



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:18 PM UTC

PDB ID : 1DUX / pdb_00001dux
Title : ELK-1/DNA STRUCTURE REVEALS HOW RESIDUES DISTAL FROM
DNA-BINDING SURFACE AFFECT DNA-RECOGNITION
Authors : Mo, Y.; Vaessen, B.; Johnston, K.; Marmorstein, R.
Deposited on : 2000-01-19
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

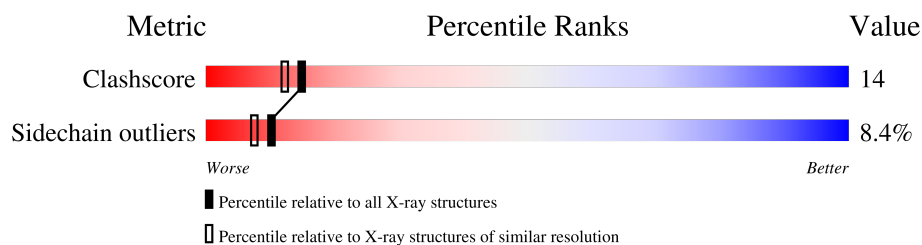
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	190562	7164 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	13	54% 46%
1	D	13	77% 23%
2	B	13	54% 38% 8%
2	E	13	54% 38% 8%
3	C	94	63% 19% 10% 9%
3	F	94	62% 22% 7% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2775 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 DNA chain called DNA (5'-D(*TP*GP*AP*CP*CP*GP*GP*AP*AP*GP*TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	13	Total	C	N	O	P	0	0	0
			268	128	52	76	12			
1	D	13	Total	C	N	O	P	0	0	0
			268	128	52	76	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*AP*CP*TP*TP*CP*CP*GP*GP*TP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			259	125	46	76	12			
2	E	13	Total	C	N	O	P	0	0	0
			259	125	46	76	12			

- Molecule 3 is a protein called ETS-DOMAIN PROTEIN ELK-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	86	Total	C	N	O	S	0	2	0
			748	482	134	131	1			
3	F	86	Total	C	N	O	S	0	2	0
			748	482	134	131	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	22	Total	O	0	0
			22	22		
4	D	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	22	Total 22	O 22	0	0
4	C	73	Total 73	O 73	0	0
4	F	67	Total 67	O 67	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

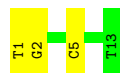
- Molecule 1: DNA (5'-D(*TP*GP*AP*CP*CP*GP*GP*AP*AP*GP*TP*GP*T)-3')

Chain A: 



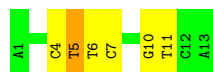
- Molecule 1: DNA (5'-D(*TP*GP*AP*CP*CP*GP*GP*AP*AP*GP*TP*GP*T)-3')

Chain D: 



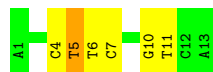
- Molecule 2: DNA (5'-D(*AP*CP*AP*CP*TP*TP*CP*CP*GP*GP*TP*CP*A)-3')

Chain B: 



- Molecule 2: DNA (5'-D(*AP*CP*AP*CP*TP*TP*CP*CP*GP*GP*TP*CP*A)-3')

Chain E: 



- Molecule 3: ETS-DOMAIN PROTEIN ELK-1

Chain C: 



- Molecule 3: ETS-DOMAIN PROTEIN ELK-1

Chain F: 

