-C2'	-7.21	96.61	103.10
27	Aa	31	DG	O4'-C1'-C2'	-7.19	100.15	105.90
1	AA	1281	DA	N1-C6-N6	-7.19	114.29	118.60
6	AF	2	DG	O4'-C1'-C2'	-7.18	100.15	105.90
1	AA	1080	DA	P-O3'-C3'	7.18	128.31	119.70
1	AA	1219	DG	O4'-C1'-C2'	-7.17	100.16	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	826	DG	O4'-C1'-N9	7.17	113.02	108.00
1	AA	976	DC	C1'-O4'-C4'	-7.16	102.94	110.10
11	AK	24	DG	O4'-C1'-C2'	-7.15	100.18	105.90
1	AA	1126	DC	O4'-C1'-C2'	-7.15	100.18	105.90
1	AA	170	DC	P-O3'-C3'	7.13	128.26	119.70
24	AX	9	DT	P-O3'-C3'	7.12	128.24	119.70
2	AB	32	DG	O4'-C1'-C2'	-7.12	100.21	105.90
36	Aj	13	DA	N1-C6-N6	-7.11	114.33	118.60
1	AA	766	DG	C5-C6-O6	-7.11	124.34	128.60
16	AP	6	DC	O4'-C4'-C3'	-7.09	101.66	104.50
36	Aj	1	DC	O4'-C1'-C2'	-7.09	100.23	105.90
1	AA	1156	DG	O4'-C1'-C2'	-7.08	100.23	105.90
1	AA	867	DC	P-O3'-C3'	7.07	128.18	119.70
1	AA	812	DA	O4'-C4'-C3'	-7.07	101.67	104.50
1	AA	272	DC	C6-N1-C1'	-7.05	112.34	120.80
1	AA	157	DA	P-O3'-C3'	7.04	128.15	119.70
4	AD	3	DA	O4'-C1'-C2'	-7.04	100.27	105.90
1	AA	1240	DG	O4'-C1'-C2'	-7.02	100.28	105.90
1	AA	405	DG	O4'-C1'-C2'	-7.00	100.30	105.90
25	AY	22	DA	P-O3'-C3'	7.00	128.09	119.70
27	Aa	41	DA	O4'-C1'-C2'	-7.00	100.30	105.90
1	AA	1222	DC	O4'-C1'-C2'	-6.99	100.31	105.90
14	AN	20	DA	C4'-C3'-C2'	-6.99	96.81	103.10
1	AA	297	DT	C4'-C3'-C2'	-6.99	96.81	103.10
1	AA	744	DG	P-O3'-C3'	6.99	128.08	119.70
1	AA	838	DG	O4'-C1'-C2'	-6.98	100.31	105.90
29	Ac	5	DA	C4'-C3'-C2'	-6.98	96.82	103.10
1	AA	676	DC	O4'-C1'-C2'	-6.98	100.31	105.90
1	AA	45	DG	C1'-O4'-C4'	-6.97	103.13	110.10
1	AA	177	DA	C4'-C3'-C2'	-6.97	96.83	103.10
14	AN	20	DA	O4'-C4'-C3'	-6.96	101.72	104.50
1	AA	944	DC	P-O3'-C3'	6.95	128.04	119.70
34	Ah	34	DG	O4'-C1'-C2'	-6.95	100.34	105.90
1	AA	969	DG	P-O3'-C3'	6.94	128.03	119.70
1	AA	1042	DG	O4'-C1'-C2'	-6.94	100.35	105.90
34	Ah	16	DG	O4'-C1'-C2'	-6.93	100.35	105.90
23	AW	25	DT	O4'-C4'-C3'	-6.92	101.73	104.50
1	AA	1246	DG	C1'-O4'-C4'	-6.91	103.19	110.10
1	AA	1163	DA	P-O3'-C3'	6.90	127.98	119.70
1	AA	867	DC	O4'-C1'-C2'	-6.89	100.38	105.90
21	AU	7	DG	O4'-C1'-C2'	-6.89	100.39	105.90
27	Aa	47	DA	N1-C6-N6	-6.88	114.47	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AQ	37	DC	O4'-C1'-C2'	-6.88	100.39	105.90
4	AD	3	DA	C1'-O4'-C4'	-6.88	103.22	110.10
23	AW	19	DC	C4'-C3'-C2'	-6.87	96.92	103.10
8	AH	17	DC	P-O3'-C3'	6.87	127.95	119.70
30	Ad	32	DA	O4'-C1'-C2'	-6.87	100.41	105.90
13	AM	21	DG	C1'-O4'-C4'	-6.86	103.24	110.10
15	AO	18	DG	C1'-O4'-C4'	-6.86	103.24	110.10
4	AD	20	DT	O4'-C1'-C2'	-6.86	100.42	105.90
33	Ag	31	DA	O4'-C1'-C2'	-6.85	100.42	105.90
1	AA	283	DC	C4'-C3'-C2'	-6.84	96.94	103.10
10	AJ	25	DA	N1-C6-N6	-6.83	114.50	118.60
1	AA	372	DG	O4'-C1'-C2'	-6.83	100.44	105.90
1	AA	1118	DT	O4'-C1'-C2'	-6.82	100.44	105.90
1	AA	1265	DA	O4'-C1'-C2'	-6.80	100.46	105.90
27	Aa	9	DA	C4'-C3'-C2'	-6.80	96.98	103.10
1	AA	157	DA	O4'-C1'-N9	6.79	112.76	108.00
18	AR	13	DC	O4'-C4'-C3'	-6.79	101.78	104.50
1	AA	1163	DA	O4'-C1'-C2'	-6.77	100.48	105.90
2	AB	23	DC	O4'-C1'-C2'	-6.77	100.48	105.90
19	AS	26	DA	N1-C6-N6	-6.76	114.54	118.60
33	Ag	10	DG	O4'-C1'-C2'	-6.76	100.49	105.90
1	AA	952	DG	O4'-C1'-C2'	-6.75	100.50	105.90
1	AA	250	DA	O4'-C1'-C2'	-6.75	100.50	105.90
18	AR	10	DG	C1'-O4'-C4'	-6.74	103.36	110.10
8	AH	29	DG	O4'-C1'-C2'	-6.72	100.52	105.90
10	AJ	9	DC	C1'-O4'-C4'	-6.71	103.39	110.10
1	AA	1118	DT	P-O3'-C3'	6.71	127.75	119.70
1	AA	766	DG	N1-C6-O6	6.70	123.92	119.90
1	AA	331	DC	O4'-C1'-C2'	-6.68	100.55	105.90
35	Ai	26	DG	C4'-C3'-C2'	-6.68	97.08	103.10
22	AV	14	DA	P-O3'-C3'	6.68	127.72	119.70
25	AY	4	DG	O4'-C1'-C2'	-6.67	100.56	105.90
1	AA	378	DG	C4'-C3'-C2'	-6.67	97.09	103.10
1	AA	1008	DC	O4'-C1'-C2'	-6.67	100.57	105.90
16	AP	22	DA	C4'-C3'-C2'	-6.66	97.10	103.10
1	AA	812	DA	C4'-C3'-C2'	-6.66	97.11	103.10
37	Ak	5	DG	O4'-C4'-C3'	-6.66	101.84	104.50
1	AA	976	DC	O4'-C1'-N1	6.65	112.66	108.00
36	Aj	20	DT	C4'-C3'-C2'	-6.65	97.11	103.10
1	AA	1104	DG	C1'-O4'-C4'	-6.64	103.46	110.10
1	AA	942	DG	O4'-C1'-C2'	-6.63	100.60	105.90
1	AA	126	DA	P-O3'-C3'	6.62	127.65	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	939	DG	O4'-C1'-C2'	-6.62	100.61	105.90
1	AA	603	DT	O4'-C1'-C2'	-6.61	100.61	105.90
1	AA	360	DG	O4'-C4'-C3'	-6.59	101.86	104.50
1	AA	759	DG	P-O3'-C3'	6.59	127.61	119.70
17	AQ	24	DG	O4'-C1'-C2'	-6.58	100.63	105.90
34	Ah	15	DG	O4'-C1'-N9	6.58	112.61	108.00
1	AA	530	DC	O4'-C1'-C2'	-6.58	100.64	105.90
27	Aa	16	DC	O4'-C1'-C2'	-6.56	100.65	105.90
4	AD	3	DA	P-O3'-C3'	6.56	127.57	119.70
4	AD	12	DG	O4'-C1'-C2'	-6.54	100.67	105.90
1	AA	921	DG	O4'-C4'-C3'	-6.53	101.89	104.50
1	AA	16	DG	C1'-O4'-C4'	-6.53	103.57	110.10
1	AA	1093	DG	O4'-C1'-C2'	-6.53	100.68	105.90
1	AA	1248	DT	O4'-C1'-C2'	-6.52	100.68	105.90
1	AA	625	DC	C4'-C3'-C2'	-6.51	97.24	103.10
4	AD	3	DA	O4'-C1'-N9	6.51	112.56	108.00
1	AA	937	DT	O4'-C4'-C3'	-6.50	101.90	104.50
9	AI	30	DG	O4'-C1'-C2'	-6.50	100.70	105.90
1	AA	651	DG	P-O3'-C3'	6.50	127.50	119.70
29	Ac	1	DT	C4'-C3'-C2'	-6.50	97.25	103.10
1	AA	261	DG	C4'-C3'-C2'	-6.49	97.26	103.10
33	Ag	6	DT	O4'-C4'-C3'	-6.49	101.90	104.50
1	AA	303	DA	P-O3'-C3'	6.49	127.48	119.70
1	AA	937	DT	C4'-C3'-C2'	-6.49	97.26	103.10
1	AA	1207	DG	C1'-O4'-C4'	-6.49	103.61	110.10
20	AT	32	DA	O4'-C1'-C2'	-6.48	100.72	105.90
1	AA	250	DA	P-O3'-C3'	6.48	127.47	119.70
33	Ag	29	DG	O4'-C1'-C2'	-6.47	100.72	105.90
1	AA	633	DT	O4'-C1'-C2'	-6.46	100.73	105.90
7	AG	2	DG	O4'-C4'-C3'	-6.46	101.92	104.50
1	AA	462	DT	C4'-C3'-C2'	-6.45	97.29	103.10
29	Ac	17	DG	O4'-C1'-N9	6.44	112.51	108.00
20	AT	30	DG	O4'-C4'-C3'	-6.44	101.92	104.50
1	AA	797	DA	C1'-O4'-C4'	-6.44	103.66	110.10
1	AA	686	DT	O4'-C1'-C2'	-6.43	100.75	105.90
20	AT	8	DG	O4'-C1'-C2'	-6.43	100.75	105.90
1	AA	682	DA	C4'-C3'-C2'	-6.43	97.31	103.10
29	Ac	2	DT	O4'-C1'-C2'	-6.42	100.76	105.90
1	AA	294	DT	C4'-C3'-C2'	-6.42	97.32	103.10
29	Ac	36	DT	C1'-O4'-C4'	-6.41	103.69	110.10
1	AA	339	DA	O4'-C1'-C2'	-6.41	100.77	105.90
11	AK	40	DT	P-O3'-C3'	6.41	127.39	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	6	DG	N1-C6-O6	6.40	123.74	119.90
1	AA	789	DA	P-O3'-C3'	6.40	127.38	119.70
11	AK	39	DG	C4'-C3'-C2'	-6.40	97.34	103.10
1	AA	806	DA	O4'-C1'-C2'	-6.39	100.79	105.90
2	AB	26	DG	N1-C6-O6	6.39	123.73	119.90
1	AA	977	DG	N1-C6-O6	6.39	123.73	119.90
5	AE	10	DT	C1'-O4'-C4'	-6.39	103.71	110.10
9	AI	12	DC	C6-N1-C2	-6.38	117.75	120.30
15	AO	33	DG	C4'-C3'-C2'	-6.35	97.38	103.10
1	AA	111	DG	O4'-C1'-C2'	-6.34	100.83	105.90
1	AA	991	DA	O4'-C1'-C2'	-6.34	100.83	105.90
6	AF	21	DT	C4'-C3'-C2'	-6.34	97.39	103.10
29	Ac	5	DA	O4'-C4'-C3'	-6.34	101.96	104.50
1	AA	1163	DA	C1'-O4'-C4'	-6.33	103.77	110.10
21	AU	1	DG	C1'-O4'-C4'	-6.33	103.77	110.10
1	AA	1255	DA	N1-C6-N6	-6.33	114.80	118.60
25	AY	6	DG	C5-C6-O6	-6.33	124.80	128.60
1	AA	74	DA	C4'-C3'-C2'	-6.33	97.41	103.10
7	AG	28	DG	O4'-C4'-C3'	-6.33	101.97	104.50
1	AA	1101	DG	C1'-O4'-C4'	-6.32	103.78	110.10
1	AA	1288	DG	O4'-C1'-C2'	-6.31	100.85	105.90
1	AA	165	DC	O4'-C1'-C2'	-6.31	100.85	105.90
5	AE	10	DT	O4'-C1'-C2'	-6.31	100.85	105.90
1	AA	356	DA	P-O3'-C3'	6.31	127.27	119.70
1	AA	762	DG	O4'-C1'-C2'	-6.30	100.86	105.90
7	AG	2	DG	C4'-C3'-C2'	-6.30	97.43	103.10
25	AY	30	DA	O4'-C1'-C2'	-6.30	100.86	105.90
13	AM	15	DT	C4'-C3'-C2'	-6.29	97.44	103.10
33	Ag	13	DT	O4'-C1'-C2'	-6.29	100.87	105.90
16	AP	16	DG	C1'-O4'-C4'	-6.29	103.81	110.10
14	AN	8	DT	O4'-C1'-C2'	-6.28	100.87	105.90
8	AH	28	DG	O4'-C1'-C2'	-6.28	100.88	105.90
11	AK	31	DG	N1-C6-O6	6.28	123.67	119.90
25	AY	12	DG	C1'-O4'-C4'	-6.27	103.83	110.10
11	AK	24	DG	P-O3'-C3'	6.27	127.23	119.70
1	AA	241	DG	O4'-C1'-C2'	-6.27	100.89	105.90
34	Ah	7	DG	O4'-C1'-C2'	-6.26	100.89	105.90
6	AF	8	DA	P-O3'-C3'	6.26	127.21	119.70
7	AG	47	DA	C4'-C3'-C2'	-6.25	97.47	103.10
1	AA	791	DG	C5-C6-O6	-6.25	124.85	128.60
33	Ag	6	DT	C4'-C3'-C2'	-6.25	97.47	103.10
1	AA	1315	DG	O4'-C1'-C2'	-6.23	100.92	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	596	DG	P-O3'-C3'	6.23	127.17	119.70
1	AA	697	DA	C1'-O4'-C4'	-6.22	103.88	110.10
5	AE	14	DC	C6-N1-C2	-6.22	117.81	120.30
15	AO	32	DG	C1'-O4'-C4'	-6.21	103.89	110.10
28	Ab	32	DA	C4'-C3'-C2'	-6.21	97.51	103.10
30	Ad	19	DC	O4'-C1'-C2'	-6.20	100.94	105.90
1	AA	220	DG	O4'-C4'-C3'	-6.20	102.02	104.50
1	AA	540	DC	C4'-C3'-C2'	-6.20	97.52	103.10
1	AA	41	DC	C1'-O4'-C4'	-6.20	103.91	110.10
1	AA	558	DC	P-O3'-C3'	6.19	127.13	119.70
27	Aa	30	DT	O4'-C1'-C2'	-6.19	100.95	105.90
13	AM	35	DG	O4'-C1'-C2'	-6.19	100.95	105.90
2	AB	30	DG	O4'-C1'-C2'	-6.18	100.95	105.90
24	AX	16	DT	O4'-C1'-C2'	-6.18	100.95	105.90
1	AA	360	DG	C4'-C3'-C2'	-6.18	97.54	103.10
5	AE	13	DC	O4'-C1'-C2'	-6.18	100.95	105.90
1	AA	830	DA	N1-C6-N6	-6.18	114.89	118.60
12	AL	28	DG	O4'-C1'-C2'	-6.17	100.97	105.90
1	AA	415	DT	P-O3'-C3'	6.17	127.10	119.70
1	AA	390	DA	O4'-C1'-C2'	-6.16	100.97	105.90
1	AA	1229	DT	O4'-C1'-N1	6.16	112.31	108.00
1	AA	860	DA	O4'-C4'-C3'	-6.15	102.04	104.50
1	AA	547	DA	N1-C6-N6	-6.15	114.91	118.60
1	AA	736	DC	O4'-C1'-C2'	-6.14	100.99	105.90
16	AP	43	DG	O4'-C1'-C2'	-6.13	100.99	105.90
1	AA	820	DG	O4'-C1'-C2'	-6.12	101.00	105.90
5	AE	2	DG	C5-C6-O6	-6.12	124.93	128.60
1	AA	238	DG	P-O3'-C3'	6.12	127.04	119.70
1	AA	545	DA	O4'-C4'-C3'	-6.11	102.06	104.50
1	AA	1153	DT	O4'-C4'-C3'	-6.11	102.06	104.50
8	AH	16	DA	P-O3'-C3'	6.11	127.03	119.70
11	AK	7	DG	O4'-C1'-C2'	-6.11	101.02	105.90
1	AA	413	DT	C4'-C3'-C2'	-6.10	97.61	103.10
11	AK	31	DG	C5-C6-O6	-6.10	124.94	128.60
31	Ae	1	DT	O4'-C1'-C2'	-6.10	101.02	105.90
36	Aj	18	DG	O4'-C4'-C3'	-6.10	102.06	104.50
1	AA	813	DT	P-O5'-C5'	6.10	130.66	120.90
1	AA	272	DC	O4'-C1'-C2'	-6.09	101.02	105.90
1	AA	493	DT	O4'-C4'-C3'	-6.09	102.06	104.50
25	AY	19	DC	P-O3'-C3'	6.09	127.01	119.70
1	AA	224	DT	O4'-C1'-C2'	-6.09	101.03	105.90
1	AA	383	DT	C4'-C3'-C2'	-6.09	97.62	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	745	DG	O4'-C1'-N9	6.08	112.26	108.00
8	AH	16	DA	O4'-C1'-N9	6.08	112.26	108.00
25	AY	9	DG	P-O3'-C3'	6.08	126.99	119.70
1	AA	842	DC	P-O3'-C3'	6.08	126.99	119.70
1	AA	1049	DC	C1'-O4'-C4'	-6.07	104.03	110.10
24	AX	10	DA	C4'-C3'-C2'	-6.07	97.64	103.10
1	AA	325	DT	C4'-C3'-C2'	-6.05	97.65	103.10
1	AA	1008	DC	P-O3'-C3'	6.05	126.96	119.70
1	AA	253	DG	O4'-C1'-C2'	-6.05	101.06	105.90
1	AA	1183	DT	C4'-C3'-C2'	-6.04	97.66	103.10
1	AA	860	DA	C4'-C3'-C2'	-6.04	97.67	103.10
6	AF	8	DA	O4'-C1'-C2'	-6.02	101.08	105.90
1	AA	394	DG	C4'-C3'-C2'	-6.01	97.69	103.10
1	AA	1081	DG	O4'-C1'-C2'	-6.01	101.09	105.90
7	AG	1	DT	O4'-C4'-C3'	-6.01	102.09	104.50
20	AT	25	DG	O4'-C1'-C2'	-6.01	101.09	105.90
1	AA	987	DT	C4'-C3'-C2'	-6.01	97.69	103.10
3	AC	19	DG	C1'-O4'-C4'	-6.01	104.09	110.10
1	AA	483	DG	P-O3'-C3'	6.01	126.91	119.70
1	AA	8	DT	C4'-C3'-C2'	-6.00	97.70	103.10
35	Ai	30	DA	O4'-C1'-C2'	-6.00	101.10	105.90
1	AA	1273	DT	P-O3'-C3'	6.00	126.90	119.70
21	AU	22	DG	P-O3'-C3'	5.98	126.88	119.70
1	AA	38	DA	P-O3'-C3'	5.98	126.88	119.70
1	AA	1257	DC	O4'-C1'-C2'	-5.98	101.12	105.90
29	Ac	17	DG	C1'-O4'-C4'	-5.98	104.12	110.10
11	AK	20	DT	C4'-C3'-C2'	-5.97	97.72	103.10
1	AA	587	DC	C2-N1-C1'	5.97	125.37	118.80
3	AC	1	DA	C1'-O4'-C4'	-5.97	104.13	110.10
1	AA	828	DT	C6-C5-C7	5.97	126.48	122.90
1	AA	615	DC	C4'-C3'-C2'	-5.96	97.73	103.10
2	AB	37	DT	P-O3'-C3'	5.96	126.85	119.70
4	AD	20	DT	C1'-O4'-C4'	-5.95	104.15	110.10
1	AA	1259	DT	O4'-C4'-C3'	-5.95	102.12	104.50
1	AA	248	DC	C4'-C3'-C2'	-5.95	97.75	103.10
4	AD	13	DA	P-O3'-C3'	5.95	126.84	119.70
37	Ak	39	DG	C1'-O4'-C4'	-5.94	104.16	110.10
1	AA	856	DC	C4'-C3'-C2'	-5.94	97.76	103.10
1	AA	601	DG	O4'-C1'-N9	5.93	112.15	108.00
1	AA	969	DG	O4'-C1'-C2'	-5.93	101.16	105.90
32	Af	7	DG	O4'-C4'-C3'	-5.93	102.13	104.50
2	AB	13	DG	O4'-C4'-C3'	-5.93	102.13	104.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	AK	15	DA	O4'-C4'-C3'	-5.93	102.13	104.50
1	AA	673	DC	P-O3'-C3'	5.93	126.81	119.70
14	AN	2	DT	P-O3'-C3'	5.92	126.81	119.70
8	AH	26	DG	O4'-C1'-C2'	-5.92	101.16	105.90
1	AA	615	DC	O4'-C4'-C3'	-5.92	102.13	104.50
16	AP	16	DG	O4'-C1'-C2'	-5.92	101.16	105.90
1	AA	630	DG	C5-C6-O6	-5.91	125.06	128.60
1	AA	957	DC	O4'-C4'-C3'	-5.91	102.14	104.50
5	AE	18	DG	C1'-O4'-C4'	-5.91	104.19	110.10
23	AW	40	DG	O4'-C4'-C3'	-5.91	102.14	104.50
1	AA	27	DT	C4'-C3'-C2'	-5.90	97.79	103.10
4	AD	29	DT	P-O3'-C3'	5.90	126.78	119.70
1	AA	837	DA	O4'-C1'-C2'	-5.89	101.18	105.90
1	AA	1201	DC	O4'-C1'-C2'	-5.89	101.19	105.90
19	AS	14	DA	O4'-C1'-C2'	-5.89	101.19	105.90
11	AK	36	DC	O4'-C1'-C2'	-5.89	101.19	105.90
13	AM	34	DG	O4'-C1'-C2'	-5.89	101.19	105.90
34	Ah	15	DG	C1'-O4'-C4'	-5.88	104.22	110.10
1	AA	455	DC	O4'-C1'-C2'	-5.88	101.19	105.90
24	AX	3	DT	C4'-C3'-C2'	-5.88	97.81	103.10
1	AA	180	DG	O4'-C1'-C2'	-5.88	101.20	105.90
1	AA	1060	DA	O4'-C1'-C2'	-5.87	101.20	105.90
15	AO	14	DG	P-O3'-C3'	5.87	126.75	119.70
1	AA	632	DG	O4'-C1'-C2'	-5.87	101.20	105.90
37	Ak	5	DG	C1'-O4'-C4'	-5.86	104.24	110.10
35	Ai	4	DT	C4'-C3'-C2'	-5.86	97.83	103.10
37	Ak	23	DG	O4'-C1'-C2'	-5.86	101.21	105.90
16	AP	34	DT	P-O3'-C3'	5.86	126.73	119.70
37	Ak	9	DG	C4'-C3'-C2'	-5.86	97.83	103.10
1	AA	1081	DG	C1'-O4'-C4'	-5.85	104.25	110.10
23	AW	2	DG	C4'-C3'-C2'	-5.84	97.84	103.10
1	AA	826	DG	C1'-O4'-C4'	-5.84	104.26	110.10
1	AA	516	DG	O4'-C1'-C2'	-5.83	101.23	105.90
3	AC	1	DA	O4'-C4'-C3'	-5.83	102.17	104.50
3	AC	37	DT	P-O3'-C3'	5.83	126.70	119.70
1	AA	818	DG	O4'-C1'-C2'	-5.83	101.24	105.90
1	AA	854	DC	P-O5'-C5'	5.82	130.22	120.90
19	AS	8	DG	O4'-C1'-C2'	-5.81	101.25	105.90
1	AA	119	DA	O4'-C1'-C2'	-5.80	101.26	105.90
1	AA	1229	DT	P-O3'-C3'	5.80	126.67	119.70
12	AL	5	DA	N1-C6-N6	-5.80	115.12	118.60
33	Ag	12	DG	O4'-C1'-C2'	-5.80	101.26	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Ae	2	DT	C1'-O4'-C4'	-5.80	104.30	110.10
21	AU	11	DT	C4'-C3'-C2'	-5.79	97.88	103.10
1	AA	676	DC	C1'-O4'-C4'	-5.79	104.31	110.10
6	AF	27	DA	O4'-C1'-C2'	-5.79	101.27	105.90
31	Ae	18	DG	C4'-C3'-C2'	-5.79	97.89	103.10
2	AB	26	DG	C5-C6-O6	-5.78	125.13	128.60
36	Aj	18	DG	C1'-O4'-C4'	-5.78	104.32	110.10
1	AA	104	DT	C4'-C3'-C2'	-5.78	97.90	103.10
1	AA	394	DG	O4'-C4'-C3'	-5.78	102.19	104.50
28	Ab	33	DC	P-O3'-C3'	5.78	126.63	119.70
37	Ak	18	DC	P-O5'-C5'	5.77	130.13	120.90
24	AX	14	DA	C4'-C3'-C2'	-5.77	97.91	103.10
4	AD	16	DG	O4'-C1'-C2'	-5.76	101.29	105.90
1	AA	666	DA	O4'-C1'-C2'	-5.76	101.29	105.90
1	AA	820	DG	C1'-O4'-C4'	-5.75	104.34	110.10
12	AL	25	DT	C1'-O4'-C4'	-5.75	104.35	110.10
1	AA	1283	DA	P-O3'-C3'	5.75	126.60	119.70
14	AN	13	DG	O4'-C1'-C2'	-5.74	101.31	105.90
1	AA	1265	DA	C1'-O4'-C4'	-5.73	104.37	110.10
21	AU	22	DG	C1'-O4'-C4'	-5.73	104.37	110.10
1	AA	601	DG	O4'-C1'-C2'	-5.73	101.32	105.90
1	AA	975	DG	O4'-C1'-N9	5.73	112.01	108.00
36	Aj	1	DC	C1'-O4'-C4'	-5.73	104.37	110.10
1	AA	906	DT	C4'-C3'-C2'	-5.71	97.96	103.10
1	AA	887	DA	O4'-C1'-C2'	-5.71	101.33	105.90
8	AH	4	DG	O4'-C1'-C2'	-5.71	101.33	105.90
1	AA	875	DA	O4'-C1'-C2'	-5.71	101.33	105.90
16	AP	42	DC	P-O3'-C3'	5.71	126.55	119.70
10	AJ	28	DT	C4'-C3'-C2'	-5.71	97.97	103.10
1	AA	1080	DA	O4'-C1'-N9	5.70	111.99	108.00
17	AQ	31	DG	O4'-C1'-C2'	-5.70	101.34	105.90
1	AA	1283	DA	O4'-C1'-C2'	-5.69	101.35	105.90
1	AA	575	DG	O4'-C1'-C2'	-5.69	101.35	105.90
1	AA	1181	DA	O4'-C1'-N9	-5.69	104.02	108.00
34	Ah	30	DA	O4'-C1'-C2'	-5.69	101.35	105.90
9	AI	16	DA	P-O3'-C3'	5.66	126.50	119.70
1	AA	47	DG	O4'-C4'-C3'	-5.66	102.23	104.50
1	AA	520	DG	O4'-C1'-C2'	-5.66	101.37	105.90
34	Ah	7	DG	C1'-O4'-C4'	-5.66	104.44	110.10
1	AA	467	DG	C1'-O4'-C4'	-5.66	104.44	110.10
1	AA	1156	DG	C1'-O4'-C4'	-5.66	104.44	110.10
8	AH	28	DG	O4'-C1'-N9	5.66	111.96	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	AR	1	DT	C1'-O4'-C4'	-5.66	104.44	110.10
1	AA	129	DC	C1'-O4'-C4'	-5.65	104.45	110.10
5	AE	18	DG	P-O3'-C3'	5.65	126.48	119.70
8	AH	9	DA	O4'-C1'-C2'	-5.64	101.39	105.90
1	AA	997	DG	O4'-C1'-C2'	-5.64	101.39	105.90
1	AA	427	DA	O4'-C1'-C2'	-5.63	101.39	105.90
21	AU	41	DA	O4'-C1'-C2'	-5.63	101.39	105.90
28	Ab	22	DT	C1'-O4'-C4'	-5.63	104.47	110.10
12	AL	36	DG	O4'-C1'-N9	5.63	111.94	108.00
30	Ad	21	DA	O4'-C1'-C2'	-5.63	101.40	105.90
12	AL	25	DT	O4'-C4'-C3'	-5.63	102.25	104.50
25	AY	16	DA	O4'-C1'-C2'	-5.62	101.40	105.90
1	AA	607	DC	C4'-C3'-C2'	-5.62	98.05	103.10
1	AA	791	DG	N1-C6-O6	5.61	123.27	119.90
24	AX	21	DG	O4'-C1'-C2'	-5.61	101.41	105.90
25	AY	22	DA	O4'-C1'-C2'	-5.61	101.41	105.90
1	AA	1163	DA	O4'-C1'-N9	5.61	111.92	108.00
15	AO	36	DA	P-O3'-C3'	5.61	126.43	119.70
33	Ag	4	DC	C4'-C3'-C2'	-5.61	98.05	103.10
1	AA	62	DC	P-O3'-C3'	5.60	126.42	119.70
1	AA	849	DC	C4'-C3'-C2'	-5.60	98.06	103.10
33	Ag	9	DT	O4'-C1'-C2'	-5.60	101.42	105.90
3	AC	19	DG	O4'-C4'-C3'	-5.60	102.26	104.50
37	Ak	30	DG	O4'-C1'-C2'	-5.59	101.42	105.90
1	AA	455	DC	C4'-C3'-C2'	-5.59	98.07	103.10
1	AA	20	DG	C4'-C3'-C2'	-5.59	98.07	103.10
1	AA	838	DG	C1'-O4'-C4'	-5.59	104.51	110.10
26	AZ	9	DA	O4'-C4'-C3'	-5.58	102.27	104.50
6	AF	21	DT	O4'-C4'-C3'	-5.58	102.27	104.50
7	AG	12	DG	P-O3'-C3'	5.58	126.40	119.70
7	AG	24	DA	O4'-C1'-C2'	-5.58	101.44	105.90
4	AD	29	DT	O4'-C1'-C2'	-5.57	101.44	105.90
1	AA	618	DC	C2-N1-C1'	5.57	124.93	118.80
11	AK	39	DG	O4'-C4'-C3'	-5.57	102.27	104.50
3	AC	15	DT	C4'-C3'-C2'	-5.57	98.09	103.10
1	AA	1112	DG	C1'-O4'-C4'	-5.56	104.54	110.10
1	AA	910	DC	O4'-C1'-C2'	-5.56	101.45	105.90
1	AA	769	DC	O4'-C1'-C2'	-5.55	101.46	105.90
1	AA	852	DT	C4'-C3'-C2'	-5.54	98.11	103.10
19	AS	29	DT	C4'-C3'-C2'	-5.54	98.11	103.10
1	AA	74	DA	O4'-C4'-C3'	-5.53	102.29	104.50
1	AA	1140	DC	C1'-O4'-C4'	-5.53	104.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	134	DG	O4'-C1'-C2'	-5.53	101.48	105.90
8	AH	26	DG	O4'-C1'-N9	5.53	111.87	108.00
1	AA	842	DC	O4'-C1'-C2'	-5.52	101.48	105.90
27	Aa	31	DG	C1'-O4'-C4'	-5.52	104.58	110.10
31	Ae	2	DT	O4'-C4'-C3'	-5.52	102.29	104.50
1	AA	1085	DC	P-O5'-C5'	5.51	129.72	120.90
1	AA	631	DA	O4'-C1'-N9	-5.51	104.14	108.00
8	AH	28	DG	P-O3'-C3'	5.51	126.31	119.70
1	AA	255	DT	O4'-C4'-C3'	-5.50	102.30	104.50
1	AA	603	DT	P-O3'-C3'	5.50	126.30	119.70
1	AA	895	DC	C4'-C3'-C2'	-5.49	98.16	103.10
1	AA	97	DG	C1'-O4'-C4'	-5.48	104.62	110.10
21	AU	17	DT	C4'-C3'-C2'	-5.48	98.17	103.10
1	AA	1039	DG	C1'-O4'-C4'	-5.48	104.62	110.10
20	AT	8	DG	C3'-C2'-C1'	-5.48	95.92	102.50
1	AA	1222	DC	C1'-O4'-C4'	-5.48	104.62	110.10
1	AA	952	DG	C1'-O4'-C4'	-5.47	104.63	110.10
9	AI	12	DC	C2-N1-C1'	5.47	124.82	118.80
1	AA	1044	DT	C4'-C3'-C2'	-5.47	98.18	103.10
1	AA	789	DA	C1'-O4'-C4'	-5.46	104.64	110.10
22	AV	35	DC	P-O3'-C3'	5.46	126.25	119.70
1	AA	235	DA	P-O3'-C3'	5.46	126.25	119.70
23	AW	16	DC	C2-N1-C1'	5.46	124.80	118.80
1	AA	536	DG	O4'-C1'-C2'	-5.45	101.54	105.90
1	AA	745	DG	O4'-C1'-C2'	-5.45	101.54	105.90
1	AA	2	DC	P-O3'-C3'	5.45	126.24	119.70
1	AA	601	DG	P-O3'-C3'	5.45	126.24	119.70
1	AA	457	DG	C1'-O4'-C4'	-5.45	104.65	110.10
15	AO	3	DG	O4'-C1'-C2'	-5.45	101.54	105.90
35	Ai	16	DC	C2-N1-C1'	5.45	124.79	118.80
1	AA	798	DG	N1-C6-O6	5.44	123.17	119.90
1	AA	1036	DG	O4'-C1'-C2'	-5.44	101.55	105.90
1	AA	727	DG	O4'-C1'-C2'	-5.44	101.55	105.90
12	AL	9	DC	P-O3'-C3'	5.43	126.22	119.70
1	AA	285	DC	C4'-C3'-C2'	-5.43	98.22	103.10
31	Ae	5	DG	O4'-C1'-C2'	-5.42	101.56	105.90
33	Ag	10	DG	C1'-O4'-C4'	-5.42	104.68	110.10
1	AA	934	DT	P-O3'-C3'	5.42	126.20	119.70
31	Ae	17	DA	N1-C6-N6	-5.41	115.35	118.60
1	AA	159	DC	P-O3'-C3'	5.41	126.19	119.70
22	AV	36	DG	C5-C6-O6	-5.41	125.35	128.60
9	AI	31	DA	N1-C6-N6	-5.41	115.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	374	DC	C1'-O4'-C4'	-5.39	104.71	110.10
1	AA	727	DG	O4'-C1'-N9	5.39	111.78	108.00
13	AM	12	DG	O4'-C1'-C2'	-5.39	101.58	105.90
1	AA	744	DG	O4'-C1'-C2'	-5.38	101.59	105.90
12	AL	12	DT	P-O3'-C3'	-5.38	113.24	119.70
1	AA	694	DG	O4'-C4'-C3'	-5.38	102.35	104.50
1	AA	220	DG	O4'-C1'-N9	5.38	111.76	108.00
28	Ab	11	DT	C4'-C3'-C2'	-5.38	98.26	103.10
35	Ai	5	DC	O4'-C1'-N1	-5.38	104.24	108.00
1	AA	566	DC	C6-N1-C2	-5.38	118.15	120.30
1	AA	1054	DG	O4'-C1'-C2'	-5.38	101.60	105.90
7	AG	1	DT	C1'-O4'-C4'	-5.38	104.72	110.10
1	AA	960	DT	O4'-C1'-C2'	-5.37	101.60	105.90
1	AA	1118	DT	C1'-O4'-C4'	-5.37	104.73	110.10
19	AS	21	DA	O4'-C1'-C2'	-5.37	101.60	105.90
28	Ab	26	DG	C4'-C3'-C2'	-5.37	98.27	103.10
1	AA	511	DG	O4'-C1'-C2'	-5.37	101.61	105.90
35	Ai	39	DT	O4'-C4'-C3'	-5.37	102.35	104.50
23	AW	19	DC	O4'-C4'-C3'	-5.37	102.35	104.50
35	Ai	15	DG	O4'-C1'-C2'	-5.37	101.61	105.90
37	Ak	16	DA	N1-C6-N6	-5.37	115.38	118.60
1	AA	1246	DG	O4'-C1'-N9	5.36	111.75	108.00
1	AA	946	DT	C4'-C3'-C2'	-5.36	98.28	103.10
16	AP	6	DC	C4'-C3'-C2'	-5.36	98.28	103.10
35	Ai	1	DC	C1'-O4'-C4'	-5.36	104.75	110.10
5	AE	2	DG	N1-C6-O6	5.35	123.11	119.90
7	AG	22	DA	C4'-C3'-C2'	-5.35	98.29	103.10
20	AT	22	DT	C4'-C3'-C2'	-5.34	98.29	103.10
1	AA	253	DG	C5-C6-O6	-5.34	125.39	128.60
1	AA	934	DT	O4'-C1'-C2'	-5.34	101.63	105.90
1	AA	181	DG	O4'-C1'-N9	5.34	111.74	108.00
1	AA	965	DA	P-O3'-C3'	5.33	126.10	119.70
17	AQ	36	DG	C5-C6-O6	-5.33	125.40	128.60
12	AL	9	DC	O4'-C1'-N1	5.33	111.73	108.00
23	AW	6	DG	N1-C6-O6	5.33	123.10	119.90
35	Ai	39	DT	C4'-C3'-C2'	-5.33	98.30	103.10
1	AA	1237	DG	O4'-C1'-C2'	-5.33	101.64	105.90
27	Aa	5	DG	O4'-C1'-C2'	-5.33	101.64	105.90
1	AA	1229	DT	C1'-O4'-C4'	-5.32	104.78	110.10
1	AA	724	DA	O4'-C1'-C2'	-5.32	101.64	105.90
17	AQ	39	DA	C4'-C3'-C2'	-5.32	98.31	103.10
1	AA	731	DC	C4'-C3'-C2'	-5.32	98.31	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	AY	30	DA	P-O3'-C3'	5.32	126.08	119.70
1	AA	900	DA	O4'-C1'-C2'	-5.31	101.65	105.90
1	AA	572	DC	C1'-O4'-C4'	-5.31	104.79	110.10
25	AY	9	DG	O4'-C1'-C2'	-5.31	101.66	105.90
1	AA	698	DG	C5-C6-O6	-5.30	125.42	128.60
10	AJ	19	DA	P-O3'-C3'	5.30	126.06	119.70
18	AR	13	DC	C4'-C3'-C2'	-5.30	98.33	103.10
37	Ak	39	DG	P-O3'-C3'	5.30	126.06	119.70
33	Ag	1	DG	O4'-C4'-C3'	-5.29	102.38	104.50
1	AA	828	DT	C4-C5-C7	-5.29	115.83	119.00
1	AA	253	DG	N1-C6-O6	5.29	123.07	119.90
1	AA	826	DG	O4'-C1'-C2'	-5.29	101.67	105.90
1	AA	1283	DA	C1'-O4'-C4'	-5.28	104.82	110.10
33	Ag	19	DA	C4'-C3'-C2'	-5.28	98.35	103.10
16	AP	21	DG	C4'-C3'-C2'	-5.28	98.35	103.10
9	AI	9	DT	C1'-O4'-C4'	-5.28	104.82	110.10
9	AI	33	DT	O4'-C1'-C2'	-5.27	101.69	105.90
10	AJ	9	DC	P-O3'-C3'	5.27	126.02	119.70
1	AA	745	DG	P-O3'-C3'	5.27	126.02	119.70
11	AK	45	DC	C6-N1-C2	-5.26	118.19	120.30
1	AA	455	DC	C6-N1-C2	-5.26	118.19	120.30
1	AA	843	DC	C6-N1-C2	-5.26	118.19	120.30
1	AA	310	DT	O4'-C1'-C2'	-5.26	101.69	105.90
16	AP	1	DG	C5-C6-O6	-5.26	125.45	128.60
1	AA	111	DG	C1'-O4'-C4'	-5.25	104.85	110.10
1	AA	1311	DG	O4'-C1'-C2'	-5.25	101.70	105.90
21	AU	1	DG	O4'-C1'-C2'	-5.25	101.70	105.90
36	Aj	23	DG	P-O3'-C3'	5.25	125.99	119.70
1	AA	894	DG	C4'-C3'-C2'	-5.24	98.38	103.10
1	AA	924	DA	O4'-C1'-C2'	-5.24	101.70	105.90
6	AF	35	DC	O4'-C1'-C2'	-5.24	101.70	105.90
1	AA	707	DA	C1'-O4'-C4'	-5.24	104.86	110.10
1	AA	1302	DA	O4'-C1'-C2'	-5.24	101.71	105.90
1	AA	879	DT	C4'-C3'-C2'	-5.24	98.39	103.10
4	AD	22	DA	O4'-C1'-C2'	-5.24	101.71	105.90
1	AA	526	DT	C4'-C3'-C2'	-5.23	98.39	103.10
1	AA	545	DA	C4'-C3'-C2'	-5.23	98.39	103.10
1	AA	1030	DG	O4'-C1'-N9	5.22	111.66	108.00
26	AZ	5	DG	C4'-C3'-C2'	-5.22	98.40	103.10
2	AB	1	DC	C1'-O4'-C4'	-5.22	104.88	110.10
1	AA	708	DG	N1-C6-O6	5.22	123.03	119.90
1	AA	640	DT	C4'-C3'-C2'	-5.22	98.41	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Ag	40	DC	O4'-C1'-C2'	-5.21	101.73	105.90
33	Ag	4	DC	O4'-C1'-N1	5.21	111.65	108.00
21	AU	11	DT	O4'-C4'-C3'	-5.21	102.42	104.50
27	Aa	3	DT	C4'-C3'-C2'	-5.21	98.41	103.10
1	AA	682	DA	O4'-C4'-C3'	-5.21	102.42	104.50
1	AA	884	DG	O4'-C1'-C2'	-5.21	101.73	105.90
1	AA	47	DG	C4'-C3'-C2'	-5.21	98.42	103.10
1	AA	176	DA	N1-C6-N6	-5.20	115.48	118.60
1	AA	873	DG	C5-C6-O6	-5.20	125.48	128.60
1	AA	892	DG	O4'-C4'-C3'	-5.20	102.42	104.50
1	AA	993	DG	O4'-C1'-C2'	-5.20	101.74	105.90
1	AA	618	DC	O4'-C1'-C2'	-5.20	101.74	105.90
5	AE	11	DA	C4'-C3'-C2'	-5.20	98.42	103.10
1	AA	493	DT	C1'-O4'-C4'	-5.20	104.90	110.10
3	AC	1	DA	P-O3'-C3'	5.20	125.94	119.70
29	Ac	43	DT	C4'-C3'-C2'	-5.20	98.42	103.10
1	AA	1147	DA	O4'-C1'-C2'	-5.19	101.75	105.90
26	AZ	27	DG	N1-C6-O6	5.19	123.01	119.90
1	AA	363	DC	P-O3'-C3'	5.19	125.92	119.70
15	AO	23	DG	P-O3'-C3'	5.19	125.92	119.70
1	AA	713	DG	C4'-C3'-C2'	-5.18	98.44	103.10
5	AE	18	DG	O4'-C1'-N9	5.18	111.63	108.00
7	AG	4	DT	C4'-C3'-C2'	-5.18	98.44	103.10
18	AR	9	DT	C4'-C3'-C2'	-5.18	98.44	103.10
28	Ab	16	DT	C4'-C3'-C2'	-5.18	98.44	103.10
29	Ac	26	DC	O4'-C1'-N1	-5.18	104.38	108.00
5	AE	24	DC	O4'-C1'-C2'	-5.17	101.76	105.90
33	Ag	29	DG	O4'-C4'-C3'	-5.17	102.43	104.50
1	AA	336	DG	C5-C6-O6	-5.17	125.50	128.60
6	AF	33	DC	C6-N1-C2	-5.17	118.23	120.30
25	AY	34	DT	C4'-C3'-C2'	-5.17	98.44	103.10
34	Ah	28	DC	O4'-C1'-N1	-5.17	104.38	108.00
1	AA	178	DC	P-O5'-C5'	5.17	129.17	120.90
28	Ab	21	DG	C5-C6-O6	-5.17	125.50	128.60
22	AV	36	DG	N1-C6-O6	5.17	123.00	119.90
28	Ab	28	DG	O4'-C1'-C2'	-5.17	101.77	105.90
29	Ac	14	DT	O4'-C4'-C3'	-5.17	102.43	104.50
2	AB	32	DG	P-O3'-C3'	5.17	125.90	119.70
1	AA	727	DG	P-O3'-C3'	5.16	125.90	119.70
6	AF	25	DG	O4'-C1'-C2'	-5.16	101.77	105.90
18	AR	6	DA	O4'-C1'-C2'	-5.16	101.77	105.90
1	AA	1175	DT	C4'-C3'-C2'	-5.16	98.46	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	Aj	13	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	342	DC	P-O3'-C3'	5.15	125.88	119.70
23	AW	21	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	630	DG	N1-C6-O6	5.15	122.99	119.90
30	Ad	14	DG	O4'-C1'-C2'	-5.15	101.78	105.90
26	AZ	8	DA	O4'-C1'-C2'	-5.15	101.78	105.90
1	AA	405	DG	O4'-C1'-N9	5.14	111.60	108.00
32	Af	29	DC	O4'-C1'-C2'	-5.14	101.78	105.90
1	AA	21	DT	C4'-C3'-C2'	-5.14	98.47	103.10
1	AA	260	DA	N1-C6-N6	-5.14	115.51	118.60
1	AA	1139	DA	O4'-C1'-N9	-5.14	104.40	108.00
1	AA	219	DG	O4'-C1'-C2'	-5.14	101.79	105.90
1	AA	1060	DA	P-O3'-C3'	5.14	125.86	119.70
30	Ad	6	DC	P-O5'-C5'	5.14	129.12	120.90
1	AA	487	DG	O4'-C1'-C2'	-5.13	101.79	105.90
1	AA	632	DG	C1'-O4'-C4'	-5.13	104.97	110.10
1	AA	1032	DT	C4'-C3'-C2'	-5.12	98.49	103.10
30	Ad	32	DA	C1'-O4'-C4'	-5.12	104.97	110.10
1	AA	336	DG	N1-C6-O6	5.12	122.97	119.90
1	AA	1237	DG	C5-C6-O6	-5.12	125.53	128.60
6	AF	2	DG	C1'-O4'-C4'	-5.12	104.98	110.10
13	AM	35	DG	P-O3'-C3'	5.12	125.84	119.70
17	AQ	17	DC	O4'-C4'-C3'	-5.12	102.45	104.50
5	AE	27	DA	O4'-C1'-N9	-5.12	104.42	108.00
1	AA	168	DG	O4'-C1'-C2'	-5.12	101.81	105.90
13	AM	16	DA	P-O3'-C3'	5.11	125.84	119.70
35	Ai	1	DC	C6-N1-C2	-5.11	118.25	120.30
1	AA	742	DT	C4'-C3'-C2'	-5.11	98.50	103.10
1	AA	1286	DG	C4'-C3'-C2'	-5.11	98.50	103.10
30	Ad	29	DG	O4'-C1'-C2'	-5.11	101.81	105.90
6	AF	2	DG	P-O3'-C3'	5.10	125.82	119.70
1	AA	559	DC	O4'-C1'-N1	5.10	111.57	108.00
20	AT	1	DC	P-O3'-C3'	5.10	125.82	119.70
23	AW	13	DG	C5-C6-O6	-5.09	125.55	128.60
27	Aa	30	DT	O4'-C4'-C3'	-5.09	102.46	104.50
1	AA	1100	DT	O4'-C1'-C2'	-5.09	101.83	105.90
2	AB	27	DC	C4'-C3'-C2'	-5.09	98.52	103.10
1	AA	542	DG	C5-C6-O6	-5.09	125.55	128.60
19	AS	14	DA	P-O3'-C3'	5.09	125.80	119.70
7	AG	32	DA	P-O3'-C3'	5.08	125.80	119.70
37	Ak	20	DG	O4'-C1'-C2'	-5.08	101.83	105.90
1	AA	135	DT	P-O3'-C3'	5.08	125.80	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	AM	22	DC	O4'-C1'-N1	-5.08	104.44	108.00
31	Ae	24	DC	P-O5'-C5'	5.08	129.02	120.90
1	AA	355	DG	O4'-C1'-C2'	-5.08	101.84	105.90
19	AS	16	DC	P-O3'-C3'	5.08	125.79	119.70
5	AE	10	DT	P-O3'-C3'	5.07	125.79	119.70
1	AA	454	DT	P-O3'-C3'	5.07	125.78	119.70
28	Ab	15	DG	O4'-C1'-C2'	-5.07	101.85	105.90
1	AA	842	DC	O4'-C1'-N1	5.07	111.55	108.00
24	AX	16	DT	C1'-O4'-C4'	-5.07	105.03	110.10
1	AA	697	DA	O4'-C1'-C2'	-5.06	101.85	105.90
1	AA	1067	DC	C4'-C3'-C2'	-5.06	98.54	103.10
23	AW	9	DA	C1'-O4'-C4'	-5.06	105.04	110.10
1	AA	1080	DA	O4'-C1'-C2'	-5.06	101.85	105.90
25	AY	22	DA	C1'-O4'-C4'	-5.06	105.04	110.10
8	AH	26	DG	C1'-O4'-C4'	-5.05	105.05	110.10
11	AK	36	DC	P-O3'-C3'	5.05	125.77	119.70
37	Ak	33	DC	P-O5'-C5'	5.05	128.99	120.90
23	AW	13	DG	N1-C6-O6	5.05	122.93	119.90
1	AA	759	DG	O4'-C1'-C2'	-5.05	101.86	105.90
1	AA	1021	DG	O4'-C1'-C2'	-5.05	101.86	105.90
1	AA	1064	DA	O4'-C1'-C2'	-5.05	101.86	105.90
6	AF	8	DA	O4'-C1'-N9	5.05	111.53	108.00
21	AU	39	DG	O4'-C4'-C3'	-5.04	102.48	104.50
1	AA	692	DG	O4'-C1'-C2'	-5.03	101.87	105.90
19	AS	14	DA	C1'-O4'-C4'	-5.03	105.07	110.10
1	AA	244	DT	C4'-C3'-C2'	-5.03	98.57	103.10
1	AA	1259	DT	C4'-C3'-C2'	-5.03	98.57	103.10
1	AA	362	DT	C4'-C3'-C2'	-5.03	98.57	103.10
1	AA	397	DG	O4'-C1'-C2'	-5.03	101.88	105.90
1	AA	1238	DA	N1-C6-N6	-5.02	115.59	118.60
3	AC	38	DG	O4'-C1'-C2'	-5.02	101.88	105.90
1	AA	610	DT	C4'-C3'-C2'	-5.02	98.58	103.10
1	AA	798	DG	C5-C6-O6	-5.02	125.59	128.60
16	AP	32	DA	O4'-C1'-C2'	-5.02	101.89	105.90
1	AA	991	DA	P-O3'-C3'	5.01	125.72	119.70
1	AA	323	DG	N1-C6-O6	5.01	122.91	119.90
13	AM	18	DT	O4'-C1'-C2'	-5.01	101.89	105.90
27	Aa	26	DA	C1'-O4'-C4'	-5.01	105.09	110.10
1	AA	1090	DG	O4'-C1'-C2'	-5.01	101.89	105.90
11	AK	27	DA	O4'-C1'-C2'	-5.01	101.89	105.90
11	AK	21	DC	P-O3'-C3'	5.00	125.70	119.70
1	AA	5	DA	C4'-C3'-C2'	-5.00	98.60	103.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	Ai	32	DT	C4'-C3'-C2'	-5.00	98.60	103.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	272	DC	C4',C3'
1	AA	1272	DC	C3'
28	Ab	35	DT	C3'

