

Supplementary material: Information on the 145 nucleic acid crystal structures with deposited structure factor data analyzed in this work.

Data set I refers to the 105 structures whose quality is surveyed in this study. Data set II refers to a subset of 6 high quality nucleic acid structures that were used to analyze the quality of nucleic acid subgroups, and to investigate the effect of using different dictionaries in the crystallographic refinement. Whenever necessary, the last column gives the reason for which the structure was not included in the analysis.

NDB ID	PDB ID	Citation	Refinement program	Low resolution	High resolution	Sigma cutoff	Completeness	R (%)	Space group	Set
ADF073	257D	B.H.Mooers, G.P.Schroth, W.W.Baxter, P.S.Ho. <i>J.Mol.Biol.</i> 249, 772-784, 1995	X-PLOR (Brünger, 1993)	8.0	2.3	2	78.8	16.4	C 2 2 21	I
ADFB62	254D	B.H.Mooers, G.P.Schroth, W.W.Baxter, P.S.Ho. <i>J.Mol.Biol.</i> 249, 772-784, 1995	X-PLOR (Brünger, 1993)	8.0	1.9	2	76.9	19.7	C 2 2 21	I
ADFB63	275D	B.H.Mooers, G.P.Schroth, W.W.Baxter, P.S.Ho. <i>J.Mol.Biol.</i> 249, 772-784, 1995	X-PLOR (Brünger, 1993)	8.0	2.0	2	47.9	17.2	C 2 2 21	I
ADFB72	256D	B.H.Mooers, G.P.Schroth, W.W.Baxter, P.S.Ho. <i>J.Mol.Biol.</i> 249, 772-784, 1995	X-PLOR (Brünger, 1993)	8.0	2.2	2	64.1	16.5	C 2 2 21	I
ADFB97	343D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published.	X-PLOR (Brünger, 1993)	8.0	2.1	3	n.a.	20.4	P 1	I
ADH007	3ANA	H.Lauble, R.Frank, H.Bloecker, U.Heinemann. <i>Nucleic Acids Res.</i> 16, 7799-7816, 1988	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	2.5	3	n.a.	16.6	P 61	I,II
ADH008	9DNA	U.Heinemann, H.Lauble, R.Frank, H.Bloecker. <i>Nucleic Acids Res.</i> 15, 9531-9550, 1987	NUCLSQ (Westhof <i>et al</i> , 1985)	6.0	1.8	3	n.a.	17.1	P 43 21 2	I
ADH038	1D78	N.Thota, X.H.Li, C.Bingman, M.Sundaralingam. <i>Acta Crystallogr.</i> , D 49, 282-291, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	5.0	1.4	2	n.a.	19.8	P 61 2 2	I,II

ADH039	1D79	N.Thota, X.H.Li, C.Bingman, M.Sundaralingam. <i>Acta Crystallogr.</i> , D49, 282-291, 1993	NUCLSQ (Westhof <i>et al.</i> , 1985)	5.0	1.45	2	n.a.	19.1	P 61 2 2	I
ADH047	118D	C.Bingman, X.Li, G.Zon, M.Sundaralingam. <i>Biochemistry</i> 31, 12803-12812, 1992	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.64	2	n.a.	15.4	P 43 21 2	I
ADH078	317D	D.B.Tippin, M.Sundaralingam <i>Acta Crystallogr.</i> , D52, 997-1003, 1996	X-PLOR (Brünger, 1993)	8.0	1.9	1	n.a.	16.4	P 43 21 2	I
ADHB100	345D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	1.85	3	n.a.	20.6	P 43 21 2	I
ADHB101	346D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	2.1	3	n.a.	20.4	P 43 21 2	I
ADHB91	337D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	1.85	3	n.a.	21	P 43 21 2	I
ADHB92	338D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	1.85	3	n.a.	20.2	P 43 21 2	I
ADHB93	339D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	2.2	3	n.a.	17.4	P 43 21 2	I
ADHB94	340D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	1.6	3	n.a.	20.5	P 43 21 2	I
ADHB95	341D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	7.7	1.75	3	n.a.	18.5	P 43 21 2	I
ADHB96	342D	B.H.M.Mooers, B.F.Eichman, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	2.1	3	n.a.	18.9	P 43 21 2	I
ADHP36	1D26	U.Heinemann, L.-N.Rudolph, C.Alings, M.Morr, W.Heikens, R.Frank, H.Bloecker <i>Nucleic Acids Res.</i> 19, 427-433, 1991	NUCLSQ (Westhof <i>et al.</i> , 1985)	6.0	2.12	3	n.a.	16	P 43 21 2	I
ADJ081	320D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.15	1	n.a.	16.2	P 21 21 21	I
ADJ082	321D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.15	1	n.a.	15.3	P 21 21 21	I
ADJB79	318D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.0	1	n.a.	16.2	P 61	I
ADJB80	319D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.2	1	n.a.	15	P 21 21 21	I
ADJB83	322D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.5	1	n.a.	17.5	P 61	I
ADJB84	323D	D.B.Tippin, M.Sundaralingam <i>J.Mol.Biol.</i> 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.15	1	n.a.	15.5	P 21 21 21	I

