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Supporting information for article:

Structural insight into DNA recognition by bacterial transcriptional regulators of the SorC/DeoR family

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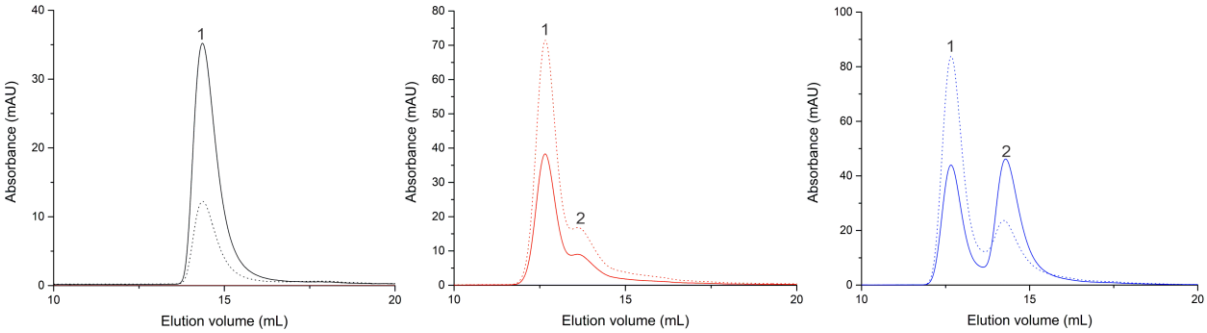
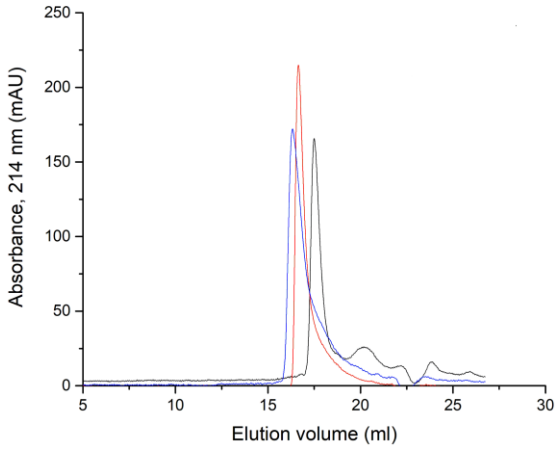


Sample	*bs*DeoR$_{DBD}$	O_{15} DNA		*bs*DeoR/O_{15} complex	
Peak	1	1	2	1	2
Theoretical MW_{theor}	6.28 kDa	9.14 kDa		NA	
Apparent MW_{app}[a]	12.31 kDa	NA		NA	12.7 kDa
Assembly[b]	dimer	NA		NA	dimer
Elution volume	14.36 ml	12.7 ml	13.6 ml	12.66 ml	14.28 ml
$A(280)_{max}$	35.20	38.3	9.02	43.97	46.18
$A(260)_{max}$	12.23	71.4	16.8	83.88	23.65
$A(280)_{max}$/ $A(260)_{max}$	2.88	0.54	0.54	0.52	1.95

[a] $MW_{app} = 3{,}735 \times e^{-0.398 \times V_e}$

[b] Assembly = MW_{theor}/MW_{app}

Figure S1 Size exclusion chromatography analysis of (a) *bs*DeoR$_{DBD}$, (b) O_{15} oligonucleotide, (c) *bs*DeoR$_{DBD}$/O_{15} complex. The absorption profiles at 280 nm and 260 nm are shown in solid and dashed line, respectively. Peak 1 in the chromatogram (c) represents the elution of unbound DNA. Inferring from the A280/A260 ratio and the slight shift in elution volume, peak 2 indicates protein/DNA formation. Peak 2 in the chromatogram (b) was evaluated because of the control of the DNA purity.



