



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:48 PM UTC

PDB ID : 6Y93 / pdb_00006y93
Title : Crystal structure of the DNA-binding domain of the Nucleoid Occlusion Factor (Noc) complexed to the Noc-binding site (NBS)
Authors : Jalal, A.S.B.; Tran, N.T.; Stevenson, C.E.M.; Chan, E.; Lo, R.; Tan, X.; Noy, A.; Lawson, D.M.; Le, T.B.K.
Deposited on : 2020-03-06
Resolution : 2.23 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

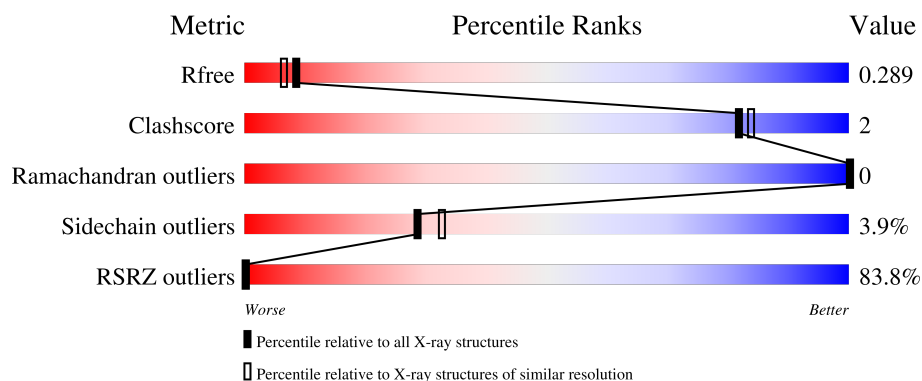
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	146	64% 64% 7% 28%
1	B	146	68% 74% 5% 21%
2	C	22	73% 95% 5%
2	D	22	59% 86% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2591 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein called Nucleoid occlusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			824	517	147	158	2			
1	B	116	Total	C	N	O	S	0	0	0
			871	549	151	169	2			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MET	-	initiating methionine	UNP P37524
A	243	LYS	-	expression tag	UNP P37524
A	244	LEU	-	expression tag	UNP P37524
A	245	ALA	-	expression tag	UNP P37524
A	246	ALA	-	expression tag	UNP P37524
A	247	ALA	-	expression tag	UNP P37524
A	248	LEU	-	expression tag	UNP P37524
A	249	GLU	-	expression tag	UNP P37524
A	250	HIS	-	expression tag	UNP P37524
A	251	HIS	-	expression tag	UNP P37524
A	252	HIS	-	expression tag	UNP P37524
A	253	HIS	-	expression tag	UNP P37524
A	254	HIS	-	expression tag	UNP P37524
A	255	HIS	-	expression tag	UNP P37524
B	110	MET	-	initiating methionine	UNP P37524
B	243	LYS	-	expression tag	UNP P37524
B	244	LEU	-	expression tag	UNP P37524
B	245	ALA	-	expression tag	UNP P37524
B	246	ALA	-	expression tag	UNP P37524
B	247	ALA	-	expression tag	UNP P37524
B	248	LEU	-	expression tag	UNP P37524
B	249	GLU	-	expression tag	UNP P37524
B	250	HIS	-	expression tag	UNP P37524
B	251	HIS	-	expression tag	UNP P37524
B	252	HIS	-	expression tag	UNP P37524

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Chain	Residue	Modelled	Actual	Comment	Reference
B	253	HIS	-	expression tag	UNP P37524
B	254	HIS	-	expression tag	UNP P37524
B	255	HIS	-	expression tag	UNP P37524

- Molecule 2 is a DNA chain called Noc Binding Site (NBS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total 448	C 215	N 82	O 130	P 21	0	0	0
2	D	22	Total 448	C 215	N 82	O 130	P 21	0	0	0

G1	G2	A3	T4	A5	T6	T7	T8	C9	C10	C11	G12	G13	A16	A17	T18	A19	T20	C21	C22
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.14Å 60.57Å 81.05Å 90.00° 116.88° 90.00°	Depositor
Resolution (Å)	72.30 – 2.23 72.30 – 2.23	Depositor EDS
% Data completeness (in resolution range)	38.1 (72.30-2.23) 38.1 (72.30-2.23)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.231 , 0.279 0.248 , 0.289	Depositor DCC
R_{free} test set	599 reflections (5.53%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2591	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	1.01	0/831	1.68	0/1122
1	B	1.04	0/878	1.72	0/1191
2	C	0.31	0/502	0.64	0/773
2	D	0.31	0/502	0.64	0/773
All	All	0.83	0/2713	1.38	0/3859