ADJB85	324D	D.B.Tippin, M.Sundaralingam J.Mol.Biol. 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.15	1	n.a.	12.6	P 21 21 21	I
ADJB86	325D	D.B.Tippin, M.Sundaralingam J.Mol.Biol. 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.5	1	n.a.	16.3	P 61	I
ADJB87	326D	D.B.Tippin, M.Sundaralingam J.Mol.Biol. 267, 1171-1185, 1997	X-PLOR (Brünger, 1993)	8.0	2.15	1	n.a.	14	P 21 21 21	I
ADJB88	327D	D.B.Tippin, B.Ramakrishnan, M.Sundaralingam J.Mol.Biol. 270, 247- 258, 1997	X-PLOR (Brünger, 1993)	8.0	1.94	1	n.a.	19.1	P 61 2 2	I
ADL045	116D	C.A.Bingman, G.Zon, M.Sundaralingam J.Mol.Biol. 227, 738-756, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.5	2	n.a.	15	P 61 2 2	I
ADL046	117D	C.Bingman, S.Jain, G.Zon, M.Sundaralingam Nucleic Acids Res. 20, 6637-6647, 1992	NUCLSQ (Westhof <i>et al</i> , 1985) (Westhof <i>et al</i> , 1985)	8.0	2.55	2	n.a.	14.2	P 61 2 2	I
AHH071	246D	M.C.Wahl, C.Ban, C.Sekharudu, B.Ramakrishnan, M.Sundaralingam Acta Crystallogr., D52, 655-667, 1996	X-PLOR (Brünger, 1993)	10.0	2.2	2	86	15.6	R 3	I
ARL048	157D	G.A.Leonard, K.E.McAuley-Hecht, S.Ebel, D.M.Lough, T.Brown, W.N.Hunter Structure 2, 483-494, 1994	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	1.8	3	n.a.	19	P 21	I
BDJ017	1BD1	U.Heinemann, C.Alings J.Mol.Biol. 210, 369-381, 1989	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	1.6	3	n.a.	16	C 2	I
BDJ031	1D49	J.R.Quintana, K.Grzeskowiak, K.Yanagi, R.E.Dickerson J.Mol.Biol. 225, 379-395, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.5	2	n.a.	15.7	P 21 21 21	I,II
BDJ036	1D56	H.Yuan, J.Quintana, R.E.Dickerson Biochemistry 31, 8009-8021, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.7	2	n.a.	17.8	P 21 21 21	I
BDJ037	1D57	H.Yuan, J.Quintana, R.E.Dickerson Biochemistry 31, 8009-8021, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.0	2	n.a.	16.5	P 21 21 21	I
BDJ039	1CGC	U.Heinemann, C.Alings, M.Bansal Embo J. 11, 1931-1939, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.2	1	n.a.	16.7	R 3	I
BDJ051	126D	D.S.Goodsell, M.L.Kopka, D.Cascio, R.E.Dickerson Proc.Nat.Acad.Sci.USA 90, 2930-2934, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.0	2	n.a.	19.6	P 21 21 21	I
BDJ060	196D	D.S.Goodsell, K.Grzeskowiak, R.E.Dickerson Biochemistry 34, 1022- 1029, 1995	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.7	2	n.a.	20	C 2	I
BDJB27	2D25	U.Heinemann, M.Hahn J.Biol.Chem. 267, 7332-7341, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.75	2	n.a.	17.4	P 6	I