Sample	*bs*CggR$_{DBD}$	O_L DNA	*bs*CggR/O_L complex
Theoretical MW_{theor}	10.92 kDa	9.14 kDa	30.98 kDa
Apparent MW_{app}[a]	22.42 kDa	NA	39.99 kDa
Assembly[b]	dimer	NA	tetramer
Elution volume	17.49 ml	16.65 ml	16.33 ml

[a] $MW_{app} = 10^{(-0.2167 \times V_e + 8.1407)}$

[b] Assembly = MW_{theor}/MW_{app}

Figure S2 Size exclusion chromatography analysis of *bs*CggR$_{DBD}$, O_L 16bp oligonucleotide (DNA) and *bs*CggR$_{DBD}$/O_L complex. The colour code of the chromatogram profiles is indicated in the table.

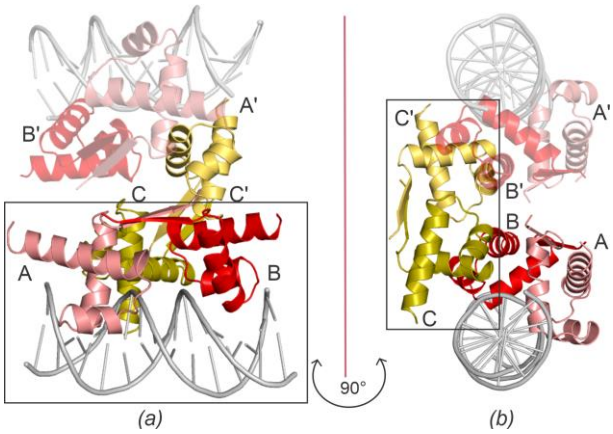


Figure S3 Representation of the composition of two asymmetric units connected via the monomers from each unit that form DNA-free dimer (C and C'). (a) A front view. The DNA-bound biological unit is framed with a rectangle. (b) A side view. The DNA-free dimer is framed with a rectangle.

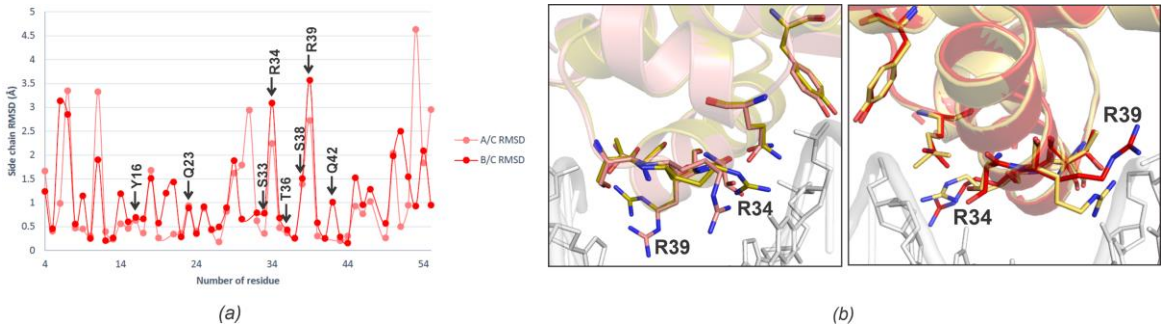


Figure S4 Superposition of the DNA-bound and unbound protein units. (a) Residual r.m.s.d. analysis calculated by Superpose program from the CCP4 package. Results of the superposition of chains A and C are in salmon, chains B and C in red. Positions of residues that contribute to the DNA binding are labelled. (b) A zoomed ribbon representation of the superposed DNA-bound and DNA-free states. DNA-recognition residues are distinguished as sticks, base-interacting residues are labelled.

