

		α_D1	α_D2	α_D3	β_D1	β_D2	
		hhhhhhhhhhhhhh	hhhhhhh	hhhhhhhhhhhhhh	ssss	ssss	
DasR (S.c.)	1	-----MSTDVSSA-ENEGGATVRTARVPKYRLKHLDDMT--RTQTPGTPVPPERTLAAEFDTSRRTTVRQALQELVVEGRLERIQGKGFVA-KPK					88
PhnF (M.s.)	1	-----MTAGAA---PRILKHQVVRaelDRML--DGMRIgDPPFAEREIAEQFEVARETVRQALRELLIDGRVER-RGRTTVVA-RPK					75
NagR (B.s.)	1	-----MNINKQSPIPIIYQIMEQLKTQIKNGELQPDMLPSEREYAEQFGISRMTVRQALSNLVNEGLLYRLKGRGTFVS-KPK					78
ScuR (S.c.)	1	-----MSLDLSVDRSSPVPLYFQLSQQLEAAIEHGALTPGSLGNETELAARLGLSRPTVRQAIQSLVDKGLLVRRRGVGTQVV-HSK					82
PsuR (P.s.)	1	-----MPTPPA---ASSLAAQMGESpAPLYARVKHMIALQIQNGTWPPHHRVPSESELVTQLGFSRMTINRALRELTVEGLLVRMQGVGTQVVA-EPK					88
CguR (C.g.)	1	-----MTTEAPIWPAELFEDLDRNGPIPLYFQVAQRLEDGIRSGVLPGARLENEISVAKHLNVSRTPTVRRAIQEVVDKGLLVRRRGVGTQVV-QSH					91
BbuR (B.b.)	1	MAEARPDSLTRSRAAKPA-----GEGAAFSPLYRQIKELLVQSLDRGEWKPGELIPSEIDLAAARFQVSQGTVRKAVDELAEEHLLRRQGKGFVA-THH					94
EfuR (E.f.)	1	-----MVQNIPIYIQIHDKIKEDIKGVWSIGDRLPSERELALKFDVSRMTLRQAIQTLADEGILERKIGSGTYVA-RKK					74
YurK (B.s.)	1	-----MLNNGSSTPLYIQLKQIITDDIKKGVYSPtakLPENELCTKYNVSRITVRKALDLVEEGYLIRQQGKGFVK-SPK					77
PhnF (E.c.)	1	-----MHLSTHPTSYPTRYQEIAAKLEQELR-QHYRCGDYLPaeQQLAARFEVNRHTLRRaidQLVEKGVQRRQGVGLVL-MRP					79
SauR (S.a.)	1	-----MTFGEQPAYLRVAGDLRKKIVDGSLLPpHTRLPSQARIREEYGVSDTVALEARKVLMAEGLVEGRSGSGTYVR-ERP					75
EcuR (E.c.)	1	-----MRAMKSLSKSSQIPLYQVVEWIRESIYTGDLVEDDRIPSEYQIMDMLEVSRGTVKKAVAQLVKEGVLIQVQGKGFVK-KEN					82
TreR (B.s.)	1	-----MKVNFITIIYKDIAQQIEGGRWKAEEILPSEHELTAQYGTSRRETVRKALHMLAQNGYIQKIRGKGSVVLNREK					73
StuR (St.a.)	1	-----MLKYEHIAKQLNAFIHQSNFKPGDKLPNVTQLKERYQVSKSTIIKALGLLEQDGLIYQAQGSQTYVR-NIA					70
BcuR (B.c.)	1	-----MASGSTQVKYLGIIYQKMKQQILDGEYKINEKIPSSPILAEFGVSVLTIKKALDLLVRDGYIIRRRGSGTVVQ-DWR					76
YydK (B.s.)	1	-----MLKYQQIATEIETYIEEHQLQQGDKLPVLETLMAQFEVSKSTIITKSLELLEQKGAIFQVRGSGIFVR-KHK					70
BauR (B.a.)	1	-----MASGSTQVKYLGIIYQKMKQQILDGEYKINEKIPSSPVLAEFGVSVLTIKKALDLLVRDGYIIRRRGSGTVVQ-DWR					76
TraR (S.p.)	1	-----MAYRAQGAGYADVAEHYRSRIKAGELAPGDALPSVTDIRQQFDVAAKTVSRALAVLKRVLVTSRGALGTVVA-KSP					76

Residues of NagR involved in DNA binding

S4 Fig. Sequence alignment of structurally characterized members of the GntR/HutC transcription factor family. The sequence alignment was performed with CLUSTAL OMEGA [59] using the canonical protein sequences of the structurally characterized (full or partial) GntR/HutC family members specified in Supplemental Table S2. Secondary structure elements refer to the topology of DasR and are marked with (h) or (s) for α -helices and β -strands, respectively. For a detailed classification, the familiar nomenclature $\alpha_{D/E}$ and $\beta_{D/E}$ is used. Residues involved in DNA binding in NagR [11] and effector binding in DasR or NagR are highlighted by a coloured background. Residues involved in of DNA and effector binding, e.g. those forming base-specific contacts with the DNA, or hydrogen bonds as well as hydrophobic and CH/ π interactions with the phosphorylated sugar, are additionally marked by a black arrow.