BDJB43	1D60	A.Lipanov, M.L.Kopka, M.Kaczor-Grzeskowiak, J.Quintana, R.E.Dickerson Biochemistry 32, 1373-1389, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.2	2	n.a.	16.2	P 32 2 1	I
BDJB44	1D61	A.Lipanov, M.L.Kopka, M.Kaczor-Grzeskowiak, J.Quintana, R.E.Dickerson Biochemistry 32, 1373-1389, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.3	2	n.a.	15.2	C 2	I
BDJB48	1DA3	I.Baikalov, K.Grzeskowiak, K.Yanagi, J.Quintana, R.E.Dickerson J.Mol.Biol. 231, 768-784, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.0	2	n.a.	17.2	P 32 2 1	I
BDJB77	286D	M.Shatzky-Schwartz, N.D.Ar buckle, M.Eisenstein, D.Rabinovich, A.Bareket-Samish, T.E.Haran, B.F.Luisi, Z.Shakked J.Mol.Biol. 267, 595- 623, 1997	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.5	2	n.a.	20.3	P 31	I
BDL028	1D28	N.Narayana, S.L.Ginell, I.M.Russu, H.M.Berman Biochemistry 30, 4449-4455, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	2.7	n.a.	n.a.	17	P 21 21 21	I
BDL029	1D29	T.A.Larsen, M.L.Kopka, R.E.Dickerson Biochemistry 30, 4443-4449, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	2.5	n.a.	n.a.	15.8	P 21 21 21	I
BDL038	1D65	K.J.Edwards, D.G.Brown, N.Spink, S.Neidle J.Mol.Biol. 226, 1161-1173, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.2	n.a.	n.a.	18.1	P 21 21 21	I
BDL042	119D	G.A.Leonard, W.N.Hunter J.Mol.Biol. 234, 198-208, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	2.25	2	n.a.	13.8	C 2	I
BDL046	1D80	J.V.Skelly, K.J.Edwards, T.C.Jenkins, S.Neidle Proc.Nat.Acad.Sci.USA 90, 804-808, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.2	n.a.	n.a.	18.8	P 21 21 21	I
BDL075	271D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.02	4	92.9	17.6	P 21 21 21	I
BDL078	287D	M.Shatzky-Schwartz, N.D.Ar buckle, M.Eisenstein, D.Rabinovich, A.Bareket-Samish, T.E.Haran, B.F.Luisi, Z.Shakked J.Mol.Biol. 267, 595-623, 1997	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.2	2	n.a.	15	P 21 21 21	I
BDLB72	265D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.01	4	86.2	17.2	P 21 21 21	I
BDLB73	266D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.03	4	81.2	16.6	P 21 21 21	I
BDLB74	270D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.01	n.a.	83.9	17.6	P 21 21 21	I

BDLB76	285D	M.Shatzky-Schwartz, N.D.Ar buckle, M.Eisenstein, D.Rabinovich, A.Bareket-Samish, T.E.Haran, B.F.Luisi, Z.Shakked J.Mol.Biol. 267, 595-623, 1997	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.5	2	n.a.	20.6	P 21 21 21	I
BDLB82	297D	M.Shatzky-Schwartz, N.D.Ar buckle, M.Eisenstein, D.Rabinovich, A.Bareket-Samish, T.E.Haran, B.F.Luisi, Z.Shakked J.Mol.Biol. 267, 595-623, 1997	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.5	n.a.	n.a.	22.1	P 21 21 21	I
DDF039	110D	G.A.Leonard, T.W.Hambley, K.McAuley-Hecht, T.Brown, W.N.Hunter Acta Crystallogr., D49, 458-467, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	1.9	2	n.a.	20.8	P 41 21 2	I
DDF040	1DA9	G.A.Leonard, T.W.Hambley, K.McAuley-Hecht, T.Brown, W.N.Hunter Acta Crystallogr., D49, 458-467, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	1.7	2	n.a.	21.6	P 41 21 2	I
DDF041	2DES	M.Cirilli, F.Bachechi, G.Ughetto, F.P.Colonna, M.L.Capobianco J.Mol.Biol. 230, 878-889, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	1.5	2	n.a.	19.2	P 1	I
DDFB70	308D	Y.-G.Gao, H.Robinson, E.R.Wijsman, G.A.Van Der Marel, J.H.Van Boom, A.H.-J.Wang J.Am.Chem.Soc. 119, 1496-1497, 1997	X-PLOR (Brünger, 1993)	10.0	1.5	2	n.a.	17.5	P 1	I
GDJ054	334D	M.L.Kopka, D.S.Goodsell, G.W.Han, T.K.Chiu, J.W.Lown, R.E.Dickerson Structure 5, 1033-1046, 1997	NUCLSQ (Westhof <i>et al</i> , 1985) (Westhof <i>et al</i> , 1985)	8.0	1.8	1	92	20	P 21 21 21	I
GDL002	1DNH	M.-K.Teng, N.Usman, C.A.Frederick, A.H.-J.Wang Nucleic Acids Res. 16, 2671-2690, 1988	NUCLSQ (Westhof <i>et al</i> , 1985)	20.0	2.25	2	n.a.	15.7	P 21 21 21	I
GDL008	1D30	T.Larsen, D.S.Goodsell, D.Cascio, K.Grzeskowiak, R.E.Dickerson J.Biomol.Struct.Dyn. 7, 477-491, 1989	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	2.4	2	n.a.	22.2	P 21 21 21	I
GDL010	1D43	J.R.Quintana, A.A.Lipanov, R.E.Dickerson Biochemistry 30, 10294-10306, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.0	2	n.a.	15.7	P 21 21 21	I
GDL012	1D45	J.R.Quintana, A.A.Lipanov, R.E.Dickerson Biochemistry 30, 10294-10306, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.9	2	n.a.	15.2	P 21 21 21	I
GDL013	1D46	J.R.Quintana, A.A.Lipanov, R.E.Dickerson Biochemistry 30, 10294-10306, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	2.0	2	n.a.	14.9	P 21 21 21	I

