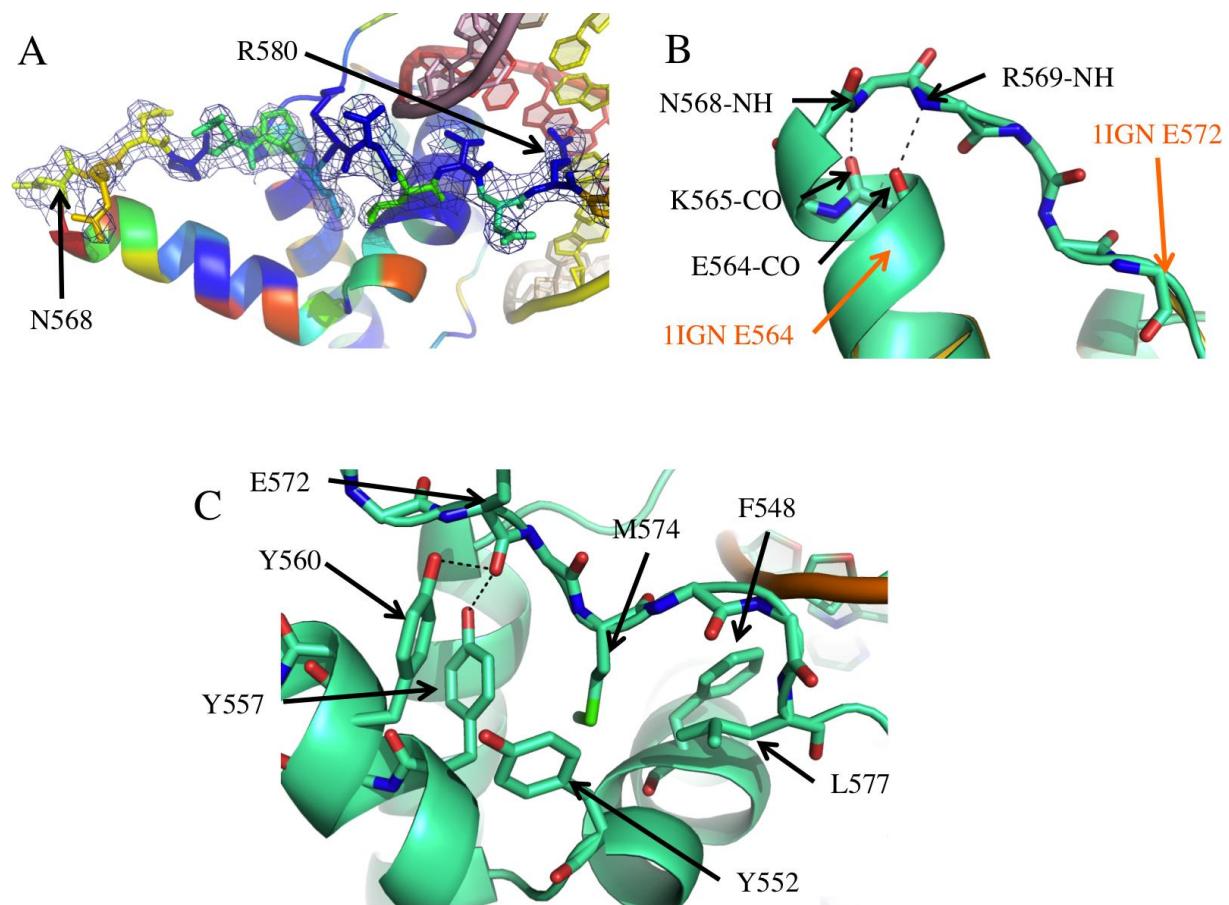


## Supplementary Material



**Supplementary Figure S1.** A. Cartoon representation of SG19 structure region 565-580 in green cyan. The DNA C-rich and G-rich strands are coloured red and yellow, respectively, with the hemi-site in bright colours. The protein is coloured according to conservative scores from *CONSURF*.  $2Fo - Fc$  electron-density map is also represented at  $1\sigma$  contour level around 567-601 region. B. Enlargement of region 564-569, showing tight interaction involved in  $\beta$ -turn. The limits of the lign structure are also indicated in bright yellow. C. Polar interaction and hydrophobic network driving loop 565-580 towards the DNA major groove.