All (662) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1	DA	Sidechain
1	AA	1001	DC	Sidechain
1	AA	101	DA	Sidechain
1	AA	1015	DG	Sidechain
1	AA	1020	DC	Sidechain
1	AA	1021	DG	Sidechain
1	AA	1023	DA	Sidechain
1	AA	1024	DA	Sidechain
1	AA	1029	DA	Sidechain
1	AA	1031	DG	Sidechain
1	AA	1034	DA	Sidechain
1	AA	1035	DA	Sidechain
1	AA	1038	DT	Sidechain
1	AA	1047	DT	Sidechain
1	AA	1051	DT	Sidechain
1	AA	1053	DC	Sidechain
1	AA	1055	DA	Sidechain
1	AA	1061	DC	Sidechain
1	AA	1064	DA	Sidechain
1	AA	1065	DG	Sidechain
1	AA	1070	DC	Sidechain
1	AA	1071	DT	Sidechain
1	AA	1074	DA	Sidechain
1	AA	1096	DC	Sidechain
1	AA	1097	DC	Sidechain
1	AA	1102	DC	Sidechain
1	AA	1106	DT	Sidechain
1	AA	1114	DG	Sidechain
1	AA	1125	DC	Sidechain
1	AA	1127	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1130	DA	Sidechain
1	AA	1131	DG	Sidechain
1	AA	1133	DT	Sidechain
1	AA	1136	DA	Sidechain
1	AA	1137	DG	Sidechain
1	AA	1138	DT	Sidechain
1	AA	1144	DT	Sidechain
1	AA	1146	DC	Sidechain
1	AA	1147	DA	Sidechain
1	AA	1149	DA	Sidechain
1	AA	1150	DG	Sidechain
1	AA	1151	DC	Sidechain
1	AA	1156	DG	Sidechain
1	AA	1157	DT	Sidechain
1	AA	1158	DT	Sidechain
1	AA	1163	DA	Sidechain
1	AA	1164	DC	Sidechain
1	AA	1169	DC	Sidechain
1	AA	117	DG	Sidechain
1	AA	1171	DG	Sidechain
1	AA	1175	DT	Sidechain
1	AA	1177	DC	Sidechain
1	AA	1182	DC	Sidechain
1	AA	1185	DC	Sidechain
1	AA	1186	DC	Sidechain
1	AA	1193	DT	Sidechain
1	AA	1196	DC	Sidechain
1	AA	12	DG	Sidechain
1	AA	1200	DC	Sidechain
1	AA	1202	DC	Sidechain
1	AA	121	DC	Sidechain
1	AA	1220	DA	Sidechain
1	AA	1223	DG	Sidechain
1	AA	1225	DG	Sidechain
1	AA	1227	DT	Sidechain
1	AA	1229	DT	Sidechain
1	AA	1232	DA	Sidechain
1	AA	1234	DT	Sidechain
1	AA	1235	DT	Sidechain
1	AA	1238	DA	Sidechain
1	AA	1250	DT	Sidechain
1	AA	1252	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1258	DG	Sidechain
1	AA	1259	DT	Sidechain
1	AA	1261	DA	Sidechain
1	AA	1263	DC	Sidechain
1	AA	1266	DG	Sidechain
1	AA	1269	DC	Sidechain
1	AA	1271	DC	Sidechain
1	AA	1274	DC	Sidechain
1	AA	1277	DT	Sidechain
1	AA	1278	DG	Sidechain
1	AA	1280	DA	Sidechain
1	AA	1281	DA	Sidechain
1	AA	1282	DG	Sidechain
1	AA	1289	DA	Sidechain
1	AA	1290	DG	Sidechain
1	AA	1292	DT	Sidechain
1	AA	1293	DC	Sidechain
1	AA	1298	DA	Sidechain
1	AA	1299	DC	Sidechain
1	AA	1304	DT	Sidechain
1	AA	1308	DA	Sidechain
1	AA	1315	DG	Sidechain
1	AA	138	DC	Sidechain
1	AA	15	DC	Sidechain
1	AA	151	DG	Sidechain
1	AA	152	DT	Sidechain
1	AA	157	DA	Sidechain
1	AA	158	DC	Sidechain
1	AA	159	DC	Sidechain
1	AA	161	DC	Sidechain
1	AA	169	DG	Sidechain
1	AA	170	DC	Sidechain
1	AA	176	DA	Sidechain
1	AA	177	DA	Sidechain
1	AA	179	DC	Sidechain
1	AA	18	DC	Sidechain
1	AA	183	DT	Sidechain
1	AA	184	DC	Sidechain
1	AA	187	DC	Sidechain
1	AA	208	DG	Sidechain
1	AA	209	DA	Sidechain
1	AA	21	DT	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	22	DC	Sidechain
1	AA	224	DT	Sidechain
1	AA	226	DA	Sidechain
1	AA	228	DC	Sidechain
1	AA	229	DT	Sidechain
1	AA	232	DC	Sidechain
1	AA	235	DA	Sidechain
1	AA	239	DA	Sidechain
1	AA	24	DG	Sidechain
1	AA	241	DG	Sidechain
1	AA	243	DC	Sidechain
1	AA	255	DT	Sidechain
1	AA	256	DG	Sidechain
1	AA	264	DC	Sidechain
1	AA	265	DG	Sidechain
1	AA	27	DT	Sidechain
1	AA	270	DT	Sidechain
1	AA	271	DG	Sidechain
1	AA	274	DG	Sidechain
1	AA	284	DA	Sidechain
1	AA	287	DC	Sidechain
1	AA	290	DC	Sidechain
1	AA	292	DG	Sidechain
1	AA	295	DG	Sidechain
1	AA	297	DT	Sidechain
1	AA	3	DC	Sidechain
1	AA	301	DT	Sidechain
1	AA	303	DA	Sidechain
1	AA	305	DG	Sidechain
1	AA	31	DC	Sidechain
1	AA	310	DT	Sidechain
1	AA	319	DT	Sidechain
1	AA	325	DT	Sidechain
1	AA	327	DG	Sidechain
1	AA	335	DA	Sidechain
1	AA	337	DC	Sidechain
1	AA	338	DC	Sidechain
1	AA	350	DA	Sidechain
1	AA	356	DA	Sidechain
1	AA	365	DG	Sidechain
1	AA	366	DT	Sidechain
1	AA	370	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	371	DA	Sidechain
1	AA	375	DT	Sidechain
1	AA	376	DG	Sidechain
1	AA	377	DG	Sidechain
1	AA	39	DA	Sidechain
1	AA	391	DT	Sidechain
1	AA	394	DG	Sidechain
1	AA	401	DG	Sidechain
1	AA	403	DC	Sidechain
1	AA	405	DG	Sidechain
1	AA	41	DC	Sidechain
1	AA	410	DC	Sidechain
1	AA	412	DC	Sidechain
1	AA	421	DA	Sidechain
1	AA	434	DC	Sidechain
1	AA	440	DT	Sidechain
1	AA	443	DG	Sidechain
1	AA	444	DG	Sidechain
1	AA	447	DG	Sidechain
1	AA	448	DG	Sidechain
1	AA	451	DC	Sidechain
1	AA	456	DT	Sidechain
1	AA	459	DG	Sidechain
1	AA	463	DA	Sidechain
1	AA	465	DA	Sidechain
1	AA	475	DT	Sidechain
1	AA	480	DC	Sidechain
1	AA	485	DG	Sidechain
1	AA	493	DT	Sidechain
1	AA	498	DG	Sidechain
1	AA	5	DA	Sidechain
1	AA	50	DG	Sidechain
1	AA	503	DT	Sidechain
1	AA	509	DG	Sidechain
1	AA	524	DG	Sidechain
1	AA	526	DT	Sidechain
1	AA	527	DA	Sidechain
1	AA	528	DC	Sidechain
1	AA	529	DG	Sidechain
1	AA	531	DG	Sidechain
1	AA	537	DT	Sidechain
1	AA	548	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	55	DG	Sidechain
1	AA	552	DC	Sidechain
1	AA	557	DG	Sidechain
1	AA	559	DC	Sidechain
1	AA	56	DC	Sidechain
1	AA	569	DG	Sidechain
1	AA	57	DT	Sidechain
1	AA	578	DA	Sidechain
1	AA	586	DT	Sidechain
1	AA	590	DG	Sidechain
1	AA	591	DC	Sidechain
1	AA	594	DT	Sidechain
1	AA	595	DC	Sidechain
1	AA	597	DC	Sidechain
1	AA	601	DG	Sidechain
1	AA	602	DA	Sidechain
1	AA	603	DT	Sidechain
1	AA	604	DA	Sidechain
1	AA	607	DC	Sidechain
1	AA	613	DT	Sidechain
1	AA	617	DC	Sidechain
1	AA	618	DC	Sidechain
1	AA	62	DC	Sidechain
1	AA	63	DC	Sidechain
1	AA	630	DG	Sidechain
1	AA	631	DA	Sidechain
1	AA	632	DG	Sidechain
1	AA	633	DT	Sidechain
1	AA	634	DC	Sidechain
1	AA	639	DT	Sidechain
1	AA	644	DT	Sidechain
1	AA	65	DA	Sidechain
1	AA	657	DT	Sidechain
1	AA	659	DG	Sidechain
1	AA	660	DT	Sidechain
1	AA	674	DA	Sidechain
1	AA	675	DA	Sidechain
1	AA	678	DC	Sidechain
1	AA	679	DT	Sidechain
1	AA	68	DG	Sidechain
1	AA	682	DA	Sidechain
1	AA	684	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	685	DC	Sidechain
1	AA	691	DC	Sidechain
1	AA	699	DC	Sidechain
1	AA	702	DG	Sidechain
1	AA	703	DT	Sidechain
1	AA	704	DC	Sidechain
1	AA	705	DA	Sidechain
1	AA	706	DC	Sidechain
1	AA	708	DG	Sidechain
1	AA	713	DG	Sidechain
1	AA	72	DG	Sidechain
1	AA	725	DC	Sidechain
1	AA	73	DT	Sidechain
1	AA	733	DC	Sidechain
1	AA	735	DC	Sidechain
1	AA	738	DC	Sidechain
1	AA	74	DA	Sidechain
1	AA	744	DG	Sidechain
1	AA	745	DG	Sidechain
1	AA	746	DC	Sidechain
1	AA	750	DT	Sidechain
1	AA	751	DT	Sidechain
1	AA	757	DA	Sidechain
1	AA	765	DG	Sidechain
1	AA	766	DG	Sidechain
1	AA	768	DA	Sidechain
1	AA	771	DA	Sidechain
1	AA	772	DC	Sidechain
1	AA	773	DA	Sidechain
1	AA	779	DC	Sidechain
1	AA	783	DA	Sidechain
1	AA	792	DC	Sidechain
1	AA	795	DG	Sidechain
1	AA	805	DC	Sidechain
1	AA	807	DA	Sidechain
1	AA	811	DA	Sidechain
1	AA	813	DT	Sidechain
1	AA	823	DT	Sidechain
1	AA	825	DA	Sidechain
1	AA	826	DG	Sidechain
1	AA	828	DT	Sidechain
1	AA	830	DA	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	838	DG	Sidechain
1	AA	842	DC	Sidechain
1	AA	846	DA	Sidechain
1	AA	848	DG	Sidechain
1	AA	854	DC	Sidechain
1	AA	859	DT	Sidechain
1	AA	871	DT	Sidechain
1	AA	874	DT	Sidechain
1	AA	888	DT	Sidechain
1	AA	906	DT	Sidechain
1	AA	914	DT	Sidechain
1	AA	92	DT	Sidechain
1	AA	922	DA	Sidechain
1	AA	928	DG	Sidechain
1	AA	930	DG	Sidechain
1	AA	937	DT	Sidechain
1	AA	940	DA	Sidechain
1	AA	943	DG	Sidechain
1	AA	944	DC	Sidechain
1	AA	949	DT	Sidechain
1	AA	950	DC	Sidechain
1	AA	967	DG	Sidechain
1	AA	97	DG	Sidechain
1	AA	970	DT	Sidechain
1	AA	971	DT	Sidechain
1	AA	975	DG	Sidechain
1	AA	976	DC	Sidechain
1	AA	988	DC	Sidechain
1	AA	989	DG	Sidechain
1	AA	99	DT	Sidechain
1	AA	990	DT	Sidechain
2	AB	14	DC	Sidechain
2	AB	16	DC	Sidechain
2	AB	18	DG	Sidechain
2	AB	26	DG	Sidechain
2	AB	29	DC	Sidechain
2	AB	34	DT	Sidechain
2	AB	38	DC	Sidechain
2	AB	42	DT	Sidechain
2	AB	44	DG	Sidechain
2	AB	45	DC	Sidechain
2	AB	8	DG	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	9	DG	Sidechain
3	AC	13	DG	Sidechain
3	AC	2	DC	Sidechain
3	AC	22	DG	Sidechain
3	AC	24	DC	Sidechain
3	AC	26	DG	Sidechain
3	AC	27	DG	Sidechain
3	AC	3	DT	Sidechain
3	AC	35	DG	Sidechain
3	AC	4	DC	Sidechain
3	AC	7	DA	Sidechain
3	AC	9	DT	Sidechain
4	AD	11	DA	Sidechain
4	AD	12	DG	Sidechain
4	AD	13	DA	Sidechain
4	AD	14	DA	Sidechain
4	AD	17	DT	Sidechain
4	AD	20	DT	Sidechain
4	AD	26	DC	Sidechain
4	AD	27	DT	Sidechain
4	AD	3	DA	Sidechain
4	AD	30	DC	Sidechain
4	AD	33	DG	Sidechain
4	AD	7	DT	Sidechain
5	AE	1	DT	Sidechain
5	AE	10	DT	Sidechain
5	AE	13	DC	Sidechain
5	AE	14	DC	Sidechain
5	AE	15	DG	Sidechain
5	AE	27	DA	Sidechain
5	AE	7	DT	Sidechain
5	AE	9	DT	Sidechain
6	AF	12	DT	Sidechain
6	AF	14	DA	Sidechain
6	AF	15	DC	Sidechain
6	AF	21	DT	Sidechain
6	AF	26	DA	Sidechain
6	AF	3	DA	Sidechain
6	AF	30	DG	Sidechain
6	AF	31	DG	Sidechain
6	AF	34	DG	Sidechain
6	AF	5	DC	Sidechain