GDL015	1D64	K.J.Edwards, T.C.Jenkins, S.Neidle Biochemistry 31, 7104-7109, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	2.1	n.a.	n.a.	19.4	P 21 21 21	I
GDL016	1D63	D.G.Brown, M.R.Sanderson, E.Garman, S.Neidle J.Mol.Biol. 226, 481-490, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	2.0	2	n.a.	18.3	P 21 21 21	I
GDL023	1PRP	C.M.Nunn, T.C.Jenkins, S.Neidle Biochemistry 32, 13838-13843, 1993	X-PLOR (Brünger, 1993)	8.0	2.1	2	n.a.	17.4	P 21 21 21	I
GDL027	166D	C.M.Nunn, T.C.Jenkins, S.Neidle Eur.J.Biochem. 226, 953-961, 1994	X-PLOR (Brünger, 1993)	8.0	2.2	2	97.4	18.9	P 21 21 21	I
GDL032	102D	C.M.Nunn, S.Neidle J.Med.Chem. 38, 2317-2325, 1995	X-PLOR (Brünger, 1993)	8.0	2.2	2	90.8	15.5	P 21 21 21	I
GDL033	109D	A.A.Wood, C.M.Nunn, A.Czarny, D.W.Boykin, S.Neidle Nucleic Acids Res. 23, 3678-3684, 1995	X-PLOR (Brünger, 1993)	8.0	2.0	2	n.a.	19.7	P 21 21 21	I
GDL039	263D	G.R.Clark, E.J.Gray, S.Neidle, Y.-H.Li, W.Leupin Biochemistry 35, 13745- 13752, 1996	X-PLOR (Brünger, 1993)	8.0	2.2	2	92.3	17.4	P 21 21 21	I
GDL044	298D	J.O.Trent, G.R.Clark, A.Kumar, W.D.Wilson, D.W.Boykin, J.E.Hall, R.R.Tidwell, B.L.Blagburn, S.Neidle J.Med.Chem. 39, 4554-4562, 1996	X-PLOR (Brünger, 1993)	8.0	2.2	2	n.a.	16.9	P 21 21 21	I
GDL045	289D	J.O.Trent, G.R.Clark, A.Kumar, W.D.Wilson, D.W.Boykin, J.E.Hall, R.R.Tidwell, B.L.Blagburn, S.Neidle J.Med.Chem. 39, 4554-4562, 1996	X-PLOR (Brünger, 1993)	8.0	2.2	2	n.a.	18.6	P 21 21 21	I
GDL047	302D	G.R.Clark, C.J.Squire, E.J.Gray, W.Leupin, S.Neidle Nucleic Acids Res. 24, 4882-4889, 1996	X-PLOR (Brünger, 1993)	8.0	2.2	2	n.a.	20.2	P 21 21 21	I
GDL048	303D	G.R.Clark, C.J.Squire, E.J.Gray, W.Leupin, S.Neidle Nucleic Acids Res. 24, 4882-4889, 1996	X-PLOR (Brünger, 1993)	8.0	2.2	2	n.a.	20.4	P 21 21 21	I
GDL052	311D	G.R.Clark, D.W.Boykin, A.Czarny, S.Neidle Nucleic Acids Res. 25, 1510- 1515, 1997	X-PLOR (Brünger, 1993)	8.0	2.2	2	n.a.	19.5	P 21 21 21	I
GDL053	328D	C.J.Squire, G.R.Clark, W.A.Denny Nucleic Acids Res. 25, 4072-4078, 1997	X-PLOR (Brünger, 1993)	8.0	2.6	2	n.a.	17.8	P 21 21 21	I
GDLB41	267D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.0	4	76.4	15.6	P 21 21 21	I
GDLB42	268D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.02	4	90.5	16	P 21 21 21	I