## Supplementary Table S1

Referenced crystallization conditions used to calculate our protein/DNA specific screen.

REF	pH	Buffer	Prec	[Prec]	Add1	[Add1]	Add2	[Add2]
Ng et al., 2008	8.0	Tris	PEG4000	30%	MgCl <sub>2</sub>	0.2M		
Genis et al., 2008	7.0	Tris	PEGmme550	15%	MgCl <sub>2</sub>	5mM		
Pereira et al., 2008	6.0	Caco	PEG4000	15%	MgCl <sub>2</sub>	0.1M		
Pereira et al., 2008			PEG3350	20%	K/Na tartrate	0.1M	MgCl <sub>2</sub>	0.05M
Suwa et al., 2008	5-5.5	Caco	PEG3350	25%	MgAc	0.08M		
Redondo et al., 2007	4.5-5.5	Na Ac	PEG4000	5.6%	glycerol	30%		
Textor et al., 2007	9.0	Bis-Tris	PEG3350, PEG400	15%, 10%				
Shanmuganatham et al., 2007	5.7	Na Citrate	Amm Sulf, Eth glycol	1.4M, 21%	DTT	10mM		
Richardson et al., 2007	6.0	Na Citrate	KCl	0.2M	Amm Ac	0.1M	MgCl <sub>2</sub>	5mM
Kapetaniou et al., 2007	8.5	Tris	PEG400	28-30%	MgCl <sub>2</sub>	10mM	KCl	10mM
Watanabe et al., 2006	6.6-6.8	Bis-Tris	PEG10000	15%	Na/K tartrate	0.3M		
Vivian et al., 2006			PEG8000	13.5%	Li <sub>2</sub> SO <sub>4</sub>	0.45M	glycerol	10%
Vassylyeva et al., 2006	7.0	Hepes	PEGmme500	22.2%				
Sam et al., 2006	5.6-6.2	Na Citrate	PEG4000	30%	Amm Ac	0.2M		
Lu et al., 2006	8.5	Tris	PEG8000, PEG300	5%, 20%	glycerol	10%		
Imasaki et al., 2004	6.1	MES	PEG20000	13%	Na Ac	0.4M	6-aminocaproic acid	6%
Viadiu et al., 2003	4.6-5.0	Na Ac	MPD	32.5%	CaCl <sub>2</sub>	5-10mM		
Sam et al., 2003	6.5	Imid	NaOAc	1M				
Aono et al., 2003	8.5	Tris	PEG4000	20%	Li <sub>2</sub> SO <sub>4</sub>	0.1M		
Larivière et al., 2002			MPD	44%	t-but	4%	UDPglucose (with protein solution)	1mM
Pereira de Jesus et al., 2002	8.5	Tris	PEG4000	30%	Li <sub>2</sub> SO <sub>4</sub> or MgCl <sub>2</sub>	0.2M, 0.1M		
Hovde et al., 2002	5.6	Na Citrate	2-propanol, PEG4000	20%, 20%				
Tahirov et al., 2001	6.0	MES	PEG400	10%	KCl	0.1M	MgCl <sub>2</sub>	10mM
Tahirov et al., 2001	6.5	Caco	PEG8000	10%	KCl	0.2M	MgAc	0.1M
Vivian et al., 2001	4.6	Na Ac	PEG4000	2-7%				
O'Loughlin et al., 2000	6.5	Mes	PEG8000, Glycerol	14%, 12%	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	0.1M	CaCl <sub>2</sub>	6mM
Horton et al., 1999	5.5	Na Citrate	PEG4000	20%	NaCl	0.12M		
Schwartz et al., 1999			Amm Sulf	1.8M	Glycerol	10%		
Tamulaitiene et al., 2004	6.5	Mes	PEG6000, NaCl	8-10%, 2M	Ethylene glycol	0-4%		
Escalante et al., 2002	6.5	Na Ac	PEG3000	15%	Glycerol	5%		
Viadiu et al., 2000	4.8	Na Ac	MPD	16-20%	CaCl <sub>2</sub>	5nM		
Tan et al., 2000	5.2	Na Ac	PEG4000	6-10%	NaNO <sub>3</sub>	0.2M	Mg(NO <sub>3</sub> ) <sub>2</sub> , DTT	10mM, 10mM
Tan et al., 2000	5.5	Na Ac	PEG6000	7-10%	Amm Ac	0.1M	CaCl <sub>2</sub>	10mM
Hirsch et al., 1997	6.0	Mes	Amm Sulf	2.2M	KCl	0.2M	Glycerol	5%
Pio et al., 1995	6.5	Caco	PEG600	10%	Zn Ac	0.2M		

