



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:53 AM GMT

PDB ID : 3K3R
Title : Unrefined crystal structure of a LexA-DNA complex
Authors : Zhang, A.P.P.; Pigli, Y.Z.; Rice, P.A.
Deposited on : 2009-10-04
Resolution : 3.20 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

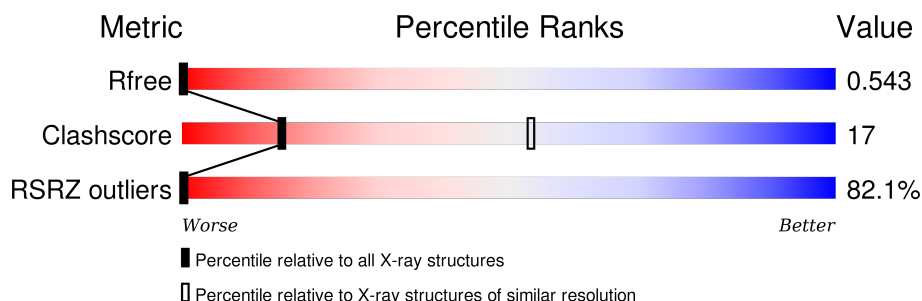
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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	E	202	<div> <div>78%</div> <div> <div>83%</div> <div>14%</div> </div> </div>
1	F	202	<div> <div>78%</div> <div> <div>83%</div> <div>14%</div> </div> </div>
2	A	29	<div> <div>24%</div> <div>97%</div> </div>
2	B	29	<div> <div>28%</div> <div>97%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 403 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 LexA repressor.

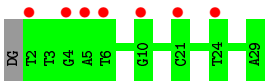
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	E	174	Total C 174 174	0	0	174
1	F	173	Total C 173 173	0	0	173

There are 2 discrepancies between the modelled and reference sequences:

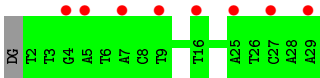
Chain	Residue	Modelled	Actual	Comment	Reference
E	156	ALA	LYS	ENGINEERED	UNP P0A7C2
F	156	ALA	LYS	ENGINEERED	UNP P0A7C2

- Molecule 2 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	A	28	Total P 28 28	0	0	28
2	B	28	Total P 28 28	0	0	28



• Molecule 2: DNA (28-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	45.36 Å 120.39 Å 149.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 35.76 – 3.19	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.20) 95.7 (35.76-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.18 Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available) 0.533 , 0.543	Depositor DCC
R_{free} test set	686 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.71 , 155.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 13754 reflections	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	403	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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 ⓘ

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	E	174	0	0	4	0
1	F	173	0	0	3	0
2	A	28	0	0	0	0
2	B	28	0	0	0	0
All	All	403	0	0	7	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 17.

All (7) 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:F:60:SER:CA	1:F:61:GLY:CA	2.78	0.60
1:F:106:LYS:CA	1:F:107:PRO:CA	2.86	0.53
1:E:22:THR:CA	1:E:23:GLY:CA	2.88	0.51
1:E:23:GLY:CA	1:E:24:MET:CA	2.90	0.50
1:E:35:LEU:CA	1:E:36:GLY:CA	2.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:ALA:CA	1:F:63:SER:CA	2.91	0.48
1:E:106:LYS:CA	1:E:107:PRO:CA	2.99	0.41

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](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 ⓘ

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	E	174/202 (86%)	11.11	158 (90%) 0 0	26, 137, 137, 137	0
1	F	173/202 (85%)	10.66	158 (91%) 0 0	137, 137, 137, 137	0
2	A	28/29 (96%)	1.13	7 (25%) 1 1	119, 119, 119, 119	0
2	B	28/29 (96%)	1.40	8 (28%) 1 0	119, 119, 119, 119	0
All	All	403/462 (87%)	9.55	331 (82%) 0 0	26, 137, 137, 137	0