MET	ASP	PRD	SER	V5	T6	L7	W8	Q9	F10	L11	L12	Q13	E17	N20	G21	H22	W26	T27	S28	R29	D30	E41	R44	L45	R49	N54	L60	R65	I72	I73	R74	F85	V86	P89	E90	VAL	ALA	GLY	CYS
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4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	33.24Å 140.52Å 38.62Å 90.00° 115.52° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.8 (50.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.236	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2775	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.25	0/301	0.62	0/464
1	D	0.25	0/301	0.61	0/464
2	B	0.26	0/289	0.69	0/443
2	E	0.27	0/289	0.69	0/443
3	C	0.38	0/765	0.91	6/1028 (0.6%)
3	F	0.38	0/765	0.91	5/1028 (0.5%)
All	All	0.33	0/2710	0.80	11/3870 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	E	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	27	THR	N-CA-C	-7.48	102.73	112.68
3	F	27	THR	N-CA-C	-7.33	102.94	112.68
3	F	29	ARG	N-CA-C	6.04	117.53	111.07
3	F	54	ASN	N-CA-C	6.00	119.90	112.59
3	C	17	GLU	N-CA-C	5.73	120.40	112.90
3	F	17	GLU	N-CA-C	5.72	120.39	112.90
3	C	54	ASN	N-CA-C	5.68	119.52	112.59
3	C	88	TYR	CA-C-N	5.36	126.53	119.84
3	C	88	TYR	C-N-CA	5.36	126.53	119.84
3	F	26	TRP	N-CA-C	-5.27	103.08	110.50
3	C	26	TRP	N-CA-C	-5.11	103.30	110.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	5	DT	Sidechain
2	E	5	DT	Sidechain

5.2 Too-close contacts

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	268	0	148	6	0
1	D	268	0	148	4	0
2	B	259	0	148	6	0
2	E	259	0	148	7	0
3	C	748	0	747	24	0
3	F	748	0	747	21	0
4	A	20	0	0	0	0
4	B	22	0	0	0	0
4	C	73	0	0	1	0
4	D	21	0	0	0	0
4	E	22	0	0	1	0
4	F	67	0	0	1	0
All	All	2775	0	2086	63	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 14.