## Supplementary Table S2

Incomplete factorial screen calculated using SAmBA (Audic et al., 1997).

Prec1	pH	Prec2	Add1	Add2
Amm Sulf 2M	4,5	Glycerol 5%	Amm Ac 0.1M	Spermine 1mM
Amm Sulf 2M	5	ter-butanol 5%	MgCl2 0.1M1	0
Amm Sulf 2M	6	Propanol-2 5%	Amm Ac 0.1M	Co-hexamine 1mM
Glycerol 20%	4,5	Ethylene glycol 5%	CaCl2 0.1M	0
Glycerol 20%	5	ter-butanol 5%	MgCl2 0.1M1	Spermine 1mM
Glycerol 20%	6,5	0	Amm Ac 0.1M	Spermine 1mM
Glycerol 20%	7,5	Propanol-2 5%	0	0
Glycerol 20%	9	0	MgCl2 0.1M1	Co-hexamine 1mM
Li2SO4 1.5M	4,5	ter-butanol 5%	Amm Ac 0.1M	0
Li2SO4 1.5M	6,5	Ethylene glycol 5%	Amm Ac 0.1M	0
Li2SO4 1.5M	9	Glycerol 5%	0	Spermine 1mM
MPD 30%	6	0	CaCl2 0.1M	Spermine 1mM
MPD 30%	7	Glycerol 5%	MgCl2 0.1M1	Co-hexamine 1mM
MPD 30%	7,5	0	CaCl2 0.1M	Co-hexamine 1mM
PEG8000 10%	5,5	Glycerol 5%	Amm Ac 0.1M	Co-hexamine 1mM
PEG8000 10%	7	0	MgCl2 0.1M1	0
PEG8000 20%	4,5	0	MgCl2 0.1M1	Co-hexamine 1mM
PEG8000 20%	5	Ethylene glycol 5%	Amm Ac 0.1M	0
PEG8000 20%	6	Propanol-2 5%	CaCl2 0.1M	0
PEG8000 20%	6,5	Glycerol 5%	0	Co-hexamine 1mM
PEG8000 20%	7	Propanol-2 5%	0	Spermine 1mM
PEG8000 20%	8	Ethylene glycol 5%	MgCl2 0.1M1	Spermine 1mM
PEG3350 15%	4,5	ter-butanol 5%	0	Co-hexamine 1mM
PEG3350 15%	6	0	MgCl2 0.1M1	0
PEG3350 15%	6,5	ter-butanol 5%	MgCl2 0.1M1	Co-hexamine 1mM
PEG3350 15%	9	Propanol-2 5%	0	Spermine 1mM
PEG3350 25%	5,5	ter-butanol 5%	MgCl2 0.1M1	0
PEG3350 25%	7	Ethylene glycol 5%	Amm Ac 0.1M	Co-hexamine 1mM
PEG3350 25%	7,5	ter-butanol 5%	CaCl2 0.1M	Spermine 1mM
PEG400 20%	4,5	Glycerol 5%	MgCl2 0.1M1	Spermine 1mM
PEG400 20%	7,5	Ethylene glycol 5%	0	Spermine 1mM
PEG400 20%	8	0	CaCl2 0.1M	Co-hexamine 1mM
PEG400 30%	5	Glycerol 5%	0	0
PEG400 30%	6	ter-butanol 5%	0	Co-hexamine 1mM
PEG400 30%	7	0	CaCl2 0.1M	0
PEG400 30%	9	0	MgCl2 0.1M1	Spermine 1mM
PEGGmme-550 20%	5	Propanol-2 5%	0	Co-hexamine 1mM
PEGGmme-550 20%	5,5	Glycerol 5%	Amm Ac 0.1M	0
PEGGmme-550 20%	6	Ethylene glycol 5%	MgCl2 0.1M1	Spermine 1mM
PEGGmme-550 20%	7,5	0	MgCl2 0.1M1	Spermine 1mM
PEGGmme-550 20%	8	Glycerol 5%	CaCl2 0.1M	0
PEGGmme-550 30%	5	Glycerol 5%	CaCl2 0.1M	Spermine 1mM
PEGGmme-550 30%	5,5	0	0	0
PEGGmme-550 30%	9	Ethylene glycol 5%	MgCl2 0.1M1	0
Propanol-2 20%	4,5	Propanol-2 5%	MgCl2 0.1M1	Spermine 1mM
Propanol-2 20%	5	0	0	Spermine 1mM
Propanol-2 20%	8	0	Amm Ac 0.1M	0