All (331) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	39	SER	40.2
1	E	55	VAL	37.1
1	F	20	SER	36.2
1	E	183	GLN	33.9
1	F	154	THR	33.8
1	F	110	ASP	33.3
1	E	109	ALA	33.0
1	F	141	ASN	32.9
1	E	189	GLU	32.7
1	E	187	THR	31.9
1	F	109	ALA	31.7
1	F	169	PRO	31.7
1	E	149	ILE	31.2
1	E	4	LEU	31.2
1	E	158	LEU	30.8
1	F	102	PRO	29.9
1	F	137	GLN	29.9
1	E	98	TYR	29.7
1	E	154	THR	29.6
1	F	191	LEU	29.5
1	F	70	GLN	29.2

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Mol	Chain	Res	Type	RSRZ
1	E	59	VAL	28.9
1	E	46	HIS	27.2
1	E	148	ARG	27.1
1	E	144	VAL	26.6
1	E	102	PRO	26.4
1	E	104	LEU	25.9
1	E	57	GLU	25.4
1	F	24	MET	25.2
1	F	123	ILE	25.1
1	E	136	THR	24.7
1	E	29	ALA	24.7
1	F	193	VAL	24.4
1	F	199	GLY	24.1
1	F	119	SER	24.1
1	E	56	ILE	23.8
1	F	95	GLU	23.4
1	F	171	ASN	22.3
1	F	153	VAL	22.2
1	E	126	MET	21.8
1	F	178	VAL	21.7
1	F	131	LEU	21.6
1	E	139	VAL	21.4
1	E	129	ASP	21.4
1	F	140	ARG	20.8
1	F	64	ARG	20.5
1	F	26	PRO	20.1
1	E	140	ARG	20.0
1	F	29	ALA	19.7
1	E	40	PRO	19.7
1	E	3	ALA	19.6
1	E	145	VAL	19.6
1	E	185	SER	19.4
1	E	190	GLY	19.2
1	E	172	SER	19.1
1	E	14	LEU	19.0
1	E	62	ALA	18.6
1	F	42	ALA	18.6
1	F	62	ALA	18.4
1	F	67	ARG	18.0
1	F	21	GLN	18.0
1	F	133	VAL	17.8
1	F	41	ASN	17.8

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Mol	Chain	Res	Type	RSRZ
1	E	155	VAL	17.5
1	E	146	VAL	17.1
1	E	26	PRO	17.0
1	E	143	GLN	17.0
1	F	30	GLU	16.8
1	E	156	ALA	16.8
1	F	39	SER	16.7
1	E	70	GLN	16.5
1	F	25	PRO	16.4
1	F	44	GLU	16.4
1	F	139	VAL	16.2
1	F	27	THR	16.2
1	E	181	LEU	16.1
1	F	174	PHE	16.0
1	F	135	LYS	15.9
1	F	38	ARG	15.6
1	F	159	LYS	15.6
1	E	178	VAL	15.5
1	E	169	PRO	15.5
1	E	142	GLY	15.4
1	F	68	LEU	15.3
1	F	142	GLY	15.2
1	E	130	LEU	15.2
1	F	164	LYS	15.2
1	F	187	THR	15.2
1	F	129	ASP	15.0
1	F	175	LYS	15.0
1	E	157	ARG	15.0
1	E	135	LYS	14.9
1	F	105	PHE	14.9
1	F	118	MET	14.9
1	F	180	ASP	14.9
1	F	113	LEU	14.8
1	E	197	ARG	14.8
1	E	25	PRO	14.6
1	E	68	LEU	14.5
1	F	31	ILE	14.5
1	F	108	ASN	14.4
1	F	120	MET	14.4
1	F	132	ALA	14.2
1	E	191	LEU	14.2
1	F	40	PRO	14.2