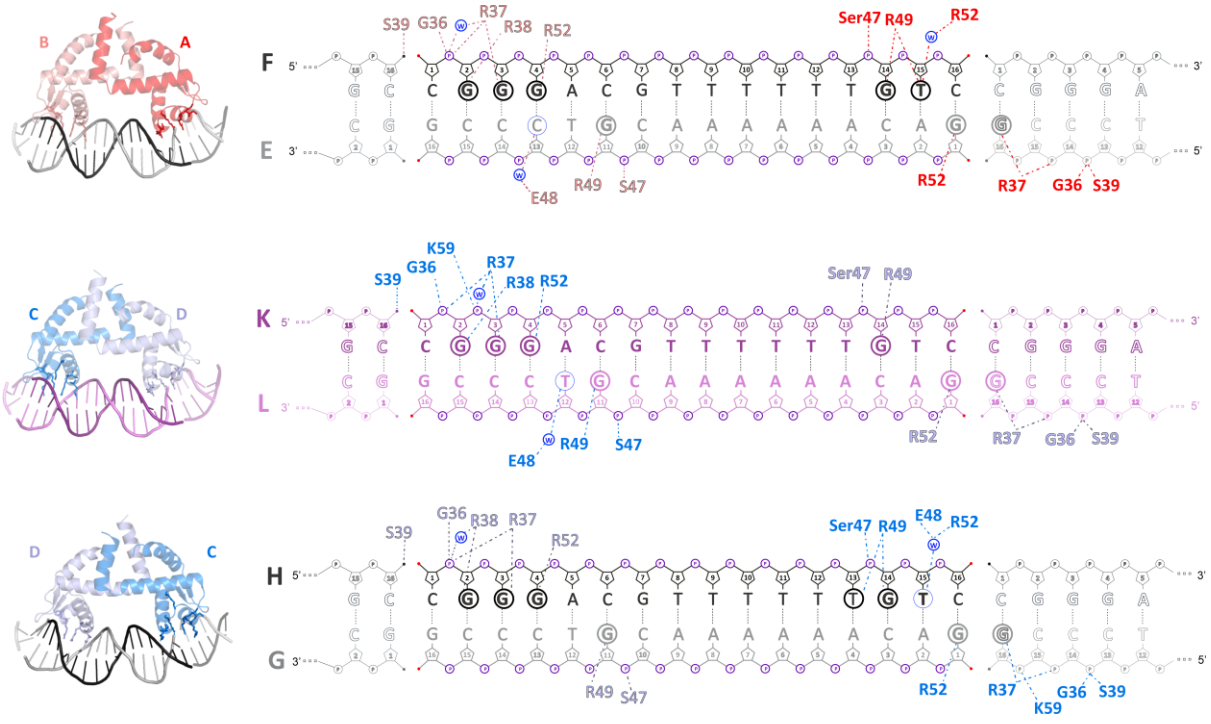


Figure S5 Schematic diagrams of *bs*CggR$_{DBD}$/O$_L$ interactions of all DNA conformers present in the asymmetric unit. GH and KL DNA duplexes in complex with the CD dimer were found as alternative conformers A and B, respectively. Scheme of the direct and indirect *bs*CggR$_{DBD}$/O$_L$ interactions based on the PISA and NUCPLOT analyses. Nucleotides interacting with the protein via bases are circled. Direct and indirect interactions of residues from monomer A and B are displayed in red and salmon, respectively, corresponding to panel a. Water molecules are indicated as a circled "W". The scheme was generated by the NUCPLOT program (Luscombe *et al.*, 1997) and subsequently adjusted.

Figure S6 Superposition of the *bs*CggR$_{DBD}$/O$_L$ (orange shades) and RosR/DNA (purple). RosR from *Halobacterium salinarum* (6QFD, (Kutnowski *et al.*, 2019) is a member of MarR/PadR family.

Table S1 *bs*DeoR$_{DBD}$ oligonucleotide designs used in crystallization trials.