**Supplementary Table S3**

Protein sequences used for conservation analysis from T-coffee alignment.

Rap1-Saccaromycescerevisiae Rap1-Saccharomycesdaiренensis Rap1-Zygosaccharomycesrouxii Rap1-Lachanceathermotolerans] Hypo-Vanderwaltozymapolyspora Rap1-Naumoviаcastellii hypo-Candidaglabrata Hypo-Kluyveromyceslactis Hypo-Ashbyagossypii Hypo-Meyerozymaguilliermondii Hypo-Pichiaguilliermondii Hypo-Clavisporalusitaniae	KASFTDEEDEFILDVVVKNPRTTHTLYDEISHY--VPNHTGNSIRHRFRVYLSKRLEY KSSFTETEDEFILDVVVKNPRTTHTLYDEISHY--VPNHTGNSIRHRFRVYLSKRLEDF KASFTEQEDEFILDVVVKNPRTTHTLYDEISHY--VPNHTGNSIRHRFRVYLSKRLEY KSSFTEEEDEFILDVVVKNPRTTHTLFDEISHY--VPKHTGNSIRHRFRVYLAKRNF KTSFTEEEDEFILDVVVKNPRTTHTLFDEISHY--VPNHTGNSIRHRFRVYLSKRLEY KASFTAEDEFILDVVVKNPRTTHTLYDEISHY--VPNHTGNSIRHRFRVYLSKRLDY KTSFTEEEDEFILDVVVKNPRTTHTLFDEISHY--VPNHTGNSIRHRFRVYLSKRLDY KSSFTKEEDEFILDVVVKNPRTTHTLYDEISHY--VPNHTGNSIRHRFRVYLSKRLEY KSSFTEEEDEFILDVVVKNPRTTHTLFDEISHY--VPNHTGNSIRHRFRVYLSKRLEY --RFNKVKDDYILKQVRMHPKYRNSHKFFDLANHPQLEGHTGNSIRSFRTHLEPKLDW --RFNKVKDDYILKQVRMHPKYRNSHKFFDLANHPQLEGHTGNSIRSFRTHLEPKLDW -TKTPPEADKYILEQVRLKPRFRTSHKFEEELSHHELLRGHTGNSRSRFRAHLEHRLDY
Rap1-Saccaromycescerevisiae Rap1-Saccharomycesdaiренensis Rap1-Zygosaccharomycesrouxii Rap1-Lachanceathermotolerans] Hypo-Vanderwaltozymapolyspora Rap1-Naumoviаcastellii hypo-Candidaglabrata Hypo-Kluyveromyceslactis Hypo-Ashbyagossypii Hypo-Meyerozymaguilliermondii Hypo-Pichiaguilliermondii Hypo-Clavisporalusitaniae	VYEVDK-FGKLVRDDDGNIKTKV--LPPSIKRKPSADEDYTLAIAVKKQFYRD-LF-QI VYEVDK-YGKLVRDEDGNIKTKL--LPPSIKKKTADEDYALAVSVKKQFYRD-LY-QI VYEVDK-DGKLIRDANGNLVHTKV--LPPSIKKKFTAEDYQLAIGIKKQFYRD-LY-QI VYQVDS-TGKLVRDDNGDLIKTTV--LPKSLKNKFTASEDYLALSVEVKQFYRD-IY-QM VYQVDS-SGKLVRDENGNLVHTKV--LPPSIKKKFTAEDDYNLAMGJTKQFYRD-LY-QV VYQVDS-YGKLVRDENGNLIKTKT--LPPSIKKKFTADEDYLALAVKKQFYRD-LY-QI VYQVQDQ-YGKLVRDENGNLIKTKV--LPPSIKKKFTADEDYELAIAIKQQFYKD-IY-QL VYQVDE-DGKLVRDQDGNIKTDI--LPNGLKRKFTSEEDYNLAVAVKKQFYRD-AF-QR VYKVD-E-NGKLLRDEKGFIKTDV--LPQGLKRKFTADEDYQLALNJKQFYKD-IY-QV VYKTAS-DGSLIKDEHGQLIRDTLNDNLPKTLKNRFTAEDYELCQAIVD-FNRAR-FFGA VYKTAS-DGSLIKDEHGQLIRDTLNDNLPKTLKNRFTAEDYELCQAIVD-FNRAR-FFGA VWKTE-YDNLVLDHEGRQIAPT-NSAKTIKNRFTAEDDYNLRCRID-HVLAN--QD