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	824	0	855	6	0
1	B	871	0	881	5	0
2	C	448	0	250	1	0
2	D	448	0	250	3	0
All	All	2591	0	2236	12	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:HIS:HB2	1:B:145:LEU:HD22	1.55	0.87
1:B:145:LEU:H	1:B:145:LEU:HD23	1.63	0.62
1:A:184:THR:OG1	2:D:13:DG:OP1	2.23	0.57
1:A:130:ILE:HG21	1:A:179:MET:HE2	1.91	0.51
1:B:167:LEU:HA	1:B:170:LEU:HD12	1.98	0.46
1:A:196:GLN:HB2	1:A:199:LEU:HD12	1.99	0.45
1:B:145:LEU:HD23	1:B:145:LEU:N	2.30	0.45
2:C:19:DA:C2	2:D:5:DA:C2	3.04	0.45
1:A:167:LEU:HA	1:A:170:LEU:HD12	2.00	0.44
1:B:172:GLN:N	1:B:173:PRO:CD	2.84	0.41
1:A:172:GLN:N	1:A:173:PRO:CD	2.83	0.41
1:A:184:THR:HG21	2:D:12:DG:H3'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	103/146 (70%)	98 (95%)	5 (5%)	0	100	100
1	B	114/146 (78%)	109 (96%)	5 (4%)	0	100	100
All	All	217/292 (74%)	207 (95%)	10 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/128 (70%)	84 (94%)	5 (6%)	19	18
1	B	90/128 (70%)	88 (98%)	2 (2%)	45	54
All	All	179/256 (70%)	172 (96%)	7 (4%)	28	33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ILE
1	A	152	GLN
1	A	154	LEU
1	A	156	LYS
1	A	184	THR
1	B	123	GLN
1	B	130	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	B	152	GLN