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Mol	Chain	Res	Type	Group
6	AF	8	DA	Sidechain
7	AG	13	DG	Sidechain
7	AG	14	DG	Sidechain
7	AG	26	DA	Sidechain
7	AG	3	DT	Sidechain
7	AG	31	DG	Sidechain
7	AG	32	DA	Sidechain
7	AG	33	DA	Sidechain
7	AG	35	DG	Sidechain
7	AG	40	DA	Sidechain
7	AG	44	DG	Sidechain
8	AH	1	DG	Sidechain
8	AH	13	DG	Sidechain
8	AH	16	DA	Sidechain
8	AH	18	DC	Sidechain
8	AH	23	DT	Sidechain
8	AH	28	DG	Sidechain
8	AH	30	DG	Sidechain
8	AH	9	DA	Sidechain
9	AI	10	DG	Sidechain
9	AI	11	DG	Sidechain
9	AI	12	DC	Sidechain
9	AI	13	DC	Sidechain
9	AI	16	DA	Sidechain
9	AI	17	DA	Sidechain
9	AI	18	DT	Sidechain
9	AI	19	DT	Sidechain
9	AI	25	DC	Sidechain
9	AI	29	DG	Sidechain
9	AI	32	DT	Sidechain
9	AI	6	DG	Sidechain
9	AI	7	DG	Sidechain
10	AJ	16	DG	Sidechain
10	AJ	2	DT	Sidechain
10	AJ	20	DC	Sidechain
10	AJ	29	DT	Sidechain
10	AJ	30	DT	Sidechain
10	AJ	9	DC	Sidechain
11	AK	10	DG	Sidechain
11	AK	11	DG	Sidechain
11	AK	15	DA	Sidechain
11	AK	19	DG	Sidechain