Rap1-Saccaromycescerevisiae Rap1-Saccharomycesdaiренensis Rap1-Zygosaccharomycesrouxii Rap1-Lachanceathermotolerans] Hypo-Vanderwaltozymapolyspora Rap1-Naumoviаcastellii hypo-Candidaglabrata Hypo-Kluyveromyceslactis Hypo-Ashbyagossypii Hypo-Meyerozymaguilliermondii Hypo-Pichiaguilliermondii Hypo-Clavisporalusitaniae	DPDTGRS-----PNHVPGESEPNFAAYRTQSRRGPIAREEFFKH DPDGSQSLISAQD-S-PTAIARRN-MTMDPNHIPGSEPGFKKEYKVNDRKGPIAREEFFKS DPDTGVSLISDED-S-PTAIAKRN-MTMDPNHVPGETPNFQDYRVSDRRGPIAREEFFKH DPDTGESLIKIDIN-A-PDGNLKG-S-FGAGSDERQNPGPSFKDFRVGERRGPVPREFFKK DPDTGESLILEBDD-S-PVAIAKRK-MTMPNHIPIGTEPNFQEYKVNBRRGPLAREEFFQ DPDTGTNLLISNED-S-PTAIARRN-MTMDPNHVPGENEPSFNDFRVNDRRGPVAREEFFKS DPVTGQSLISND-P-PARVAKRQ-MMMDPNVQRGSEPPFSKYRVGTRRGPIAREEFFQ DPDTGASLIAEDD-E-PNIVAKRQ-LVMNTIEDPSEVPSFEKYTVNDRRGPLSRREFFKL DPDTGESLIRDDD-E-PSTVAKRK-MVMDPTFIPGKEPSFQDYNVGDRRGPLSRREFFKT ADEHG--IVRDETGKPK-----EF-----DLY--GQLTVPIS--FFST ADEHG--IVRDETGKPK-----EF-----DLY--GQLTVPIS--FFST ADQL-K-VTDGSY-----EYPLNEENKFVSIVFFDE
Rap1-Saccaromycescerevisiae Rap1-Saccharomycesdaiренensis Rap1-Zygosaccharomycesrouxii Rap1-Lachanceathermotolerans] Hypo-Vanderwaltozymapolyspora Rap1-Naumoviаcastellii hypo-Candidaglabrata Hypo-Kluyveromyceslactis Hypo-Ashbyagossypii Hypo-Meyerozymaguilliermondii Hypo-Pichiaguilliermondii Hypo-Clavisporalusitaniae	FAEHAAHTENAWDRFRKFLLAYGIDDYISYYEAKAQNRREPPEPMKNLTNRPKR-PGVP FADENPTHTENAWDRYRKFLLTFGVDAYIAYYEIEBRASGREPKPMKNLTNRPKR-VNAP FGESHPTHTENAWDRFRKFLLSYGIDNYIYYYERBLGHGNDPEPMKNLTNRVKR-PGIP YADENPNHTENAWDRFRKFLLSYGIDNYITYETKEENGNEPEPEPMKNFTTRPKR-SALS FADANVSHSENAWDRFRKFLLTFGVDHYIEYFEQETNAGRKPPEPMKNLTNRPRR-KAGI FTENHPTHTESAWDRFRKFLLFGVDKYIEYYETQKANNDEPEAMKNLTIRTKR-DNFP FALEVPHTSENAWDRFRKFILFGIDSYSIISYYEKCMEEGIEPESIKNMTNRPKR-EG-P YGEKYPHSSENAWDRFRKFLLNYGIDEYIAYYENEQAHNRVPEPEPMKNMTNRVKR-PG-P LAKTNPMHTPNWSRDRYRKFVSRYGAKKYIDYYDKVTASGGVPEPIKGDSPTAKAIK-- LAKTNPMHTPNWSRDRYRKFVSRYGAKKYIDYYDKVTASGGVPEPIKGDSPTAKAIKQL YARLHPQHSSSWRDRYRKFARVYGLQKYRDYLLREKDSKEGPQPMKNLTSRASK-EKKK
Rap1-Saccaromycescerevisiae Rap1-Saccharomycesdaiренensis Rap1-Zygosaccharomycesrouxii Rap1-Lachanceathermotolerans] Hypo-Vanderwaltozymapolyspora Rap1-Naumoviаcastellii hypo-Candidaglabrata Hypo-Kluyveromyceslactis Hypo-Ashbyagossypii Hypo-Meyerozymaguilliermondii Hypo-Pichiaguilliermondii Hypo-Clavisporalusitaniae	TPGNYNSAAKRARN- TPGNYNSSVKRAR-- TPGNYNSA-KK---- TPGNYNSFAKKVK-- APGNYGSYVKILK-- TPGNYNSAIKRQR-- TPGNYGNAAKRQK-- SPGNYNTTLKKS-- APGNYNN-AKK--- -----Q- IGSNY---RKDTQS IENN--RRMKK-