All (63) 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)
3:F:20:ASN:HD22	3:F:22:HIS:H	1.28	0.79
3:C:17:GLU:HG2	3:F:45:LEU:HG	1.72	0.71
3:C:45:LEU:HG	3:F:17:GLU:HG2	1.72	0.70
3:C:74:ARG:HG2	3:C:74:ARG:HH11	1.56	0.69
3:C:69[A]:ASP:OD1	3:C:70:LYS:HD2	1.92	0.69
3:F:13:GLN:HE22	3:F:49:ARG:HH12	1.42	0.67
3:C:13:GLN:HE22	3:C:49:ARG:HH12	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:12:LEU:HD13	3:F:85:PHE:CZ	2.33	0.64
3:C:12:LEU:HD13	3:C:85:PHE:CZ	2.34	0.62
3:F:73:ILE:O	3:F:74:ARG:HD3	1.98	0.61
3:F:29:ARG:HH21	3:F:90:GLU:HG3	1.65	0.60
3:C:13:GLN:HE21	3:C:49:ARG:HH22	1.51	0.58
3:F:13:GLN:HE21	3:F:49:ARG:HH22	1.52	0.57
3:F:89:PRO:HG2	3:F:90:GLU:CD	2.29	0.57
3:F:89:PRO:HG2	3:F:90:GLU:OE1	2.08	0.54
2:E:6:DT:H2''	2:E:7:DC:H5'	1.90	0.54
3:C:13:GLN:NE2	3:C:49:ARG:HH22	2.05	0.54
2:B:6:DT:H2''	2:B:7:DC:H5'	1.89	0.54
1:D:1:DT:H4'	1:D:2:DG:H5'	1.91	0.53
3:C:6:THR:OG1	3:C:9:GLN:HG3	2.09	0.53
3:C:73:ILE:O	3:C:74:ARG:HD2	2.08	0.53
2:B:4:DC:H2'	2:B:5:DT:H72	1.91	0.53
1:A:1:DT:H4'	1:A:2:DG:H5'	1.90	0.53
1:A:1:DT:H1'	1:A:2:DG:C8	2.44	0.52
3:F:6:THR:OG1	3:F:9:GLN:HG3	2.10	0.52
3:F:41:GLU:OE2	3:F:44[A]:ARG:NH2	2.43	0.52
3:F:13:GLN:NE2	3:F:49:ARG:HH22	2.08	0.51
2:E:6:DT:H2''	2:E:7:DC:C5'	2.41	0.51
1:D:1:DT:H1'	1:D:2:DG:C8	2.46	0.50
2:E:4:DC:H2'	2:E:5:DT:H72	1.92	0.50
2:B:6:DT:H2''	2:B:7:DC:C5'	2.42	0.49
3:C:41:GLU:OE2	3:C:44[A]:ARG:NH2	2.45	0.49
3:C:13:GLN:NE2	3:C:49:ARG:HH12	2.09	0.48
3:F:20:ASN:ND2	3:F:22:HIS:H	2.02	0.48
2:E:10:DG:N7	4:E:32:HOH:O	2.35	0.48
1:A:5:DC:H2'	3:C:65:ARG:HD2	1.96	0.48
3:F:60:LEU:C	3:F:60:LEU:HD23	2.39	0.47
3:F:89:PRO:HG2	3:F:90:GLU:OE2	2.15	0.47
3:C:60:LEU:C	3:C:60:LEU:HD23	2.40	0.47
3:F:13:GLN:NE2	3:F:49:ARG:HH12	2.09	0.47
3:C:74:ARG:HG2	3:C:74:ARG:NH1	2.28	0.46
1:D:5:DC:H2'	3:F:65:ARG:HD2	1.96	0.46
3:C:72:ILE:O	3:C:86:VAL:HG13	2.16	0.45
3:F:7:LEU:HD22	3:F:11:LEU:HD22	1.98	0.45
3:C:5:VAL:HG11	4:C:104:HOH:O	2.15	0.45
3:C:7:LEU:HD22	3:C:11:LEU:HD22	2.00	0.44
3:C:74:ARG:HH11	3:C:74:ARG:CG	2.28	0.43
2:B:10:DG:C8	2:B:11:DT:H72	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:DA:H4'	3:C:80:LYS:HD2	1.99	0.42
2:B:4:DC:H2'	2:B:5:DT:C7	2.49	0.42
1:D:1:DT:O2	1:D:1:DT:O4'	2.36	0.42
2:E:10:DG:C8	2:E:11:DT:H72	2.54	0.42
3:C:87:SER:O	3:C:88:TYR:C	2.61	0.42
3:F:5:VAL:HG11	4:F:98:HOH:O	2.20	0.42
2:B:10:DG:H2''	2:B:11:DT:OP2	2.19	0.42
3:C:73:ILE:C	3:C:74:ARG:HD2	2.45	0.41
2:E:10:DG:H2''	2:E:11:DT:OP2	2.19	0.41
2:E:4:DC:H2'	2:E:5:DT:C7	2.50	0.40
3:F:72:ILE:O	3:F:86:VAL:HG13	2.21	0.40
1:A:1:DT:O2	1:A:1:DT:O4'	2.36	0.40
1:A:11:DT:H2''	1:A:12:DG:C8	2.57	0.40
3:C:12:LEU:HD12	3:C:12:LEU:HA	1.93	0.40
3:C:72:ILE:C	3:C:86:VAL:HG13	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
3	C	79/83 (95%)	72 (91%)	7 (9%)	9	6
3	F	79/83 (95%)	73 (92%)	6 (8%)	12	9
All	All	158/166 (95%)	145 (92%)	13 (8%)	10	8

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	7	LEU
3	C	11	LEU
3	C	12	LEU
3	C	45	LEU
3	C	74	ARG
3	C	80	LYS
3	C	86	VAL
3	F	7	LEU
3	F	11	LEU
3	F	12	LEU
3	F	30	ASP
3	F	45	LEU
3	F	86	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	13	GLN
3	F	13	GLN
3	F	20	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.