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Mol	Chain	Res	Type	Group
11	AK	20	DT	Sidechain
11	AK	22	DG	Sidechain
11	AK	23	DT	Sidechain
11	AK	29	DT	Sidechain
11	AK	3	DT	Sidechain
11	AK	33	DG	Sidechain
11	AK	37	DA	Sidechain
11	AK	40	DT	Sidechain
11	AK	41	DA	Sidechain
11	AK	43	DT	Sidechain
11	AK	45	DC	Sidechain
12	AL	1	DG	Sidechain
12	AL	11	DG	Sidechain
12	AL	19	DA	Sidechain
12	AL	2	DG	Sidechain
12	AL	26	DT	Sidechain
12	AL	31	DG	Sidechain
12	AL	35	DG	Sidechain
12	AL	36	DG	Sidechain
12	AL	37	DT	Sidechain
12	AL	44	DG	Sidechain
12	AL	46	DT	Sidechain
13	AM	13	DC	Sidechain
13	AM	20	DC	Sidechain
13	AM	27	DT	Sidechain
13	AM	28	DG	Sidechain
13	AM	29	DA	Sidechain
13	AM	31	DG	Sidechain
13	AM	32	DT	Sidechain
13	AM	42	DT	Sidechain
13	AM	43	DT	Sidechain
14	AN	16	DG	Sidechain
14	AN	2	DT	Sidechain
14	AN	20	DA	Sidechain
14	AN	21	DT	Sidechain
14	AN	24	DG	Sidechain
14	AN	7	DG	Sidechain
14	AN	8	DT	Sidechain
15	AO	14	DG	Sidechain
15	AO	15	DG	Sidechain
15	AO	18	DG	Sidechain
15	AO	19	DG	Sidechain