- Aono, S., Hartsch, T. & Schulze-Gahmen, U. (2003). *Acta Cryst. D***59**, 576-579.
- Escalante, C. R., Shen, L., Escalante, M. C., Brass, A. L., Edwards, T. A., Singh, H. & Aggarwal, A. K. (2002). *J. Struct. Biol.* **139**, 55-59.
- Genis, C., Scone, P., Kasahara, H. & Nam, H. J. (2008). *Acta Cryst. F***64**, 1079-1082.
- Hirsch, J. A., Wah, D. A., Dorner, L. F., Schildkraut, I. & Aggarwal, A. K. (1997). *FEBS Lett.* **403**, 136-138.
- Horton, N. C., Dorner, L. F., Schildkraut, I. & Perona, J. J. (1999). *Acta Cryst. D***55**, 1943-1945.
- Hovde, S., Brooks, A., Strong, K. & Geiger, J. H. (2002). *Acta Cryst. D***58**, 511-512.
- Imasaki, T., Hashimoto, H., Shimizu, T., Kato, M., Tsuda, J., Kita, K. & Sato, M. (2004). *Acta Cryst. D***60**, 1165-1166.
- Kapetaniou, E. G., Kotsifaki, D., Providaki, M., Rina, M., Bouriotis, V. & Kokkinidis, M. (2007). *Acta Cryst. F***63**, 12-14.
- Larivière, L., Kurzeck, J., Aschke-Sonnenborn, U., Rüger, W. & Moréra, S. (2002). *Acta Cryst. D***58**, 1484-1486.
- Lu, P., Li, Y., Gorman, A. & Chi, Y. I. (2006). *Acta Cryst. F***62**, 525-529.
- Ng, C. K., Palasingam, P., Venkatachalam, R., Baburajendran, N., Cheng, J., Jauch, R. & Kolatkar, P. R. (2008). *Acta Cryst. F***64**, 1184-1187.
- O'Loughlin, T. J., Xu, Q., Kucera, R. B., Dorner, L. F., Sweeney, S., Schildkraut, I. & Guo, H. C. (2000). *Acta Cryst. D***56**, 1652-1655.
- Pereira, J. H., Ha, S.-C. & Kim, S.-H. (2008). *Acta Cryst. F***64**, 175-178.
- Pereira de Jésus, K., Serre, L., Hervouet, N., Bouckson-Castaing, V., Zelwer, C. & Castaing, B. (2002). *Acta Cryst. D***58**, 679-682.
- Pio, F., Ni, C. Z., Mitchell, R. S., Knight, J., McKercher, S., Klemsz, M., Lombardo, A., Maki, R. A. & Ely, K. R. (1995). *J. Biol. Chem.* **270**, 24258-24263.
- Redondo, P., Prieto, J., Ramos, E., Blanco, F. J. & Montoya, G. (2007). *Acta Cryst. F***63**, 1017-1020.