GDLB43	269D	B.L.Partridge, S.A.Salisbury To be Published	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.15	4	70.3	15.6	P 21 21 21	I
TRNA08	3TRA	E.Westhof, P.Dumas, D.Moras Acta Crystallogr., A44, 112-123, 1988	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	3.0	2	n.a.	18.8	C 2 2 21	I
UDI047	253D	B.H.M.Mooers, P.S.Ho To be Published	X-PLOR (Brünger, 1993)	8.0	2.2	1	n.a.	19.31	P 42 21 2	I
UDJ049	272D	D.Vlieghe, L.Van Meervelt, A.Dautant, B.Gallois, G.Precigoux, O.Kennard Science 273, 1702-1705, 1996	SHELXL (Sheldrick, 1993)	10.0	2.0	0	n.a.	20.9	P 21 21 21	I
UHI055	1FIX	N.C.Horton, B.C.Finzel J.Mol.Biol. 264, 521-533, 1996	X-PLOR (Brünger, 1993)	5.0	2.3	2	80	14.5	P 43 2 2	I
URL050	280D	S.E.Lietzke, C.L.Barnes, C.E.Kundrot Structure 4, 917-930, 1996	X-PLOR (Brünger, 1993)	8.0	2.4	2	n.a.	19.1	P 1	I
URX035	1MME	W.G.Scott, J.T.Finch, A.Klug Cell 81, 991-1002, 1995	X-PLOR 3.1 (Brünger, 1993)	15.0	3.1	2	94.9	25.1	P 31 2 1	I
URX057	299D	W.G.Scott, J.B.Murray, J.R.P.Arnold, B.L.Stoddard, A.Klug Science 274, 2065- 2069, 1996	X-PLOR 3.1 (Brünger, 1993)	8.0	3.0	2	85.4	21.6	P 31 2 1	I
URX058	300D	W.G.Scott, J.B.Murray, J.R.P.Arnold, B.L.Stoddard, A.Klug Science 274, 2065- 2069, 1996	X-PLOR 3.1 (Brünger, 1993)	8.0	3.0	2	83.3	21.7	P 31 2 1	I
URX059	301D	W.G.Scott, J.B.Murray, J.R.P.Arnold, B.L.Stoddard, A.Klug Science 274, 2065- 2069, 1996	X-PLOR 3.1 (Brünger, 1993)	8.0	3.0	2	92.2	25.8	P 31 2 1	I
ZDF028	1D39	T.F.Kagawa, B.H.Geierstanger, A.H.- J.Wang, P.S.Ho J.Biol.Chem. 266, 20175- 20184, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	1.2	n.a.	n.a.	19.8	P 21 21 21	I
ZDFB04	1DN4	B.Chevrier, A.C.Dock, B.Hartmann, M.Leng, D.Moras, M.T.Thuong, E.Westhof J.Mol.Biol. 188, 707-719, 1986	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	1.6	3	n.a.	13.27	P 21 21 21	I
ZDFB05	1DN5	B.Chevrier, A.C.Dock, B.Hartmann, M.Leng, D.Moras, M.T.Thuong, E.Westhof J.Mol.Biol. 188, 707-719, 1986	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	1.4	2	n.a.	12.47	P 21 21 21	I
ZDFB10	1D40	B.H.Geierstanger, T.F.Kagawa, S.- L.Chen, G.J.Quigley, P.S.Ho J.Biol.Chem. 266, 20185-20191, 1991	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	1.3	n.a.	n.a.	20.9	P 21 21 21	I
ZDFB21	1D24	S.L.Ginell, S.Kuzmich, R.A.Jones, H.M.Berman Biochemistry 29, 10461- 10465, 1990	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.9	n.a.	n.a.	19	P 21 21 21	I