DNA	Sequence	Bases
O_{18}	5' - ATTGAACAAAATTTCAAT 3' - TAACTTGTTTTAAAGTTA	18
O_{16+1}	5' - TTGAACAAAATTTCAA 3' - TAACTTGTTTTAAAGTT	16/17
O_{15+2}	5' - TGAACAAAATTTCAA 3' - TAACTTGTTTTAAAGTT	15/17
O_{15} overhang	5' - TGAACAAAATTTCAA 3' - TAACTTGTTTTAAAG	15
O_{10}	5' - CGATTGAAGC 3' - GCTAACTTCG	10
O_9 overhang	5′ - ATTGAACAA 3′ - TTAACTTGT	9
O_{32}[a]	5' - ATTGAACAAAA□TTCAAATTGAACAAAA□TTCAA 3' - TAACTTGTTTT□AAGTTTAACTTGTTTT□AAGTT	32
O_{30}[a]	5' - TTGAACAAAA□TTCAATTGAACAAAA□TTCAA 3' - AACTTGTTTT□AAGTTAACTTGTTTT□AAGTT	30
O_{16b}[a]	5' - ATTGAACAAAA□TTCAA 3' - TAACTTGTTTT□AAGTT	16
O_{15}[a]	5' - TTGAACAAAA□TTCAA 3' - AACTTGTTTT□AAGTT	15
O_15b	5' - TTGAACAAAATTTCA 3' - AACTTGTTTTAAAGT	15
O_{13}[a]	5' - TGAACAAAA□TTCAA 3' - ACTTGTTTT□AAGTT	13
O_{17a}	5' - ATTGAACAAAA□TTCAA 3' - TAACTTGTTTT□AAGTT	17
O_{17b}	5' - TTGAACAAAATTTCAAT 3' - AACTTGTTTTAAAGTTA	17
O_{16b}	5' - ATTGAACAAAATTTCA 3' - TAACTTGTTTTAAAGT	16
O_{2x17a}	5' - ATTGAACAAAATTTCAAATTGAACAAAATTTCAA 3' - TAACTTGTTTTAAAGTTTAACTTGTTTTAAAGTT	34
O_{17c}	5' - AATTTACATATGTTCAA 3' - TTAAATGTATACAAGTT	17

[a] Symbol □ is used for places where a nucleotide from operator sequence was deleted in the design.

Table S2 *bs*CggR$_{DBD}$ oligonucleotide designs used in crystallization trials.

DNA	Sequence	Base pairs
Derived from O_R		
O_{R16}	5' - CGGGACATATAATGTC 3' - GCCCTGTATATTACAG	16
O_{R18}	5' - GCGGGACATATAATGTCC 3' - CGCCCTGTATATTACAGG	18
O_{R16} overhang	5' - GCGGGACATATAATGTC 3' - GCCCTGTATATTACAGC	17
O_{R17}	5' - CGGGACATATAATGTCC 3' - GCCCTGTATATTACAGG	17
O_{R19}	5' - GCGGGACATATAATGTCCA 3' - CGCCCTGTATATTACAGGT	19
Derived from OL		
O_{L16}	5' - CGGGACGTTTTTTGTC 3' - GCCCTGCAAAAAACAG	16
O_{L18}	5' - ACGGGACGTTTTTTGTCA 3' - TGCCCTGCAAAAAACAGT	18

Table S3 Volumes and concentrations of loaded samples for size exclusion chromatography

Column type	Superdex 75 Increase GL 10/300			Superdex 200 Increase GL 10/300		
Flow rate	0.8 ml/min			0.5 ml/min		
Sample	***bs*DeoR$_{DBD}$**	**O_{15}**	***bs*DeoR$_{DBD}$/O_{15}**	***bs*CggR$_{DBD}$**	**O_L**	***bs*CggR$_{DBD}$/O_L**
Volume [µl]	50	30	30	100	100	100
Concentration [µM]	54	57.6	106.3/57	140	70	131.6/68.4

Supplementary table S4
Overview of bsDeoRDBD protein/protein interactions identified by PISA server.
Only biologically relevant interactions are included. The crystal contacts and interaction of the expression tag's remnant sequence were omitted.

***bs* DeoRDBD chain A**			***bs* DeoRDBD chain B**				***bs* $DeoR_{DBD}$ atom**		
***bs* $DeoR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	***bs* $DeoR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	**Interaction type[b]**	**chain A**	**chain B**	**Distance (Å)[c]**
Ile10	α1	61.1	Met55	β1	53.4				
Ala13	α1	100.0	Val54	β1	65.9				
Arg14	α1	23.3	Met55	β1	53.4	HB/SB	NH2	O	2.83
Arg14			Met55			SB	NH2	OXT	3.61
Arg14			Met55			HB/SB	NE	OXT	3.06
Arg14			Met55			SB	NE	O	3.78
Tyr17		52.1	Ile52		62.2				
Tyr49	loop3	67.3	Met55		53.4	HB	O	N	3.02
Val50	β1	85.8	Ile52		62.2				
Gln51		24.8	Arg53		23.8	HB	O	N	3.10
Gln51			Arg53			HB	N	O	3.04
Ile52		63.5	Val50		82.2				
Arg53		29.2	Gln51		64.0	HB	O	N	2.84
Arg53			Gln51			HB	O	NE2	3.60
Arg53			Gln51			HB	N	O	3.06
Val54		92.1	Ala13	α1	100.0				
Val54			Arg14		23.3				
Met55		52.6	Ile10		61.1				
Met55			Gln51	β1	64.0	HB	O	NE2	2.81
Met55			Tyr49		57.6	HB	N	O	2.80