- Richardson, J. M., Finnegan, D. J. & Walkinshaw, M. D. (2007). *Acta Cryst. F***63**, 434-437.
- Sam, M. D., Abbani, M. A., Cascio, D., Johnson, R. C. & Clubb, R. T. (2006). *Acta Cryst. F***62**, 825-828.
- Sam, M. D., Cascio, D., Johnson, R. & Clubb, R. T. (2003). *Acta Cryst. D***59**, 1238-1240.
- Schwartz, T., Shafer, K., Lowenhaupt, K., Hanlon, E., Herbert, A. & Rich, A. (1999). *Acta Cryst. D***55**, 1362-1364.
- Shanmuganatham, K. K., Ravichandran, M., Howe, M. M. & Park, H.-W. (2007). *Acta Cryst. F***63**, 620-623.
- Suwa, Y., Nakamura, T., Toma, S., Ikemizu, S., Kai, H. & Yamagata, Y. (2008). *Acta Cryst. F***64**, 171-174.
- Tahirov, T. H., Inoue-Bungo, T., Sasaki, M., Fujikawa, A., Kimura, K., Sato, K., Adachi, S., Kamiya, N. & Ogata, K. (2001). *Acta Cryst. D***57**, 854-856.
- Tamulaitiene, G., Grazulis, S., Janulaitis, A., Janowski, R., Bujacz, G. & Jaskolski, M. (2004). *Biochim. Biophys. Acta*, **1698**, 251-254.
- Tan, S., Hunziker, Y., Pellegrini, L. & Richmond, T. J. (2000). *J. Mol. Biol.* **297**, 947-959.
- Textor, L. C., Wilmanns, M. & Holton, S. J. (2007). *Acta Cryst. F***63**, 657-661.

- Vassylyeva, M. N., Svetlov, V., Klyuyev, S., Devedjiev, Y. D., Artsimovitch, I. & Vassylyev, D. G. (2006). *Acta Cryst. F***62**, 1027-1030.
- Viadiu, H., Kucera, R., Schildkraut, I. & Aggarwal, A. K. (2000). *J. Struct. Biol.* **130**, 81-85.
- Viadiu, H., Vanamee, E. S., Jacobson, E. M., Schildkraut, I. & Aggarwal, A. K. (2003). *Acta Cryst. D***59**, 1493-1495.
- Vivian, J. P., Porter, C., Wilce, J. A. & Wilce, M. C. (2006). *Acta Cryst. F***62**, 1104-1107.
- Vivian, J. P., Wilce, J. A., Hastings, A. F. & Wilce, M. C. (2001). *Acta Cryst. D***57**, 421-424.
- Watanabe, S., Kita, A., Kobayashi, K., Takahashi, Y. & Miki, K. (2006). *Acta Cryst. F***62**, 1275-1277.