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 oligosaccharides 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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	105/146 (71%)	3.23	93 (88%) 0 0	133, 153, 170, 188	0
1	B	116/146 (79%)	3.35	100 (86%) 0 0	132, 153, 182, 194	0
2	C	22/22 (100%)	2.24	16 (72%) 0 0	136, 148, 156, 163	0
2	D	22/22 (100%)	2.01	13 (59%) 0 0	131, 148, 160, 165	0
All	All	265/336 (78%)	3.10	222 (83%) 0 0	131, 152, 176, 194	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	ALA	8.9
1	B	113	THR	8.1
1	B	142	LEU	6.8
1	B	122	LEU	6.4
1	B	227	GLN	6.1
1	A	127	LEU	5.9
1	B	228	GLY	5.9
1	B	195	LYS	5.5
1	B	117	ALA	5.5
1	B	225	LEU	5.5
1	A	209	GLU	5.4
1	B	121	ASN	5.3
1	B	116	VAL	5.3
1	B	196	GLN	5.2
1	A	139	LEU	5.2
1	A	196	GLN	5.2
1	A	199	LEU	5.1
1	B	125	GLU	5.1
1	B	222	VAL	5.0
1	A	138	ARG	5.0
1	A	146	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	127	LEU	5.0
1	A	226	GLU	4.8
1	B	172	GLN	4.8
1	B	224	MET	4.8
1	A	141	GLU	4.7
1	A	198	GLU	4.6
1	A	194	LEU	4.6
1	B	143	HIS	4.5
1	B	145	LEU	4.5
1	A	202	THR	4.5
1	B	140	LEU	4.5
1	A	222	VAL	4.5
1	A	195	LYS	4.4
1	A	144	ASP	4.4
1	A	185	GLU	4.4
1	B	144	ASP	4.4
1	B	202	THR	4.4
1	A	227	GLN	4.4
1	B	153	ARG	4.3
1	A	182	LYS	4.3
1	B	226	GLU	4.3
1	B	138	ARG	4.2
1	A	126	GLU	4.2
1	A	219	ASP	4.2
1	A	208	ILE	4.1
1	A	149	ALA	4.0
1	B	194	LEU	4.0
1	B	181	LYS	4.0
1	B	223	LYS	4.0
1	B	220	ARG	4.0
1	B	179	MET	3.9
2	C	22	DC	3.9
1	B	141	GLU	3.9
1	A	212	LEU	3.9
1	A	230	ARG	3.9
1	A	152	GLN	3.9
1	A	225	LEU	3.9
1	B	118	LEU	3.9
1	B	168	LEU	3.9
1	B	205	THR	3.9
1	A	181	LYS	3.8
1	B	126	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	209	GLU	3.8
1	B	169	LYS	3.8
1	A	145	LEU	3.8
1	A	159	SER	3.7
1	B	159	SER	3.7
1	B	182	LYS	3.7
1	A	213	ASN	3.7
1	A	140	LEU	3.6
1	A	193	PRO	3.6
1	A	148	GLU	3.6
1	B	176	GLU	3.6
1	B	198	GLU	3.6
1	A	216	GLN	3.6
1	A	228	GLY	3.6
1	A	167	LEU	3.6
1	B	199	LEU	3.6
1	B	212	LEU	3.6
1	A	210	LYS	3.6
1	A	179	MET	3.6
1	A	131	GLU	3.6
1	B	129	SER	3.5
1	B	173	PRO	3.5
1	B	152	GLN	3.5
2	C	1	DG	3.5
1	B	154	LEU	3.5
1	A	205	THR	3.5
1	A	201	VAL	3.5
1	B	115	SER	3.5
1	A	211	SER	3.4
1	A	204	LEU	3.4
1	A	229	GLN	3.4
1	B	180	GLU	3.4
1	B	146	THR	3.4
1	A	154	LEU	3.4
1	A	168	LEU	3.4
1	B	219	ASP	3.4
1	B	124	ARG	3.4
1	A	169	LYS	3.3
2	D	22	DC	3.3
1	A	197	PRO	3.3
1	A	223	LYS	3.3
1	A	142	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	153	ARG	3.3
1	B	119	ILE	3.2
1	B	200	GLN	3.2
1	B	165	LEU	3.2
1	B	137	ALA	3.2
1	B	148	GLU	3.2
1	A	135	ALA	3.2
1	A	184	THR	3.2
1	B	186	ARG	3.1
1	B	136	TYR	3.1
1	B	130	ILE	3.1
1	B	120	GLU	3.1
1	B	149	ALA	3.1
1	B	201	VAL	3.1
1	A	136	TYR	3.0
1	A	130	ILE	3.0
1	A	192	ILE	3.0
1	A	162	ALA	3.0
1	A	180	GLU	3.0
1	A	220	ARG	3.0
1	A	137	ALA	3.0
1	B	131	GLU	3.0
2	D	1	DG	3.0
1	A	163	ASN	2.9
1	B	197	PRO	2.9
1	A	143	HIS	2.9
1	A	207	ILE	2.9
1	B	183	ILE	2.9
1	A	206	GLU	2.9
1	A	173	PRO	2.9
1	A	190	ALA	2.9
1	B	207	ILE	2.9
1	B	204	LEU	2.8
1	B	160	THR	2.8
1	B	128	SER	2.8
1	B	123	GLN	2.8
2	C	2	DG	2.8
1	A	165	LEU	2.8
1	A	164	LYS	2.8
1	B	210	LYS	2.8
1	B	139	LEU	2.7
1	A	172	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	157	GLY	2.7
1	A	128	SER	2.7
1	B	166	ARG	2.7
1	A	129	SER	2.7
1	A	174	VAL	2.7
1	A	191	LEU	2.7
1	A	200	GLN	2.6
1	A	215	LYS	2.6
1	B	163	ASN	2.6
1	B	190	ALA	2.6
1	A	214	VAL	2.6
1	A	221	VAL	2.6
1	B	193	PRO	2.6
1	B	155	GLY	2.6
1	A	178	ILE	2.6
1	A	175	GLN	2.6
2	C	8	DT	2.6
1	A	217	THR	2.6
1	B	211	SER	2.6
1	B	175	GLN	2.5
1	B	203	LEU	2.5
1	B	189	ARG	2.5
1	A	160	THR	2.5
1	A	134	HIS	2.5
1	A	218	GLU	2.5
1	B	218	GLU	2.5
2	C	9	DC	2.5
1	B	208	ILE	2.5
2	D	9	DC	2.5
2	C	21	DC	2.5
1	B	156	LYS	2.4
1	B	216	GLN	2.4
1	A	189	ARG	2.4
1	B	178	ILE	2.4
1	B	134	HIS	2.4
2	D	7	DT	2.4
2	C	17	DA	2.4
1	B	133	ALA	2.4
1	B	135	ALA	2.4
1	A	203	LEU	2.4
1	B	187	HIS	2.4
2	C	15	DA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	184	THR	2.3
2	D	8	DT	2.3
1	A	187	HIS	2.3
1	B	150	LEU	2.3
1	B	214	VAL	2.3
2	D	10	DC	2.3
2	D	16	DA	2.2
1	A	150	LEU	2.2
2	C	16	DA	2.2
2	C	4	DT	2.2
2	C	20	DT	2.2
2	D	21	DC	2.2
1	A	166	ARG	2.2
2	C	7	DT	2.2
2	D	2	DG	2.2
1	B	161	ILE	2.1
2	C	18	DT	2.1
2	C	3	DA	2.1
1	B	171	PRO	2.1
2	D	20	DT	2.1
1	B	213	ASN	2.1
2	D	4	DT	2.1
1	A	170	LEU	2.1
1	A	183	ILE	2.1
1	A	171	PRO	2.1
1	B	177	ALA	2.1
1	B	206	GLU	2.1
1	A	155	GLY	2.1
1	A	177	ALA	2.0
2	C	14	DG	2.0
2	C	19	DA	2.0
2	D	18	DT	2.0
2	D	5	DA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.