***bs* DeoRDBD chain C**			***bs* DeoRDBD chain C'**				***bs* $DeoR_{DBD}$ atom**		
***bs* $DeoR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	***bs* $DeoR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	**Interaction type[b]**	**chain A**	**chain B**	**Distance (Å)[c]**
Ile10	α1	84.4	Met55	β1	51.3				
Ala13		100.0	Val54		65.7				
Arg14		27.0	Met55	β1	51.3	HB	NE	O	2.94
Arg14			Met55			HB	NH2	O	3.29
Arg14			Met55			HB	NH2	OXT	2.98
Tyr17		59.7	Lys45	α3	14.3	HB	O	NZ	3.71
Tyr49	loop3	65.5	Met55	β1	51.3	HB	O	N	2.94
Val50	β1	88.3	Ile52/Val54		69.0/65.7				
Gln51		29.8	Arg53		25.2	HB	N	O	2.84
Gln51			Arg53			HB	O	N	2.96
Ile52		70.2	Ile52		69.0				
Arg53			Ile52						
Arg53		25.0	Gln51		29.7	HB	N	O	2.96
Arg53			Gln51			HB	O	N	2.84
Val54		66.3	Ala13	α1	94.4				
Met55		51.3	Tyr49	loop3	66.2	HB	N	O	2.94
Met55			Arg14	α1	27.3	HB	O	NE	2.94
Met55			Arg14			HB	O	NH2	3.29
Met55			Arg14			HB/SB	OXT	NH2	2.98

[a] total solvent accesible area of a given residue, residues with BSA over 30% are listed

[b] HB and SB are acronyms for hydrogen bond and salt bridge, respectively

[c] for possible hydrogen bonds the distance between hydrogen bond donor and acceptor atoms are listed

Supplementary Table S5
***bs* DeoR$_{DBD}$/DNA interactions identified by PISA server and NUCPLOT**

bs DeoR$_{DBD}$ chain	*bs* DeoR$_{DBD}$ residue	Residue location	BSA[a] [%]	DNA chain	DNA residue	Hydrogen bond[b]	*bs* DeoR$_{DBD}$ atom	DNA atom	Sugar-phosphate backbone	Base	Distance (Å)
A	Tyr16	α1	34.1	**E**	T9	+	OH	OP1	1		2.43
	Ser22	loop1	53.8	**E**	T8						
	Gln23	α2	95.4	**E**	T9	+	N	OP2	1		2.85
				E	G10	+	NE2	OP2	1		2.92
	Ser33	loop2	77.7	**G**	G3	+	N	OP2	1		3.12
					G3	+	OG	OP2	1		2.44
	Arg34	α3	74.8	**E**	G10	+	NH2	O6		1	2.88
	Pro35	α3	87.6	**E**	T11						
	Thr36	α3	81.4	**G**	G3	+	OG1	OP2	1		2.40
	Ser38	α3	85.7	**E**	G10	+	OG	OP2	1		2.72
	Arg39	α3	63.3	**E**	T12	+	NH2	O4		1	3.04
				G	G3	+		O6		1	2.87
B	Lys5	α1	37.1	**E'**	A15	+	NZ	OP2	1		3.28
	Tyr16	α1	24.8	**G**	A10	+	OH	OP1	1		2.86
	Ser22	loop1	34.0	**G**	A10						
	Gln23	α2	95.9	**G**	A10	+	N	OP2	1		3.14
					T11	+	NE2	OP2	1		2.97
	Ser33	loop2	71.2	**E**	T2	+	N	OP2	1		3.04
	Arg34	α3	64.4	**G**	A10	+	NH2	N7		1	2.89
	Pro35	α3	87.4	**E/G**	T2/T11						
	Thr36	α3	90.0	**E**	T2	+	OG1	OP2	1		2.93
					T1	+	OG1	O5'	1		2.68
	Ser38	α3	96.0	**G**	T11	+	OG	OP2	1		2.67
	Arg39	α3	33.5	**E'**	A15	+	NH2	OP2	1		3.82
	Gln42	α3	31.5	**G**	T12	+	NE2	OP2	1		3.36
								Sum:	17	4	
									21		

