Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 05:35 am BST

PDB ID	:	1DUX
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

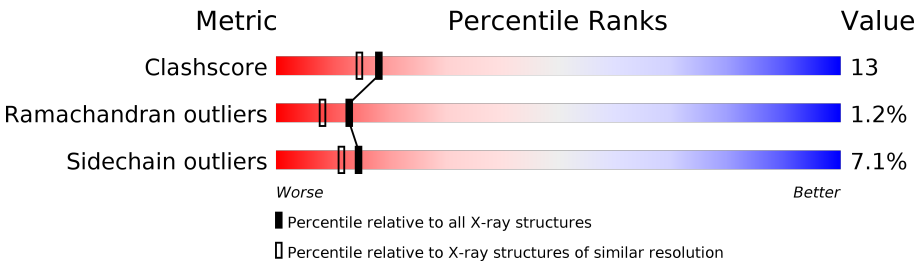
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 on 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 <=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	67% 19% 5% 9%
3	F	94	65% 20% 6% 9%

2 Entry composition (i)

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
			Total	C	N	O	P			
1	A	13	268	128	52	76	12	0	0	0
1	D	13	268	128	52	76	12	0	0	0

- 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
			Total	C	N	O	P			
2	B	13	259	125	46	76	12	0	0	0
2	E	13	259	125	46	76	12	0	0	0

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

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

- Molecule 4 is water.

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

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

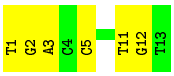
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

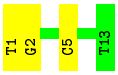
- Molecule 1: DNA (5'-D(*TP*GP*AP*CP*CP*GP*GP*AP*AP*GP*TP*GP*T)-3')

Chain A: 54% 46%



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

Chain D: 77% 23%

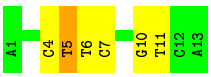


- Molecule 2: DNA (5'-D(*AP*CP*AP*CP*TP*TP*CP*CP*GP*GP*TP*CP*A)-3')

Chain B: 54% 38% 8%

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

Chain E: 54% 38% 8%

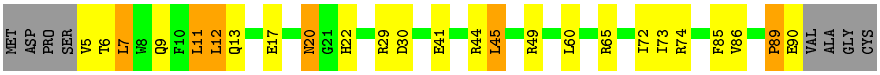


- Molecule 3: ETS-DOMAIN PROTEIN ELK-1

Chain C: 67% 19% 5% 9%

- Molecule 3: ETS-DOMAIN PROTEIN ELK-1

Chain F: 65% 20% 6% 9%


MET
ASP
PRO
SER
V5
T6
L7
W8
Q9
F10
L11
L12
Q13
E17
N20
G21
H22
R29
D30
E41
R44
L45
R49
L60
R65
I72
I73
R74
F85
V86
P89
E90
VAL
ALA
GLY
CYS

4 Data and refinement statistics (i)

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 (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	0.29	0/301	0.69	0/464
1	D	0.30	0/301	0.69	0/464
2	B	0.30	0/289	0.75	0/443
2	E	0.30	0/289	0.74	0/443
3	C	0.36	0/765	0.61	0/1028
3	F	0.36	0/765	0.62	0/1028
All	All	0.33	0/2710	0.66	0/3870

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.

There are no bond angle outliers.

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 (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	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	22	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	61	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 13.

All (61) 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:HH11	3:C:74:ARG:HG2	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
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: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
3:F:89:PRO:HG2	3:F:90:GLU:CD	2.29	0.53
1:D:1:DT:H4'	1:D:2:DG:H5'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:PRO:HG2	3:F:90:GLU:OE2	2.15	0.47
3:F:13:GLN:NE2	3:F:49:ARG:HH12	2.09	0.47
3:C:74:ARG:NH1	3:C:74:ARG:HG2	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:CG	3:C:74:ARG:HH11	2.28	0.43
2:B:10:DG:C8	2:B:11:DT:H72	2.54	0.43
3:F:60:LEU:C	3:F:60:LEU:HD23	2.39	0.42
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:60:LEU:HD23	3:C:60:LEU:C	2.40	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
2:E:10:DG:H2"	2:E:11:DT:OP2	2.19	0.41
3:C:5:VAL:HG13	3:C:5:VAL:O	2.22	0.40
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:11:DT:H2"	1:A:12:DG:C8	2.57	0.40
1:A:1:DT:O4'	1:A:1:DT:O2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HA	3:C:12:LEU:HD12	1.93	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	
3	C	86/94 (92%)	83 (96%)	2 (2%)	1 (1%)	13	8
3	F	86/94 (92%)	83 (96%)	2 (2%)	1 (1%)	13	8
All	All	172/188 (92%)	166 (96%)	4 (2%)	2 (1%)	13	8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	89	PRO
3	C	89	PRO

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%)	74 (94%)	5 (6%)	18	15
3	F	79/83 (95%)	73 (92%)	6 (8%)	13	10
All	All	158/166 (95%)	147 (93%)	11 (7%)	14	12

All (11) 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	F	7	LEU
3	F	11	LEU
3	F	12	LEU
3	F	20	ASN
3	F	30	ASP
3	F	45	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	13	GLN
3	F	13	GLN
3	F	20	ASN
3	F	22	HIS

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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.