	β^*/α^*	α_1	β_1	α_2	β_2	β_3	α_3	α_4	
	****	hhhhhhhh	s-----ssssssssss-s	hhhhhhh	ssssssssss	ssssssssshh-h	hhhhh		
DasR (S.c.)	89	VSQAL---QLTSYTEDMRAQGLEP-----TSQLLDIGYI-TADDRLAGLLDITAGGRVLRIERLRMANGEPMAIETTHLSAK-RFPALRRSLV--KYT	174						
PhnF (M.s.)	76	IRQPL---GMGSYTEAAKAQGLSA-----GRILVAWSDL-TADEVLAVGLVGVDPVQLQERVLTTDGVVVGLETTKLPAQ-RYPGLRETFD--HEA	161						
NagR (B.s.)	79	MEQAL---QGLTSFTEDMKSRGMTP-----GSRLIDYQLI-DSTEELAAIILGCGHPSSIHKITRVRRLANDIPMAIESSHIPFE-LAGELNESH---FQS	164						
ScuR (S.c.)	83	VRRPL---ELSSLYDDLEAAGQRP-----ATKVLVNTVV-PATAEIAAALGVAEDSEVHRIERLRLTHGEPMAYLCNYLPPG-LVDLDT-GQL--EAT	167						
PsuR (P.s.)	89	SQSAL--FEVHNIADIAARGHRH-----TCKVMVLKEE-AAGSERALALDMREGQRVVFHSLIVHFENDIPVQIEDRFVNAQ-VAPDYLKQDF--TLQ	175						
CguR (C.g.)	92	VTRPV---ELTSFFNDLKNANLDP-----KTRVLEHRL-LAASSAIAEKLGVSADEVLLIRRLRSTGDI PVAILENYLPPA-FNDVSL-DEL--EKG	176						
BbuR (B.b.)	95	EARVR--YRFLRLAPDEEGEGGRA-----ESRILECRRL-RAPAEIARALELRAGETVVTIRRLQSMNHMPTVIDDLWLPGT-HFRGLTLELLTASKA	183						
EfuR (E.f.)	75	VQETM--TGTTSETEITLSQNRVP-----SSRTVSYFVA-KPSSSEMELQLGPEDSLRLMERIRFADDIPICFEVASIPYS-LVSQYKSE---ITN	160						
YurK (B.s.)	78	LKREL--IAVNGYSEFMESTGKKP-----KHHVLSHDI-I-PASKPIAEKLIQPEPVPVELKRIILYNDDQPLTFEVTHYPLD-LVPGIDTFIA--DGV	164						
PhnF (E.c.)	80	FDYPL--NAQAREFQNLDDQGSHP-----TSEKLLSVLR-PASGHVADALGITEGENVIHLRLTRRVNGVALCLIDHYFADLTWPTLQ--RF--DSG	165						
SauR (S.a.)	76	VPRRV---ARSGYRFDGATPFRQEQADGAVRGTWESHSEQAEASGAIAERLDIRPGERVMCTKYVFRDAGEVMMSTWEPLA-VTGRTPVMLP--EEG	169						
EcuR (E.c.)	83	VAYPL-GEGLLSFAESLESQKIHF-----TTEVITSRIE-PANRYVAEKLRIPTGQDILYLERLRSIGDEKAMLIENRINIE-LCPGIVEIDF--NQH	170						
TreR (B.s.)	74	MQFPV--SGLVSPKELAQTLGKET-----KTTVHKFGLE-PPSELIQQLRANLDDDIWEVIRSRKIDGHEVILDKDYFFRK-HVPHLTKEI---CEN	159						
StuR (St.a.)	71	DANRINVKTNQFSKSLG--EHRM-----TSKVLVFKEMATPPKSVQDELQNLADDTVYYLERLRFVDDDLVLCIEYSYHKE-IVKYLNDI---AKG	157						
BcuR (B.c.)	77	QQEKA--RMIQTLTGTKAVYGSEV-----ESKIEFTIV-GADEIAEKLGISVGFVYKIRLRIIHSIPTIMEHTWMPIS-VIPGVEASV---LEE	162						
YydK (B.s.)	71	RKGYISLLSQGFKKDL--DFNV-----TSKVELDVR-KPTPEAAENLNIEMDEDIYYKRVRYINGQTLCEESYTKS-IVTYLNNEI---VSH	156						
BauR (B.a.)	77	QQEKA--RMIQTLTGTKAVYGSEV-----ESKIEFTIV-GADEIAEKLGISVGFVYKIRLRIIHSIPTIMEHTWMPIS-VIPGVEASV---LEE	162						
TraR (S.p.)	77	IVITG----ADRLDRMAKNGKRYAPGETSSGHRVMQRS---VYDPEVCAALDLEPGDEAVIRIRVFRQDDKPSVGVSVYPPH-TVAAVPELGQ---DER	165						
		α_5	β_4	α_6	β_5	β_6	β_7		
		h--hhhhh--h	ssssssssss	hhhhhhh	ssssssssss	ssssssssss	ssssss		