ZDFB24	1D41	G.Zhou, P.S.Ho <i>Biochemistry</i> 29, 7229-7236, 1990	NUCLSQ (Westhof <i>et al.</i> , 1985)	n.a.	1.3	n.a.	n.a.	20.8	P 21 21 21	I
ZDFB31	1D76	B.Schneider, S.L.Ginell, R.Jones, B.Gaffney, H.M.Berman <i>Biochemistry</i> 31, 9622-9628, 1992	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.3	4	n.a.	13.8	P 21 21 21	I
ZDFB37	145D	G.P.Schroth, T.F.Kagawa, P.Shing Ho <i>Biochemistry</i> 32, 13381-13392, 1993	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.25	1.5	n.a.	19.3	P 21 21 21	I
ZDFB51	242D	M.R.Peterson, S.J.Harrop, S.M.McSweeney, G.A.Leonard, A.W.Thompson, W.N.Hunter, J.R.Helliwell <i>J.Synchrotron Radia.</i> 3, 24-34, 1996	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.65	0	n.a.	17	P 21 21 21	I
ZDG054	312D	B.H.M.Moers, B.F.Eichman, P.S.Ho <i>J.Mol.Biol.</i> 269, 796-810, 1997	X-PLOR (Brünger, 1993)	8.0	1.8	3	n.a.	20.9	P 21 21 21	I,II
ZDG056	314D	B.H.M.Moers, B.F.Eichman, P.S.Ho <i>J.Mol.Biol.</i> 269, 796-810, 1997	X-PLOR (Brünger, 1993)	8.0	1.9	3	n.a.	19.1	P 21 21 21	I,II
ZDGB55	313D	B.H.M.Moers, B.F.Eichman, P.S.Ho <i>J.Mol.Biol.</i> 269, 796-810, 1997	X-PLOR (Brünger, 1993)	8.0	1.68	3	n.a.	20.7	P 21 21 21	I
ADDB01	1ANA	B.N.Conner, C.Yoon, J.L.Dickerson, R.E.Dickerson <i>J.Mol.Biol.</i> 174, 663-695, 1984	JACK-LEVITT (Jack & Levitt, 1978)	8.0	2	n.a.	n.a.	16.5	P 43 21 2	III-1
ADH006	2ANA	M.McCall, T.Brown, O.Kennard <i>J.Mol.Biol.</i> 183, 385-396, 1985	NUCLSQ (Westhof <i>et al.</i> , 1985)	10.0	2.5	2	n.a.	14	P 61	III-1
ADH023	28DN	C.Courseille, A.Dautant, M.Hospital, B.Langlois D'Estaintot, G.Precigoux, D.Molko, R.Teoule <i>Acta Crystallogr.</i> A46, Fc9-Fc12, 1990	X-PLOR (Brünger, 1993)	n.a.	2.4	n.a.	n.a.	17	P 43 21 2	III-1
ADH070	243D	D.J.Wilcock, A.Adams, C.J.Cardin, L.P.G.Wakelin <i>Acta Crystallogr.</i> , D52, 481-485, 1996	X-PLOR 3.0 (Brünger, 1992)	5.0	1.9	1	97.7	17.7	P 43 21 2	III-1
ADJ049	160D	B.Ramakrishnan, M.Sundaralingam <i>J.Mol.Biol.</i> 231, 431-444, 1993	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.65	n.a.	n.a.	18.5	P 21 21 21	III-1
ADJ050	137D	B.Ramakrishnan, M.Sundaralingam <i>Biochemistry</i> 32, 11458-11468, 1993	X-PLOR (Brünger, 1993)	8.0	1.7	3	n.a.	18.5	P 21 21 21	III-1
ADJ051	138D	B.Ramakrishnan, M.Sundaralingam <i>Biochemistry</i> 32, 11458-11468, 1993	X-PLOR (Brünger, 1993)	8.0	1.8	3	n.a.	18.3	P 61 2 2	III-1
AHJ052	161D	C.Ban, B.Ramakrishnan, M.Sundaralingam <i>J.Mol.Biol.</i> 236, 275-285, 1994	X-PLOR (Brünger, 1993)	8.0	1.9	1	n.a.	13.6	P 21 21 21	III-1