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Mol	Chain	Res	Type	RSRZ
1	E	188	ILE	14.2
1	E	22	THR	14.2
1	E	177	ILE	14.1
1	F	63	SER	14.0
1	E	152	GLU	13.9
1	E	11	VAL	13.9
1	E	6	ALA	13.6
1	F	17	ASP	13.4
1	E	113	LEU	13.3
1	E	150	ASP	13.1
1	E	176	PRO	12.9
1	E	163	ASN	12.8
1	F	163	ASN	12.8
1	E	17	ASP	12.7
1	E	147	ALA	12.7
1	E	119	SER	12.7
1	F	55	VAL	12.6
1	E	141	ASN	12.3
1	E	196	ILE	12.2
1	F	144	VAL	12.0
1	E	170	GLU	12.0
1	F	149	ILE	12.0
1	F	150	ASP	11.9
1	F	167	LEU	11.8
1	E	131	LEU	11.7
1	F	114	ARG	11.5
1	E	100	VAL	11.5
1	F	196	ILE	11.2
1	E	69	LEU	11.2
1	E	168	LEU	11.2
1	F	56	ILE	11.2
1	F	15	ILE	11.1
1	F	96	GLY	11.1
1	E	99	GLN	11.1
1	E	122	ASP	11.1
1	E	171	ASN	11.1
1	F	160	LYS	11.1
1	F	23	GLY	11.1
1	E	199	GLY	11.0
1	E	97	HIS	11.0
1	F	5	THR	11.0
1	F	107	PRO	10.9

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Mol	Chain	Res	Type	RSRZ
1	F	198	ASN	10.9
1	E	51	ALA	10.7
1	E	49	ALA	10.6
1	E	63	SER	10.6
1	F	155	VAL	10.5
1	F	100	VAL	10.5
1	E	162	GLY	10.5
1	E	120	MET	10.3
1	E	24	MET	10.2
1	F	50	LEU	10.1
1	E	106	LYS	9.9
1	E	50	LEU	9.8
1	F	59	VAL	9.8
1	E	116	SER	9.8
1	F	147	ALA	9.6
1	F	145	VAL	9.6
1	E	111	PHE	9.5
1	E	151	ASP	9.5
1	E	35	LEU	9.3
1	E	16	ARG	9.2
1	F	8	GLN	9.2
1	F	156	ALA	9.0
1	F	138	ASP	8.9
1	F	157	ARG	8.9
1	F	197	ARG	8.9
1	E	5	THR	8.8
1	E	105	PHE	8.7
1	E	134	HIS	8.5
1	F	65	GLY	8.5
2	A	24	DT	8.4
1	F	126	MET	8.3
1	F	184	GLN	8.3
1	E	96	GLY	7.9
1	F	46	HIS	7.9
1	E	15	ILE	7.7
1	E	65	GLY	7.6
1	F	168	LEU	7.6
1	F	11	VAL	7.6
1	E	124	GLY	7.6
1	F	14	LEU	7.5
1	E	186	PHE	7.5
1	F	52	ARG	7.4