DasR (S.c.)	175	SI--YALAE--VYDVHLAEAEETIETSLATPREAGLLGTDVGL---PMLMSRHSYDR-TGQPVWVRSVYRG-DRYKFVARLKRQD----	254						
PhnF (M.s.)	162	SI--YAEIRS---RGIATRTRVTDIDTALPDAREALLGADART---PMLLNRSYDQ-DDVAIEQRRSLYRG-DRMTFTAVMHAKNSAIVS	244						
NagR (B.s.)	165	SI--YDHIER--YNSIPISRAKQLEPSAATTEEANILGIQKGA---PVLLIKRTTYLQ-NGTAFEHAKSVYRG-DRYTFVHYMDRLS-----	243						
ScuR (S.c.)	168	GI--YRLMRA---AGITLHSARQSIGARAATSGEAERLGEDAGA---PLLTMERITTFDD-TGRAVEFGTHTYRP-SRYSFEFQLLVRP-----	245						
PsuR (P.s.)	176	TP--YAYLSQ---VAPLTEGEHVVEAIIAEADECKLLQIDAGE---PCLLIRRTWS--GRQPVTAAARLIHPG-SRHRLEGRFTK-----	249						
CguR (C.g.)	177	GI--YDALRS---RGVVLKIANQKIGARRAVGEESTLLDIEDGG---PLLTVERVALDN-SGQVIELGSHCYRP-DMYNFETTLVAR-----	253						
BbuR (B.b.)	184	PI--YGLFES--EFGVSMVRADEKLRAVAASPEIAPLLGVEPGR---PLLVDRISYTY-GDRPMEVRRGLYLT-DHYHYRNSLN-----	259						
EfuR (E.f.)	161	SF--YKTLA--KSGHKIGHSNQTI SAVQASEQIAEYLEIKRGD---AILRVQVSYFE-NGLPFEYVRTQYAG-SRFEFYLEK-----	235						
YurK (B.s.)	165	SM--HDILKQ--QYKVVPTHNTKLLNVVYAQQEESKYLDLDCIDG---ALFEIDKTAFTS-NDQPIYCSLFLMHT-NRVFTTINSPYT-----	242						
PhnF (E.c.)	166	SI--HDFLRE--QTGIALRRSQTRISARRAQAKECQRLEIPNMS---PLLCVRTLNRHDGESSPAEYSVSLTRA-DMIEFTMEH-----	241						
SauR (S.a.)	170	PVGGMGVYERMAAIDVIVDNTVEVGARPLAEELLTLGGVPGH---VVLVIQRTYF-A-SGRPVETADVVPVPA-DRYRVAYHLPVK-----	250						
EcuR (E.c.)	171	NI--FPTIES--LSKRKIRYSESRYAARLIGNERGHFLDISEDA---PVLHLEQLVFFS-REL PVEFGNVWLKG-NKYVLGTVLQRRELS---	251						
TreR (B.s.)	160	SI--YEYIEG--ELGLSISYAQKEIVAEPCTDEDRELLDLRGYD---HMVVVRYNYVLE-DTSLFQYTESRHL-DKFRFVDFARRGK-----	238						
StuR (St.a.)	158	SI--FDYLES--NMKLRIGFSDIFFNVDKLTSSEASLLQLSTGE---PCLRVHQTFTYM-TGKPFDDSSDIVFHY-RHAQFYIPSKK-----	234						
BcuR (B.c.)	163	SI--YSYIQN--KGLKVGTSVVRVKGIRPDDKEKQFMNLTNQD---FLMRVEQVAYLT-DGRTFEYSYADHLP-ETFEFETVITAKSYKEA-	245						
YydK (B.s.)	157	SI--FHYIRE--GLGLKIGFSDLFLHVGQLNEEEAEYLGLEAGL---PKLYTESIFHLT-NGQPFYDYSKISYNY-EQSQFVVQANSFLL----	236						
BauR (B.a.)	163	SI--YSHIQN--KGLQVGTSVVRVKGIRPDDKEKQFMNLTNQD---FLMRVEQVAYLT-DGRTFEYSYADHLP-ETFEFETVITAKSYKEA-	245						
TraR (S.p.)	166	MVAQFDQLYT-ERTGREVVKGQRTAHARQASQDELAALDAPPASHAVMVTVTVTFHD-DERALGYWEDVYAPGARVPMGE-----	245						

Residues of DasR or NagR involved in the binding of potential effectors GlcN-6-P and GlcNAc-6-P
Residues of GntR/HutC family members that might additionally/alternatively be involved in the phosphate moiety coordination of phosphorylated effectors

S4 Fig. Sequence alignment of structurally characterized members of the GntR/HutC transcription factor family (continued)