AHJ060	100D	C.Ban, B.Ramakrishnan, M.Sundaralingam <i>Nucleic Acids Res.</i> 22, 5466-5476, 1994	X-PLOR (Brünger, 1993)	8.0	1.9	1	n.a.	14.5	P 21 21 21	III-1
ARFS26	310D	D.A.Adamiak, J.Milecki, M.Popenda, R.W.Adamiak, Z.Dauter, W.R.Rypniewski <i>Nucleic Acids Res.</i> 25, 4599-4607, 1997	SHELXL-96 (Sheldrick, 1996)	8.0	1.3	0	95.3	17.2	P 61 2 2	III-2
BDJ008	3DNB	G.G.Prive, K.Yanagi, R.E.Dickerson <i>J.Mol.Biol.</i> 217, 177-199, 1991	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.3	2	n.a.	16.4	C 2	III-1
BDJ019	5DNB	G.G.Prive, K.Yanagi, R.E.Dickerson <i>J.Mol.Biol.</i> 217, 177-199, 1991	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.4	1	n.a.	16	C 2	III-1
BDJ025	1D23	K.Grzeskowiak, K.Yanagi, G.G.Prive, R.E.Dickerson <i>J.Biol.Chem.</i> 266, 8861- 8883, 1991	NUCLSQ (Westhof <i>et al.</i> , 1985)	8.0	1.5	2	n.a.	16.1	P 21 21 21	III-1
BDJ081	307D	G.W.Han, M.L.Kopka, D.Cascio, K.Grzeskowiak, R.E.Dickerson <i>J.Mol.Biol.</i> 269, 811- 826, 1997	TNT (Tronrud <i>et al.</i> , 1987)	8.0	1.85	2	93	23.3	C 2	III-2
BDL001	1BNA	H.R.Drew, R.M.Wing, T.Takano, C.Broka, S.Tanaka, K.Itakura, R.E.Dickerson <i>Proc.Nat.Acad.Sci.USA</i> 78, 2179-2183, 1981	JACK-LEVITT (Jack & Levitt, 1978)	8.0	1.9	n.a.	n.a.	17.8	P 21 21 21	III-1
BDL002	2BNA	H.R.Drew, S.Samson, R.E.Dickerson <i>Proc.Nat.Acad.Sci.USA</i> 79, 4040-4044, 1982	JACK-LEVITT (Jack & Levitt, 1978)	15.0	2.7	n.a.	n.a.	15.1	P 21 21 21	III-1
BDL005	7BNA	R.Wing, H.R.Drew, T.Takano, C.Broka, S.Tanaka, K.Itakura, R.E.Dickerson <i>Nature</i> 287, 755-758, 1980	JACK-LEVITT (Jack & Levitt, 1978)	15.0	2.7	n.a.	n.a.	15.1	P 21 21 21	III-3
BDL007	1DN9	S.R.Holbrook, R.E.Dickerson, S.-H.Kim <i>Acta Crystallogr.</i> , B41, 255-262, 1985	CORELS (Sussman <i>et al.</i> , 1977)	8.0	1.9	2	n.a.	14.9	P 21 21 21	III-1
BDL015	1BDN	C.Yoon, G.G.Prive, D.S.Goodsell, R.E.Dickerson <i>Proc.Nat.Acad.Sci.USA</i> 85, 6332-6336, 1988	X-PLOR (Brünger, 1993)	8.0	2.2	0.5	n.a.	18.9	P 21 21 21	III-1
BDL047	1D89	A.D.DiGabriele, M.R.Sanderson, T.A.Steitz <i>Proc.Nat.Acad.Sci.USA</i> 86, 1816-1820, 1989	CORELS (Sussman <i>et al.</i> , 1977)	8.0	2.6	n.a.	n.a.	20.1	P 21 21 21	I-2
BDL059	194D	A.D.DiGabriele, T.A.Steitz <i>J.Mol.Biol.</i> 231, 1024-1039, 1993	X-PLOR (Brünger, 1993)	6.0	2.3	2	n.a.	23.2	P 21 21 2	III-1