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Mol	Chain	Res	Type	Group
15	AO	21	DA	Sidechain
15	AO	30	DC	Sidechain
15	AO	31	DC	Sidechain
15	AO	5	DA	Sidechain
16	AP	1	DG	Sidechain
16	AP	10	DG	Sidechain
16	AP	11	DC	Sidechain
16	AP	14	DG	Sidechain
16	AP	15	DC	Sidechain
16	AP	16	DG	Sidechain
16	AP	17	DC	Sidechain
16	AP	18	DT	Sidechain
16	AP	19	DG	Sidechain
16	AP	23	DT	Sidechain
16	AP	3	DT	Sidechain
16	AP	31	DC	Sidechain
16	AP	34	DT	Sidechain
16	AP	36	DC	Sidechain
16	AP	4	DC	Sidechain
16	AP	7	DG	Sidechain
16	AP	8	DC	Sidechain
17	AQ	18	DT	Sidechain
17	AQ	19	DG	Sidechain
17	AQ	2	DT	Sidechain
17	AQ	20	DA	Sidechain
17	AQ	21	DA	Sidechain
17	AQ	23	DC	Sidechain
17	AQ	26	DT	Sidechain
17	AQ	27	DT	Sidechain
17	AQ	28	DT	Sidechain
17	AQ	29	DA	Sidechain
17	AQ	36	DG	Sidechain
17	AQ	39	DA	Sidechain
17	AQ	40	DC	Sidechain
18	AR	1	DT	Sidechain
18	AR	12	DA	Sidechain
18	AR	13	DC	Sidechain
18	AR	17	DG	Sidechain
18	AR	2	DT	Sidechain
18	AR	20	DA	Sidechain
18	AR	22	DA	Sidechain
18	AR	4	DG	Sidechain