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Mol	Chain	Res	Type	RSRZ
1	E	166	GLU	7.4
1	E	175	LYS	7.3
1	F	13	ASP	7.3
1	E	101	ASP	7.1
1	E	184	GLN	7.1
1	E	66	ILE	7.1
1	E	18	HIS	7.1
1	F	173	GLU	7.1
1	F	6	ALA	7.1
1	F	9	GLN	7.0
1	F	57	GLU	6.9
1	F	116	SER	6.9
1	E	54	GLY	6.8
1	F	99	GLN	6.8
1	F	58	ILE	6.7
1	F	189	GLU	6.6
1	E	30	GLU	6.6
1	F	45	GLU	6.6
1	F	34	ARG	6.6
1	E	95	GLU	6.5
1	F	195	VAL	6.5
1	E	138	ASP	6.5
1	F	61	GLY	6.4
1	E	118	MET	6.4
1	E	31	ILE	6.3
1	E	198	ASN	6.3
1	F	179	VAL	6.3
1	E	34	ARG	6.3
1	F	185	SER	6.2
1	F	66	ILE	6.2
1	F	143	GLN	6.2
1	F	101	ASP	6.2
1	E	23	GLY	6.2
1	E	153	VAL	6.2
1	E	12	PHE	6.2
1	F	181	LEU	6.1
1	F	172	SER	6.1
1	F	104	LEU	6.1
1	F	158	LEU	6.0
1	F	18	HIS	6.0
1	F	51	ALA	5.8
1	E	103	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	48	LYS	5.8
1	F	111	PHE	5.7
1	E	164	LYS	5.6
1	F	47	LEU	5.6
1	F	127	ASP	5.5
1	E	195	VAL	5.4
1	E	43	ALA	5.3
1	F	170	GLU	5.2
1	F	49	ALA	5.1
1	E	107	PRO	5.1
1	E	115	VAL	5.1
1	F	122	ASP	5.0
1	E	180	ASP	5.0
1	E	174	PHE	5.0
1	F	194	GLY	4.9
1	F	60	SER	4.8
1	F	182	ARG	4.8
1	F	98	TYR	4.8
1	F	3	ALA	4.8
1	E	38	ARG	4.8
1	F	103	SER	4.7
1	E	60	SER	4.7
1	F	165	VAL	4.6
1	E	161	GLN	4.6
2	B	4	DG	4.6
1	E	27	THR	4.6
1	F	48	LYS	4.5
1	E	64	ARG	4.5
1	F	112	LEU	4.4
1	F	176	PRO	4.3
1	F	151	ASP	4.2
1	F	134	HIS	4.2
1	E	117	GLY	4.2
1	F	7	ARG	4.2
2	B	16	DT	4.1
1	E	125	ILE	4.1
2	B	7	DA	4.1
1	E	28	ARG	4.1
1	F	186	PHE	4.1
1	E	132	ALA	4.1
1	E	44	GLU	4.0
1	F	125	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	A	5	DA	3.9
1	E	42	ALA	3.9
1	F	124	GLY	3.9
1	E	112	LEU	3.9
1	E	167	LEU	3.8
1	F	183	GLN	3.7
1	F	190	GLY	3.7
1	F	32	ALA	3.6
1	E	41	ASN	3.6
1	E	127	ASP	3.5
1	E	179	VAL	3.4
2	A	6	DT	3.4
1	E	9	GLN	3.4
1	E	110	ASP	3.4
1	F	146	VAL	3.4
1	F	4	LEU	3.4
1	F	166	GLU	3.4
1	F	162	GLY	3.3
1	E	121	LYS	3.2
1	E	7	ARG	3.2
1	F	121	LYS	3.2
1	F	161	GLN	3.1
1	F	54	GLY	3.1
1	E	37	PHE	3.1
1	E	58	ILE	3.1
2	B	29	DA	3.1
1	E	61	GLY	3.0
1	E	114	ARG	3.0
1	F	115	VAL	3.0
1	F	117	GLY	3.0
1	E	133	VAL	2.9
1	F	10	GLU	2.9
1	E	13	ASP	2.9
1	F	128	GLY	2.8
2	B	25	DA	2.7
1	E	159	LYS	2.7
1	F	130	LEU	2.6
2	A	21	DC	2.5
1	E	128	GLY	2.5
2	A	4	DG	2.5
1	E	165	VAL	2.5
1	E	193	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	43	ALA	2.4
1	F	37	PHE	2.4
1	E	194	GLY	2.4
1	E	36	GLY	2.3
2	A	10	DG	2.3
1	E	108	ASN	2.3
1	E	45	GLU	2.3
1	F	28	ARG	2.3
2	B	9	DT	2.2
1	E	173	GLU	2.2
1	E	137	GLN	2.2
1	F	33	GLN	2.2
2	B	27	DC	2.2
1	F	19	ILE	2.1
2	B	5	DA	2.0
2	A	2	DT	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.