E': symmetry related DNA strand E from the neigbouring asymmetric unit

[a] accessible surface area burried upon formation of protein/DNA complex, expressed as percentage of the total solvent accesible area of a given residue, residues with BSA over 30% are listed unless possible H-bond was detected

[b] for possible hydrogen bonds the distance between hydrogen bond donor and acceptor atoms are listed
DNA resiudes with major contribution to iteration are listed

Supplementary table S6
Overview of *bs* $CggR_{DBD}$ protein/protein interactions identified by PISA server.
Only biologically relevant interactions are included. The crystal contacts and interaction of the expression tag's remnant sequence were omitted.

***bs* $CggR_{DBD}$ chain A**			***bs* $CggR_{DBD}$ chain B**				***bs* $CggR_{DBD}$ atom**		
***bs* $CggR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	***bs* $CggR_{DBD}$ residue**	**Location**	**BSA[a] [%]**	**Interaction type[b]**	**chain A**	**chain B**	**Distance (Å)[c]**
Met1	α1	66.2	Met1	α1	90.2				
Gln3		55.6	Thr87	α5	95.3	HB	NE2	OG1	2.78
Leu4		100.0	Ile5	α1	50.4				
Ile5		34.8	Leu4		100.0				
Ala7		96.5	Leu84	α5	100.0				
Gln8		96.5	Gln8	α1	91.4	HB	OE1	NE2	2.83
						HB	NE2	OE1	2.86
Lys10		43.3	Arg22	α1	86.8				
			Leu80	α5	91.7				
Leu11	α1	100.0	Arg22	α2	86.8	HB	O	NH1	2.76
Leu12		100.0	Val18		61.6				
			Met19		99.8				
Pro13	α1	51.3	Phe57	α4	54.7				
Asp14	loop1	45.3	Arg22	α2	86.8	SB	OD1	NH1	3.00
						SB	OD1	NH2	3.71
						HB/SB	OD2	NH2	2.82
						SB	OD2	NH1	3.63
Leu15	α2	74.9	Val18		61.6				
Met19	α2	98.4	Leu12	α1	87.3				
Arg22	α2	48.0	Leu11	α1	100.0	HB	NH1	O	2.58
Phe23		34.7							
Leu26		100.0							
Phe57	α4	46.9	Pro13	α1	34.3				
Leu58	α4	100.0	Leu11	α1	100.0				
Gln61	α4	61.2	Lys10	α1	63.8	HB	O	NZ	2.96
						HB	NE2	O	3.05
Leu63	loop2	97.7	Leu11	α1	100.0				
Glu76	β2	12.5	Lys10	α1	63.8	SB	OE1	NZ	3.90
Leu80	α5	84.1	Leu11		100.0				
			Ala7		91.1				
Leu84	α5	100.0		α1					
Thr87	α5	60.1	Leu4	α1					

[a] accessible surface area burried upon formation of dimer, expressed as percentage of the total solvent accesible area of a given residue, residues with BSA over 30% are listed unless possible H-bond or Salt bridge were detected

[b] HB and SB are acronyms for hydrogen bond and salt bridge, respectively

[c] for possible hydrogen bonds the distance between hydrogen bond donor and acceptor atoms are listed