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Mol	Chain	Res	Type	Group
18	AR	8	DA	Sidechain
18	AR	9	DT	Sidechain
19	AS	1	DT	Sidechain
19	AS	11	DG	Sidechain
19	AS	12	DG	Sidechain
19	AS	15	DC	Sidechain
19	AS	17	DA	Sidechain
19	AS	2	DG	Sidechain
19	AS	22	DG	Sidechain
19	AS	29	DT	Sidechain
19	AS	30	DT	Sidechain
19	AS	31	DT	Sidechain
19	AS	32	DT	Sidechain
19	AS	9	DT	Sidechain
20	AT	15	DG	Sidechain
20	AT	16	DA	Sidechain
20	AT	2	DC	Sidechain
20	AT	26	DC	Sidechain
20	AT	27	DC	Sidechain
20	AT	32	DA	Sidechain
20	AT	36	DG	Sidechain
20	AT	5	DT	Sidechain
20	AT	6	DG	Sidechain
20	AT	8	DG	Sidechain
20	AT	9	DT	Sidechain
21	AU	15	DA	Sidechain
21	AU	2	DA	Sidechain
21	AU	22	DG	Sidechain
21	AU	33	DG	Sidechain
21	AU	35	DT	Sidechain
21	AU	42	DT	Sidechain
21	AU	8	DC	Sidechain
21	AU	9	DC	Sidechain
22	AV	12	DT	Sidechain
22	AV	13	DT	Sidechain
22	AV	14	DA	Sidechain
22	AV	18	DG	Sidechain
22	AV	19	DA	Sidechain
22	AV	27	DG	Sidechain
22	AV	28	DT	Sidechain
22	AV	34	DC	Sidechain
22	AV	36	DG	Sidechain

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Mol	Chain	Res	Type	Group
22	AV	5	DC	Sidechain
22	AV	8	DG	Sidechain
23	AW	15	DA	Sidechain
23	AW	17	DT	Sidechain
23	AW	22	DT	Sidechain
23	AW	3	DA	Sidechain
23	AW	32	DG	Sidechain
23	AW	33	DA	Sidechain
23	AW	34	DA	Sidechain
23	AW	35	DC	Sidechain
23	AW	7	DT	Sidechain
23	AW	9	DA	Sidechain
24	AX	13	DG	Sidechain
24	AX	19	DT	Sidechain
24	AX	3	DT	Sidechain
24	AX	33	DG	Sidechain
24	AX	7	DC	Sidechain
24	AX	8	DG	Sidechain
24	AX	9	DT	Sidechain
25	AY	20	DG	Sidechain
25	AY	24	DC	Sidechain
25	AY	27	DC	Sidechain
25	AY	3	DA	Sidechain
25	AY	33	DG	Sidechain
25	AY	34	DT	Sidechain
25	AY	6	DG	Sidechain
26	AZ	10	DC	Sidechain
26	AZ	2	DC	Sidechain
26	AZ	31	DA	Sidechain
26	AZ	6	DT	Sidechain
26	AZ	7	DG	Sidechain
27	Aa	13	DG	Sidechain
27	Aa	14	DC	Sidechain
27	Aa	16	DC	Sidechain
27	Aa	20	DC	Sidechain
27	Aa	21	DT	Sidechain
27	Aa	25	DA	Sidechain
27	Aa	3	DT	Sidechain
27	Aa	30	DT	Sidechain
27	Aa	38	DT	Sidechain
27	Aa	41	DA	Sidechain
27	Aa	47	DA	Sidechain

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Mol	Chain	Res	Type	Group
27	Aa	48	DC	Sidechain
27	Aa	6	DA	Sidechain
27	Aa	8	DT	Sidechain
28	Ab	20	DG	Sidechain
28	Ab	24	DG	Sidechain
28	Ab	25	DA	Sidechain
28	Ab	34	DC	Sidechain
28	Ab	35	DT	Sidechain
29	Ac	12	DC	Sidechain
29	Ac	15	DT	Sidechain
29	Ac	17	DG	Sidechain
29	Ac	18	DT	Sidechain
29	Ac	19	DT	Sidechain
29	Ac	20	DA	Sidechain
29	Ac	26	DC	Sidechain
29	Ac	3	DT	Sidechain
29	Ac	4	DG	Sidechain
29	Ac	41	DG	Sidechain
29	Ac	44	DT	Sidechain
29	Ac	46	DT	Sidechain
29	Ac	7	DT	Sidechain
29	Ac	8	DG	Sidechain
30	Ad	19	DC	Sidechain
30	Ad	33	DG	Sidechain
30	Ad	7	DC	Sidechain
30	Ad	8	DA	Sidechain
30	Ad	9	DC	Sidechain
31	Ae	12	DT	Sidechain
31	Ae	18	DG	Sidechain
31	Ae	22	DT	Sidechain
31	Ae	4	DC	Sidechain
31	Ae	5	DG	Sidechain
31	Ae	7	DA	Sidechain
31	Ae	8	DA	Sidechain
32	Af	1	DG	Sidechain
32	Af	10	DC	Sidechain
32	Af	11	DA	Sidechain
32	Af	12	DC	Sidechain
32	Af	14	DA	Sidechain
32	Af	27	DT	Sidechain
32	Af	3	DC	Sidechain
32	Af	34	DT	Sidechain

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Mol	Chain	Res	Type	Group
32	Af	35	DT	Sidechain
32	Af	36	DT	Sidechain
32	Af	7	DG	Sidechain
32	Af	8	DC	Sidechain
33	Ag	10	DG	Sidechain
33	Ag	13	DT	Sidechain
33	Ag	20	DT	Sidechain
33	Ag	21	DT	Sidechain
33	Ag	27	DT	Sidechain
33	Ag	3	DG	Sidechain
33	Ag	32	DT	Sidechain
33	Ag	35	DA	Sidechain
33	Ag	36	DT	Sidechain
33	Ag	38	DT	Sidechain
33	Ag	7	DA	Sidechain
34	Ah	15	DG	Sidechain
34	Ah	2	DG	Sidechain
34	Ah	24	DC	Sidechain
34	Ah	28	DC	Sidechain
34	Ah	29	DA	Sidechain
35	Ai	1	DC	Sidechain
35	Ai	14	DT	Sidechain
35	Ai	19	DA	Sidechain
35	Ai	22	DT	Sidechain
35	Ai	28	DG	Sidechain
35	Ai	3	DT	Sidechain
35	Ai	32	DT	Sidechain
35	Ai	39	DT	Sidechain
35	Ai	4	DT	Sidechain
36	Aj	11	DG	Sidechain
36	Aj	19	DA	Sidechain
36	Aj	2	DT	Sidechain
36	Aj	21	DG	Sidechain
36	Aj	22	DG	Sidechain
37	Ak	1	DC	Sidechain
37	Ak	10	DC	Sidechain
37	Ak	11	DT	Sidechain
37	Ak	19	DC	Sidechain
37	Ak	25	DG	Sidechain
37	Ak	27	DG	Sidechain
37	Ak	28	DA	Sidechain
37	Ak	31	DG	Sidechain

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Mol	Chain	Res	Type	Group
37	Ak	35	DA	Sidechain
37	Ak	37	DC	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	26988	0	14795	0	0
2	AB	1008	0	551	0	0
3	AC	863	0	478	0	0
4	AD	676	0	372	0	0
5	AE	546	0	307	0	0
6	AF	710	0	395	0	0
7	AG	1006	0	553	0	0
8	AH	698	0	387	0	0
9	AI	698	0	384	0	0
10	AJ	611	0	340	0	0
11	AK	936	0	519	0	0
12	AL	940	0	523	0	0
13	AM	893	0	505	0	0
14	AN	584	0	332	0	0
15	AO	826	0	449	0	0
16	AP	877	0	486	0	0
17	AQ	810	0	452	0	0
18	AR	610	0	342	0	0
19	AS	694	0	389	0	0
20	AT	831	0	456	0	0
21	AU	871	0	474	0	0
22	AV	749	0	421	0	0
23	AW	844	0	464	0	0
24	AX	668	0	376	0	0
25	AY	725	0	393	0	0
26	AZ	636	0	348	0	0
27	Aa	985	0	554	0	0
28	Ab	776	0	435	0	0
29	Ac	975	0	548	0	0
30	Ad	774	0	430	0	0
31	Ae	547	0	310	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Af	727	0	406	0	0
33	Ag	854	0	479	0	0
34	Ah	713	0	394	0	0
35	Ai	966	0	551	0	0
36	Aj	551	0	305	0	0
37	Ak	819	0	445	0	0
All	All	54985	0	30348	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

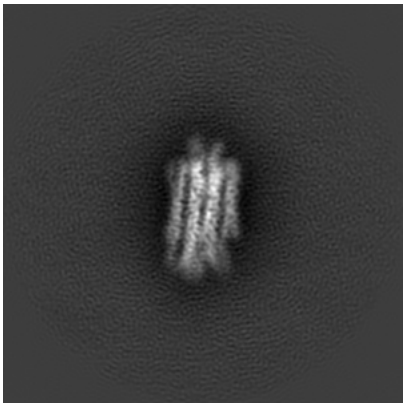
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11367. These allow visual inspection of the internal detail of the map and identification of artifacts.

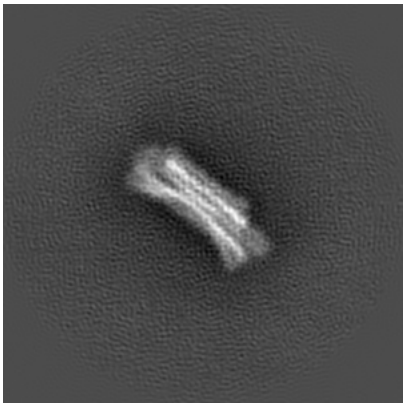
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

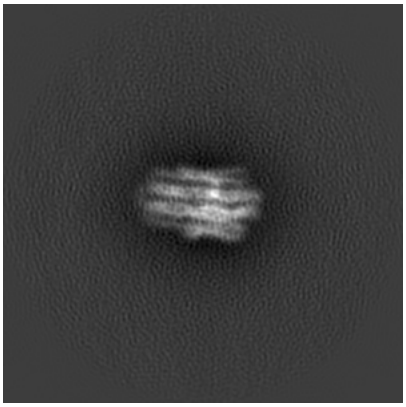
6.1.1 Primary map



X



Y

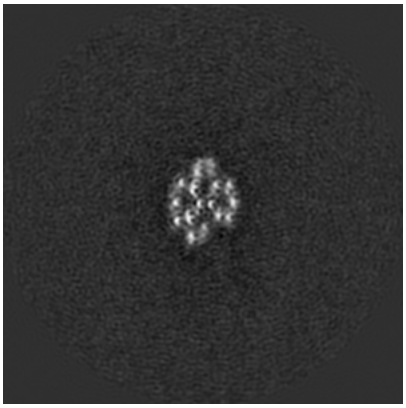


Z

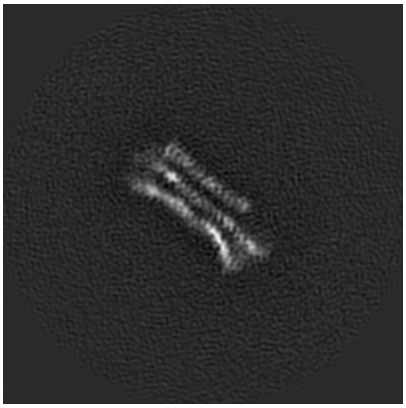
The images above show the map projected in three orthogonal directions.