BDLB03	3BNA	K.Balendiran, S.T.Rao, C.Y.Sekharudu, G.Zon, M.Sundaralingam Acta Crystallogr., D51, 190-198, 1995	X-PLOR (Brünger, 1993)	6.0	2.3	2	n.a.	14.8	P 21 21 21	III-1
BDLB04	4BNA	A.V.Fratini, M.L.Kopka, H.R.Drew, R.E.Dickerson J.Biol.Chem. 257, 14686- 14707, 1982	JACK-LEVITT (Jack & Levitt, 1978)	8.0	3.0	2	n.a.	13	P 21 21 21	III-1
BDLB26	1D27	A.V.Fratini, M.L.Kopka, H.R.Drew, R.E.Dickerson J.Biol.Chem. 257, 14686- 14707, 1982	JACK-LEVITT (Jack & Levitt, 1978)	8.0	2.3	n.a.	n.a.	21.6	P 21 21 21	III-1
DDF035	1D54	G.A.Leonard, J.Thomson, W.P.Watson, T.Brown Proc.Nat.Acad.Sci.USA 87, 9573-9576, 1990	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	2.0	3	n.a.	18.5	P 21 21 21	III-1
DDF036	1D58	G.A.Leonard, T.Brown, W.N.Hunter Eur.J.Biochem. 204, 69-74, 1992	NUCLSQ (Westhof <i>et al</i> , 1985)	7.0	1.4	3	n.a.	17	P 41 21 2	III-1
DDF038	1D67	B.Langlois D'Estaintot, B.Gallois, T.Brown, W.N.Hunter Nucleic Acids Res. 20, 3561-3566, 1992	X-PLOR (Brünger, 1993)	7.0	1.7	2	n.a.	20.2	P 41 21 2	III-1
DDF064	258D	B.Gallois, B.Langlois D'Estaintot, T.Brown, W.N.Hunter Acta Crystallogr., D49, 311-317, 1993	NUCLSQ (Westhof <i>et al</i> , 1985)	8.0	1.6	3	n.a.	22.2	P 41 21 2	III-2
DDL017	5BNA	C.K.Smith, J.A.Brannigan, M.H.Moore J.Mol.Biol. 263, 237-258, 1996	SHELXL-93 (Sheldrick, 1993)	10.69	1.58	0	94	18.8	P 21 21 21	III-3
GDHB25	159D	R.M.Wing, P.Pjura, H.R.Drew, R.E.Dickerson Embo J. 3, 1201-1206, 1984	JACK-LEVITT (Jack & Levitt, 1978)	8.0	2.6	2	n.a.	10.2	P 21 21 21	III-1
GDL006	8BNA	X.Chen, B.Ramakrishnan, S.T.Rao, M.Sundaralingam Nat.Struct.Biol. 1, 169- 175, 1994	X-PLOR (Brünger, 1993)	10.0	1.8	2	n.a.	15	P 41 2 2	III-1
GDL030	195D	P.E.Pjura, K.Grzeskowiak, R.E.Dickerson J.Biol.Chem. 197, 257-271, 1987	JACK-LEVITT (Jack & Levitt, 1978)	8.0	2.2	0	n.a.	19.1	P 21 21 21	III-1
GDLB05	6BNA	K.Balendiran, S.T.Rao, C.Y.Sekharudu, G.Zon, M.Sundaralingam Acta Crystallogr., D51, 190-198, 1995	X-PLOR (Brünger, 1993)	6.0	2.3	2	n.a.	16.2	P 21 21 21	III-1
TRNA07	2TRA	J.-A.Feng, R.C.Johnson, R.E.Dickerson Science 263, 348-355, 1994	X-PLOR (Brünger, 1993)	8.0	2.3	2	n.a.	22.8	C 2 2 21	III-2
TRNA10	4TNA	E.Westhof, P.Dumas, D.Moras Acta Crystallogr. A44, 112-123, 1988	NUCLSQ (Westhof <i>et al</i> , 1985)	10.0	3.0	2	n.a.	19.3	C 2 2 21	III-4

UDH052	284D	B.E.Hingerty, R.S.Brown, A.Jack J.Mol.Biol. 124, 523-534, 1978	JACK-LEVITT (Jack & Levitt, 1978)	n.a.	2.5	n.a.	n.a.	n.a.	P 21	III-2
UDP011	1D16	S.A.Salisbury, S.E.Wilson, H.R.Powell, O.Kennard, P.Lubini, G.M.Sheldrick, N.Escaja, E.Alazzouzi, A.Grandas, E.Pedroso Proc.Nat.Acad.Sci.USA 94, 5515-5518, 1997	SHELXL-96 (Sheldrick, 1996)	9.0	1.1	4	100	19.9	P 21 21 21	III-1
ZDD015	1ZNA	R.Chattopadhyaya, K.Grzeskowiak, R.E.Dickerson J.Mol.Biol. 211, 189-210, 1990	NUCLSQ (Westhof <i>et al</i> , 1985)	n.a.	2.1	2	n.a.	20	C 2	III-1
ZDF058	347D	H.R.Drew, R.E.Dickerson J.Mol.Biol. 152, 723-736, 1981	JACK-LEVITT (Jack & Levitt, 1978)	5.5	1.5	2	n.a.	21	B 2 21 2	III-3
ZDJ050	279D	C.Ban, B.Ramakrishnan, M.Sundaralingam Biophys.J. 71, 1215- 1221, 1996	X-PLOR (Brünger, 1993)	8.0	1.9	1	n.a.	18.6	P 65 2 2	III-1

I. Structures included in data set I

II. Structures included in data set II

III.

1. Structures missing the experimental σ values in the deposited structure factors
2. Structures refined anisotropically
3. Structures with major disordered portions
4. Structures missing B factors in the deposited structure factors