Supplementary Table S7
***bs* $CggR_{DBD}$/DNA interactions identified by PISA server and NUCPLOT**

bs $CggR_{DBD}$ chain	*bs* $CggR_{DBD}$ residue	Residue location	BSA[a] [%]	DNA chain	DNA residue	Hydrogen bond[b]	*bs* $CggR_{DBD}$ atom	DNA atom	Sugar-phospate backbone	Base	Distance (Å)
	Gly36	loop1	100.0	**E'**	C14	+	N	OP1	1		2.69
	Arg37	α3	85.0	**E'**	C15	+	N	OP2	1		2.85
				E'	G16	+	NH2	O6		1	2.75
	Arg38	α3	27.0	**E'**							
	Ser39	α3	44.8	**E'**	C14	+	N	OP2		1	3.06
	Ser47	loop3	30.9	**F**	G14	+	OG	OP1	1		2.58
A	Glu48	α4	26.9	**F**							
	Arg49	α4	81.1	**F**	G14	+	NH2	O6		1	2.58
				F	T15	+	NH2	O4		1	3.40
	Val50	loop3	50.9	**E/F**							
	Arg52	α4	45.7	**E**	G1	+	NH1	O6		1	2.89
	Lys59	α4		**E**							
	Ile66	β1	59.1	**E'**	C15						
	Thr68	loop5 (wing)	30.1	**E'/F'**	N/A						
	Gly70	loop5 (wing)	97.5	**E'**	C14						
	Met71	β2	65.3	**E'**	C15						
	Gly36	loop1	92.4	**F**	C1						
	Arg37	α3	93.2	**F**	G2	+	N	OP2	1		2.98
				F	G4	+	NH2	O6		1	3.75
				F	G3	+		O6		1	2.86
	Arg38	α3	50.2	**F**	G2	+	NH2	O6		1	2.81
	Ser39	α3	32.4	**F'**	C16	+	OG	O3'	1		3.18
B	Ser47	loop3	38.7	**E**	G11	+	OG	OP2	1		2.58
	Glu48	α4	39.9	**E**	T12/C13						
	Arg49	α4	70.8	**E**	G11	+	NE	O6		1	3.19
				E	G11	+	NH2	O6		1	2.95
	Val50	loop3	45.3	**E**	C10/G11						
	Arg52	α4	66.2	**F**	G4	+	NH1	O6		1	2.81
	Ile66	β1	61.7	**F**	G2						
	Gly70	loop5 (wing)	89.4	**F**	C1						
	Met71	β2	77.4	**F**	G2						
								Sum:	6	11	

bs $CggR_{DBD}$ chain	*bs* $CggR_{DBD}$ residue	Residue location	BSA[a] [%]	DNA chain	DNA residue	Hydrogen bond[b]	*bs* $CggR_{DBD}$ atom	DNA atom	Sugar-phospate backbone	Base	Distance (Å)
	Gly36	loop1	46.1	**G'**	C14	+	N				
	Arg37	α3	10.0	**G**	G1	+	NH2	O6		1	3.78
			42.9	**G'**	C15	+	N	OP2	1		3.01
				G'	G16	+	NH2	O6		1	2.72
	Arg38	α3	41.7	**G'**	C15/G16						
	Ser39	α3	40.4	**G'**	C13	+	OG	O3'		1	3.67
				G'	C14	+	OG	OP2	1		2.76
				G'	C14	+	N	OP2	1		3.30
	Ser47	loop3	32.2	**H**	G14	+	OG	OP2	1		2.63
C	Glu48	α4	40.8	**H**	C16						
	Arg49	α4	51.9	**H**	T13	+	NH1	O4		1	3.27
					G14	+		O6		1	3.01
	Val50	loop3	48.3	**H**	T13						
	Arg52	α4	33.9	**G**	G1	+	NH1	O6		1	2.99
	Lys59	α4	15.6	**G'**	G16	+	NZ	OP1	1		3.41
	Ile66	β1	50.4	**G'**	C15						
	Thr68	loop5 (wing)	37.6	**G'/H'**	C14/A5						
	Gly70	loop5 (wing)	50.0	**G'**	C14						
	Met71	β2	50.7	**G'**	C15						
	Gly36	loop1	42.3	**H**	C1/G2						
	Arg37	α3	45.8	**H**	G2	+	N	OP1	1		2.95
				H	G3	+	NH2	O6		1	2.63
	Arg38	α3	35.8	**H**	G2	+	NH2	O6		1	2.87
	Ser39	α3		**H'**	C16	+	OG	O3'	1		3.57
D	Ser47	loop3	35.0	**G**	G11	+	OG	OP2	1		2.41