6.2 Central slices

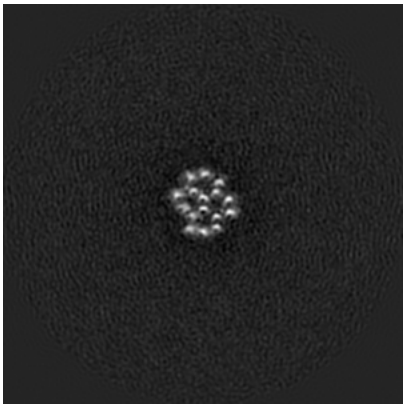
6.2.1 Primary map



X Index: 180



Y Index: 180

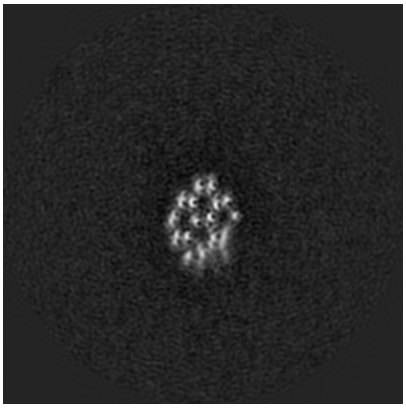


Z Index: 180

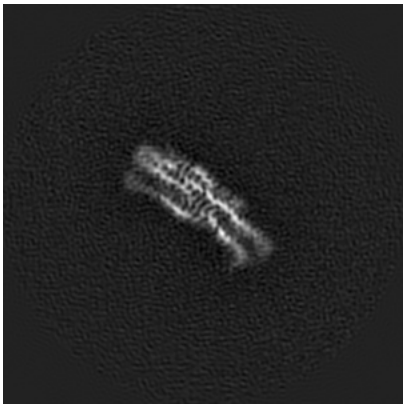
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

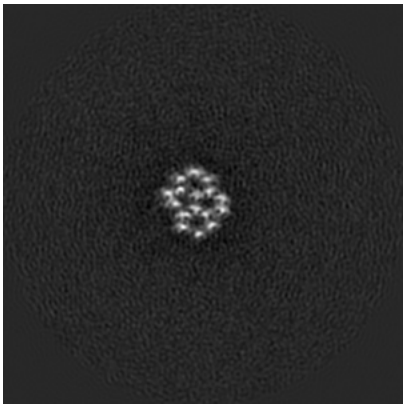
6.3.1 Primary map



X Index: 191



Y Index: 171



Z Index: 189

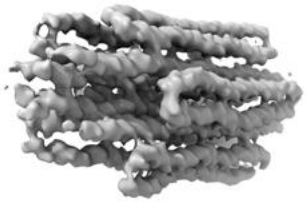
The images above show the largest variance slices of the map in three orthogonal directions.

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 0.17. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

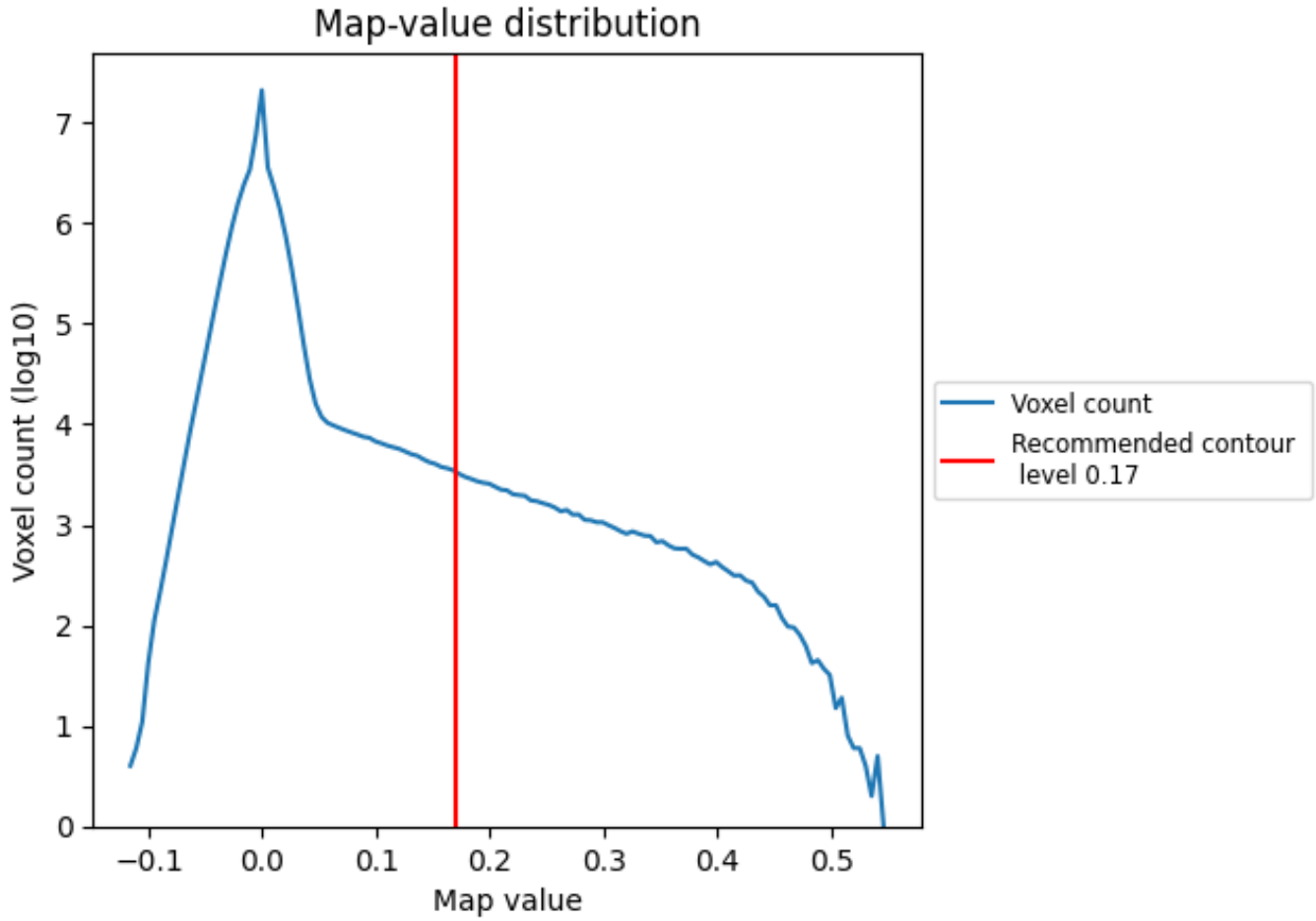
6.5 Mask visualisation (i)

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

7 Map analysis

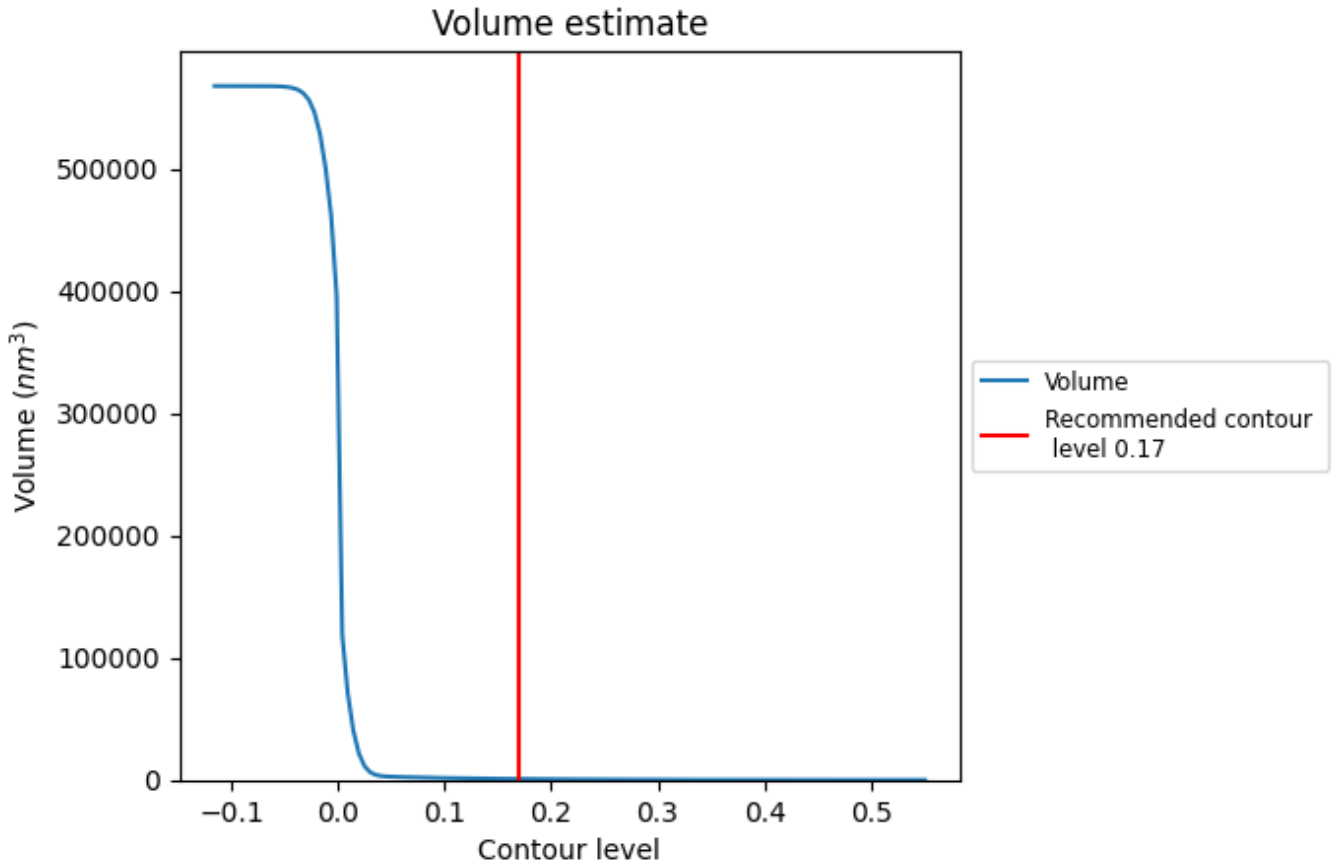
This section contains the results of statistical analysis of the map.

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.

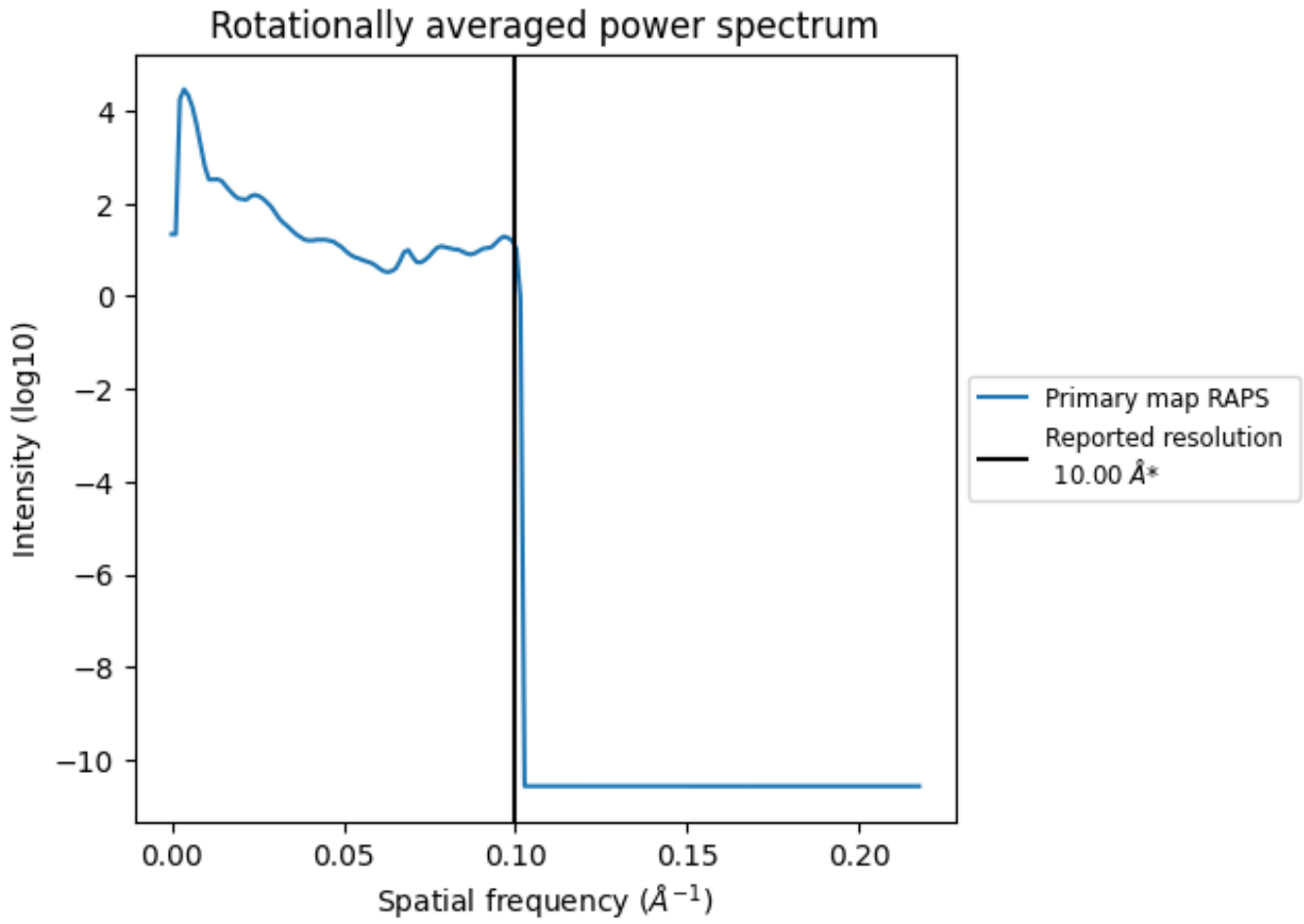
7.2 Volume estimate



The volume at the recommended contour level is 795 nm^3; this corresponds to an approximate mass of 719 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)

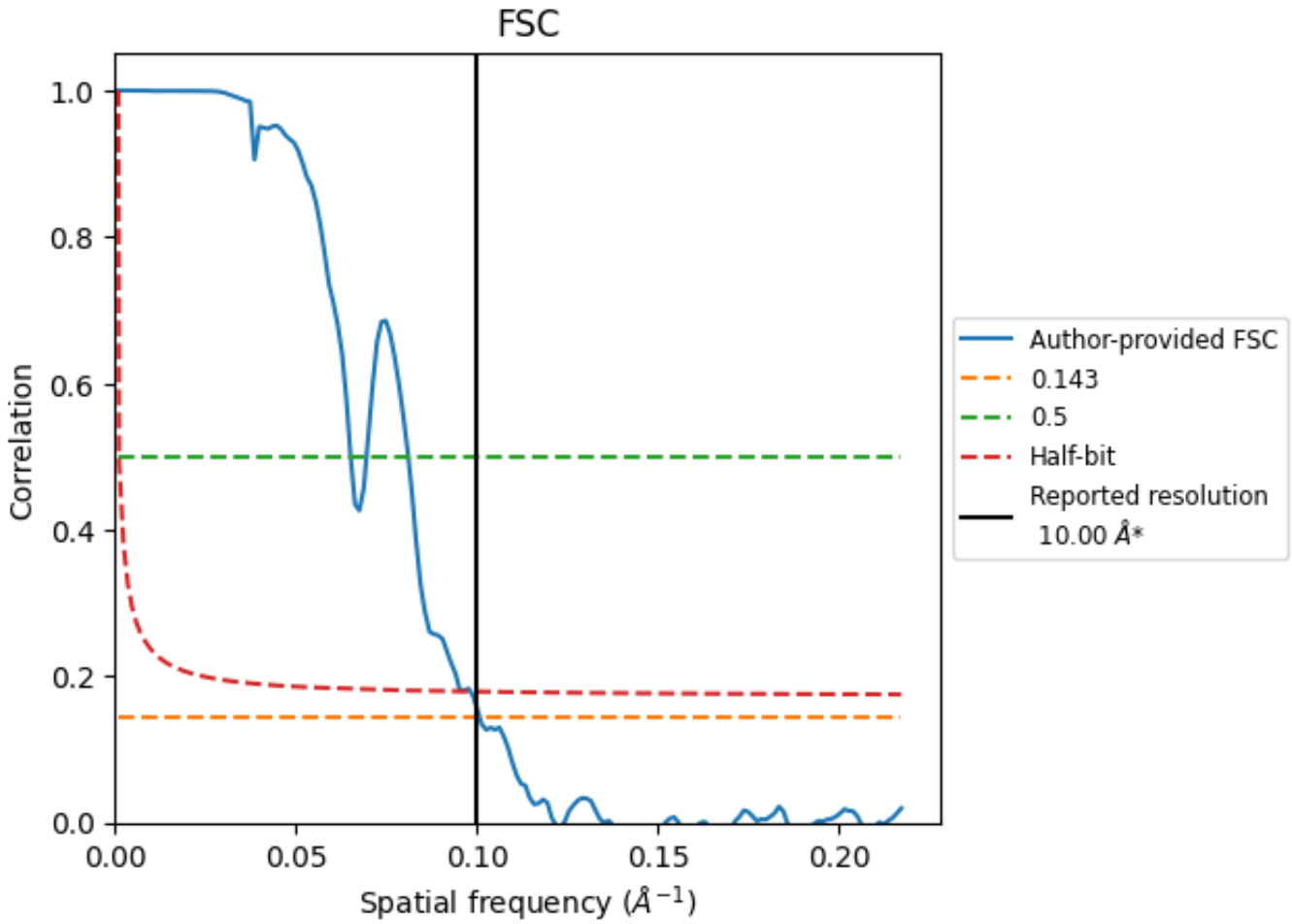


*Reported resolution corresponds to spatial frequency of 0.100 Å^{-1}

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 0.100 Å^{-1}

8.2 Resolution estimates (i)

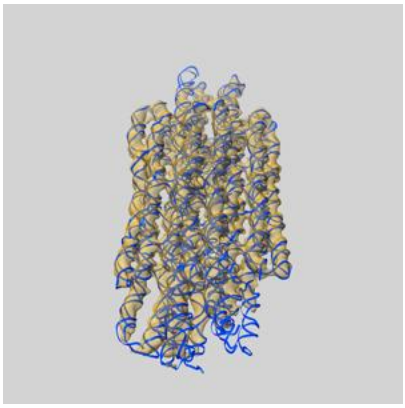
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.91	15.34	10.17
Unmasked-calculated*	-	-	-

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

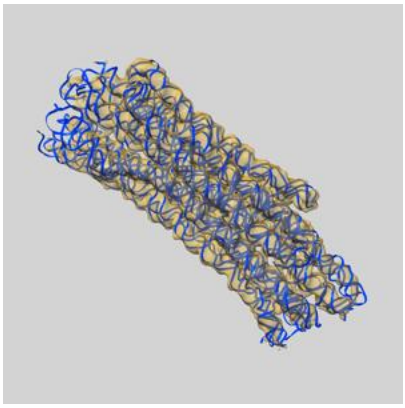
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11367 and PDB model 7ARQ. Per-residue inclusion information can be found in section 3 on page 10.

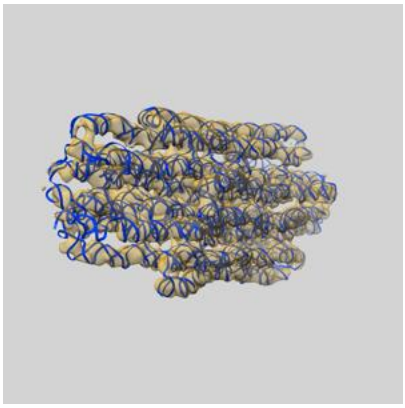
9.1 Map-model overlay



X



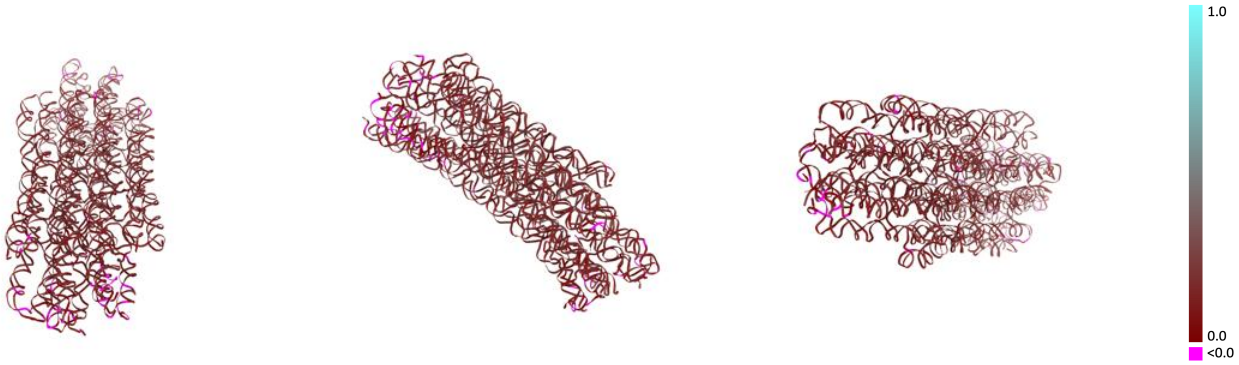
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.17 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

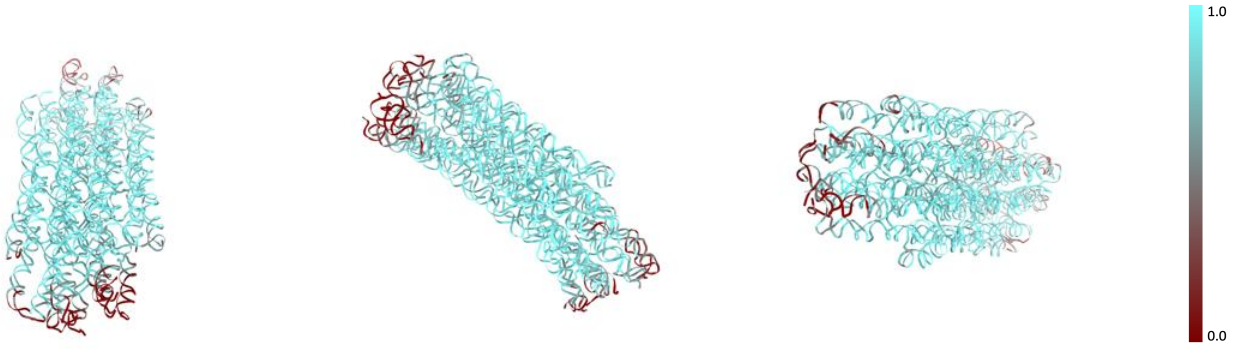
9.2 Q-score mapped to coordinate model (i)



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.

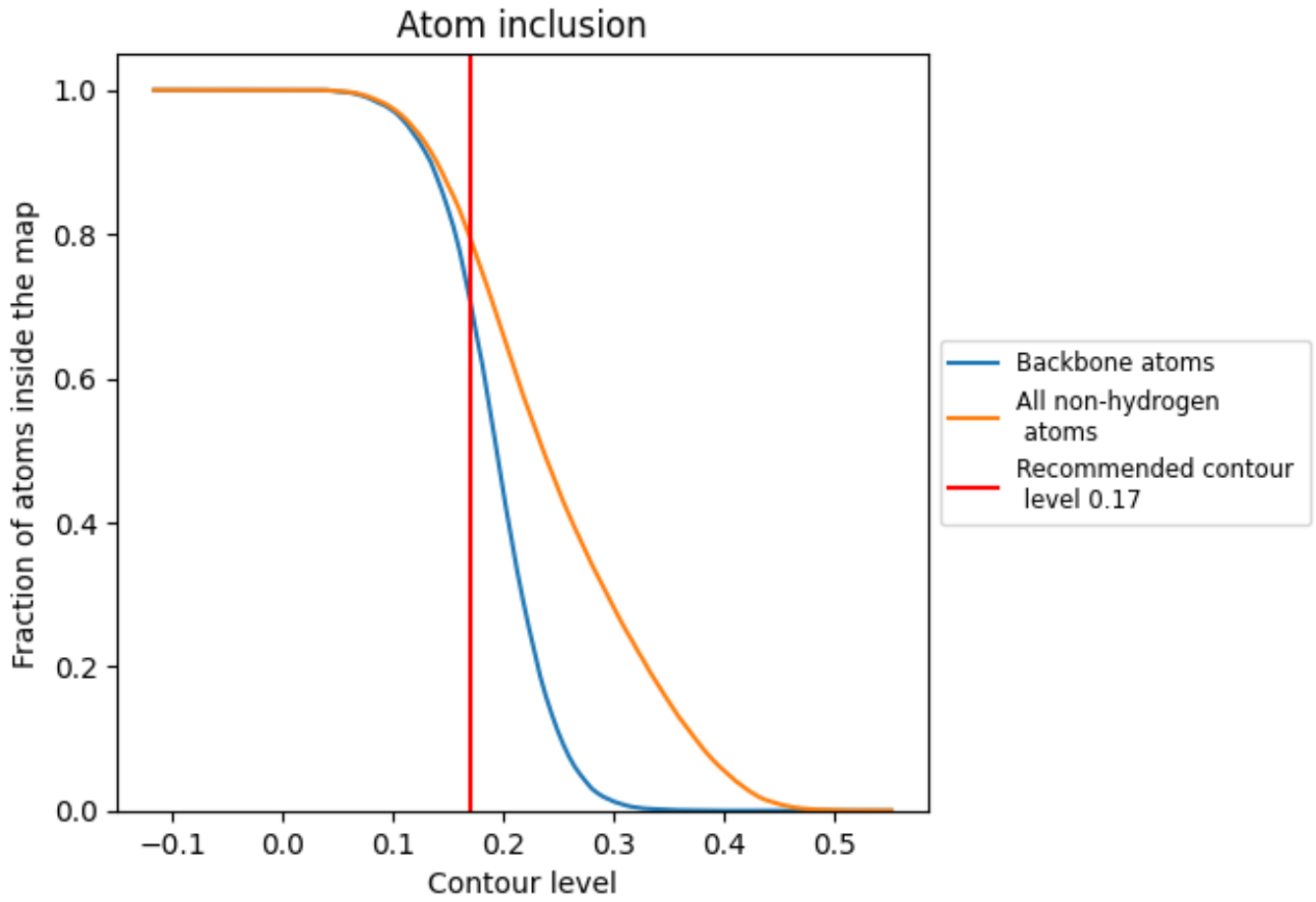
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.17).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 79% 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 (0.17) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7937	0.1570
AA	0.8086	0.1630
AB	0.8988	0.1720
AC	0.9247	0.1730
AD	0.7899	0.1620
AE	0.8974	0.1670
AF	0.9296	0.1740
AG	0.8817	0.1670
AH	0.9226	0.1810
AI	0.6662	0.1290
AJ	0.5941	0.1150
AK	0.7222	0.1160
AL	0.8798	0.1570
AM	0.3606	0.0880
AN	0.7192	0.1390
AO	0.8777	0.1680
AP	0.9008	0.1620
AQ	0.4099	0.0700
AR	0.6131	0.1220
AS	0.7421	0.1510
AT	0.8664	0.1560
AU	0.8542	0.1610
AV	0.8398	0.1720
AW	0.8353	0.1480
AX	0.8892	0.1590
AY	0.8993	0.1670
AZ	0.9214	0.1850
Aa	0.9086	0.1730
Ab	0.5361	0.1160
Ac	0.6892	0.1530
Ad	0.4677	0.1320
Ae	0.5704	0.1220
Af	0.5117	0.1410
Ag	0.9215	0.1740
Ah	0.9144	0.1770

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Chain	Atom inclusion	Q-score
Ai	0.8975	0.1660
Aj	0.8403	0.1710
Ak	0.8120	0.1530