	Glu48	α4	34.0	**G**	C13						
	Arg49	α4	48.6	**G**	G11	+	NH2	O6 (base)		1	2.69
				G	T12	+		O4 (base)		1	3.74
	Val50	loop3	50.5	**G**	C10,G11						
	Arg52	α4	42.7	**H**	G4	+	NH1	O6		1	2.85
	Ile66	β1	51.8	**H**	G2						
	Gly70	loop5 (wing)	48.8	**H**	C1						
	Met71	β2	44.2	**G**	G2						
								Sum:	8	11	

***bs* $CggR_{DBD}$ chain**	***bs* $CggR_{DBD}$ residue**	**Residue location**	**BSA[a] [%]**	**DNA chain**	**DNA residue**	**Hydrogen bond[b]**	***bs* $CggR_{DBD}$ atom**	**DNA atom**	**Sugar-phospate backbone**	**Base**	**Distance (Å)**
	Gly36	loop1	43.4	**K**	C1						
	Arg37	α3	47.0	**K**	G2	+	N	OP2	1		2.94
				K	G3	+	NH2	O6		1	2.78
				K	G4	+	NH2	O6		1	3.72
	Arg38	α3	38.1	**K**	G2	+	NH2	O6		1	2.95
	Ser39	α3	34.0	**K'**	C16	+	OG	O3'		1	3.27
	Ser47	loop3	38.8	**L**	G11	+	OG	OP2	1		2.52
C	Glu48	α4	40.1	**L**	T12, C13						
	Arg49	α4	48.1	**L**	G11	+	NE	O6		1	3.36
				L	G11	+	NH1	O6		1	3.25
	Val50	loop3	45.7	**L**	G11						
	Arg52	α4	47.4	**K**	G4	+	NH1	O6		1	2.88
	Lys59	α4	17.3	**K**	G3	+	NZ	OP1	1		3.07
	Ile66	β1	49.6	**K**	G2						
	Thr68	loop5 (wing)	16.3	**K/L**							
	Gly70	loop5 (wing)	50.0	**K**	C1						
	Met71	β2	49.3	**K**	G2						
	Gly36	loop1	46.7	**L'**	C14	+	N	OP1	1		2.95
	Arg37	α3	44.8	**L'**	C15	+	N	OP2	1		2.82
				L'	G16	+	NH2	O6 (base)		1	2.65
	Arg38	α3	44.2	**K'/L'**							
	Ser39	α3	37.6	**L'**	C13	+	OG	O3'	1		3.83
				L'	C14	+	N	OP2	1		3.34
				L'	C14	+	OG	OP2	1		2.90
D	Ser47	loop3	33.6	**K**	G14	+	OG	OP1	1		2.69
	Glu48	α4	28.9	K/L							
	Arg49	α4	51.4	**K**	G14	+	NH2	O6 (base)		1	2.56
				K	T15	+		O4 (base)		1	3.86
	Val50	loop3	49.5	**K/L**	C1/C15, G16						
	Arg52	α4	34.7	**L**	G1	+	NH1	O6 (base)		1	2.79
	Ile66	β1	48.2	**L'**	C15						
	Gly70	loop5 (wing)	51.2	**L'**	C14						
	Met71	β2	55.8	**L'**	C15						
								Sum:	9	11	

N': symmetry related DNA strands from the neigbouring asymmetric units

[a] accessible surface area burried upon formation of protein/DNA complex, expressed as percentage of the total solvent accesible area of a given residue, residues with BSA over 30% are listed unless possible H-bond was detected

[b] for possible hydrogen bonds the distance between hydrogen bond donor and acceptor atoms are listed

Supplementary references

Kutnowski, N., Shmulevich, F., Davidov, G., Shahar, A., Bar-Zvi, D., Eichler, J., Zarivach, R. & Shaanan, B. (2019). *Nucleic Acids Res* **47**, 8860-8873.
Luscombe, N. M., Laskowski, R. A. & Thornton, J. M. (1997). *Nucleic Acids Research* **25**, 4940-4945.