



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 02:04 pm GMT

PDB ID : 1LQ1
Title : DNA Complexed Structure of the Key Transcription Factor Initiating Development in Sporulation Bacteria
Authors : Zhao, H.; Msadek, T.; Zapf, J.; Madhusudan; Hoch, J.A.; Varughese, K.I.
Deposited on : 2002-05-08
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

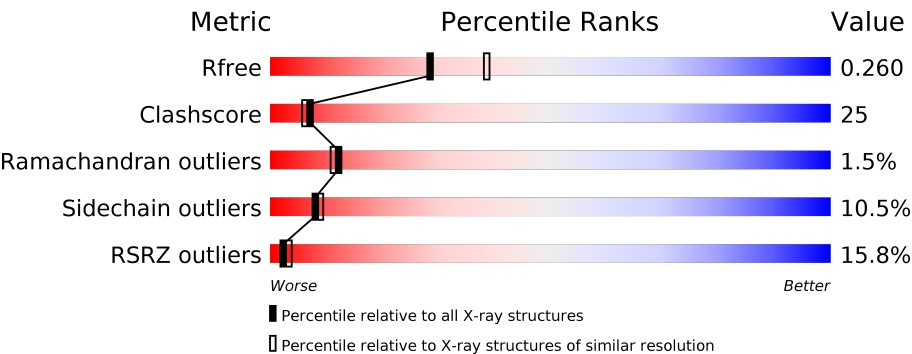
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.30 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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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	16	<div><div></div><div><div></div><div>31%</div><div>56%</div><div>13%</div></div></div>
1	G	16	<div><div>6%</div><div></div><div><div></div><div>19%</div><div>75%</div><div>6%</div></div></div>
2	F	16	<div><div></div><div><div></div><div>19%</div><div>81%</div></div></div>
2	H	16	<div><div>6%</div><div></div><div><div></div><div>94%</div></div></div>
3	A	120	<div><div>13%</div><div></div><div><div></div><div>58%</div><div>28%</div><div>• •</div><div>11%</div></div></div>
3	B	120	<div><div>40%</div><div></div><div><div></div><div>43%</div><div>38%</div><div>5%</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	C	120	<div><div></div><div>7%</div><div>55%</div><div>29%</div><div>8%</div><div>7%</div></div>
3	D	120	<div><div></div><div>4%</div><div>58%</div><div>27%</div><div>5%</div><div>11%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4909 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 5'-D(*TP*TP*CP*GP*TP*GP*TP*CP*GP*AP*AP*TP*TP*TP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	16	Total	C	N	O	P	0	0	0
			325	158	52	100	15			
1	G	16	Total	C	N	O	P	0	0	0
			325	158	52	100	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	16	Total	C	N	O	P	0	0	0
			325	156	66	88	15			
2	H	16	Total	C	N	O	P	0	0	0
			325	156	66	88	15			

- Molecule 3 is a protein called Stage 0 sporulation protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	107	Total	C	N	O	S	0	0	0
			845	541	147	155	2			
3	B	103	Total	C	N	O	S	0	0	0
			805	517	138	148	2			
3	C	112	Total	C	N	O	S	0	0	0
			870	557	153	158	2			
3	D	107	Total	C	N	O	S	0	0	0
			845	541	147	155	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	9	Total 9	O 9	0	0
4	C	51	Total 51	O 51	0	0
4	D	51	Total 51	O 51	0	0
4	E	39	Total 39	O 39	0	0
4	F	20	Total 20	O 20	0	0
4	G	18	Total 18	O 18	0	0
4	H	30	Total 30	O 30	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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: 5'-D(*TP*TP*CP*GP*TP*GP*TP*CP*GP*AP*AP*TP*TP*TP*TP*G)-3'

Chain E: 



- Molecule 1: 5'-D(*TP*TP*CP*GP*TP*GP*TP*CP*GP*AP*AP*TP*TP*TP*TP*G)-3'

Chain G: 

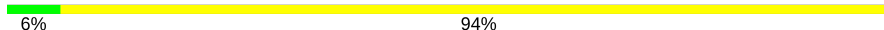


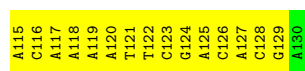
- Molecule 2: 5'-D(*AP*CP*AP*AP*AP*AP*TP*TP*CP*GP*AP*CP*AP*CP*GP*A)-3'

Chain F: 



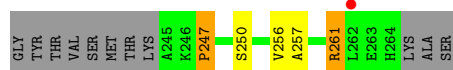
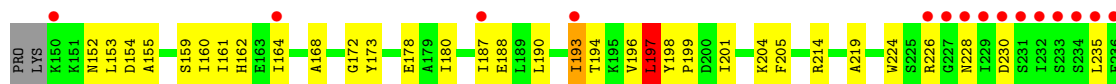
- Molecule 2: 5'-D(*AP*CP*AP*AP*AP*AP*TP*TP*CP*GP*AP*CP*AP*CP*GP*A)-3'

Chain H: 

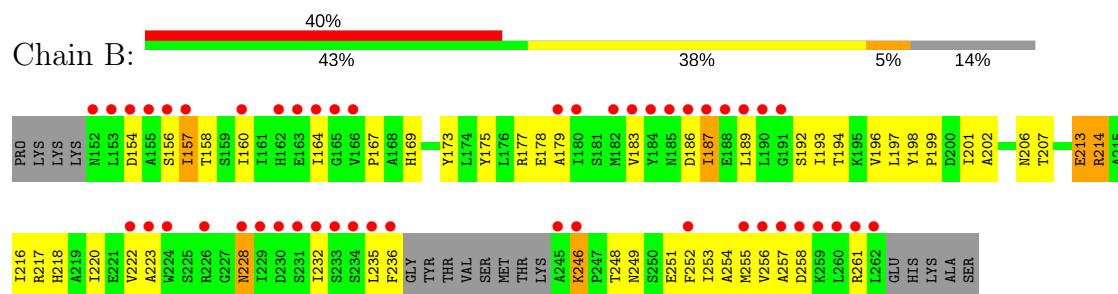


- Molecule 3: Stage 0 sporulation protein A

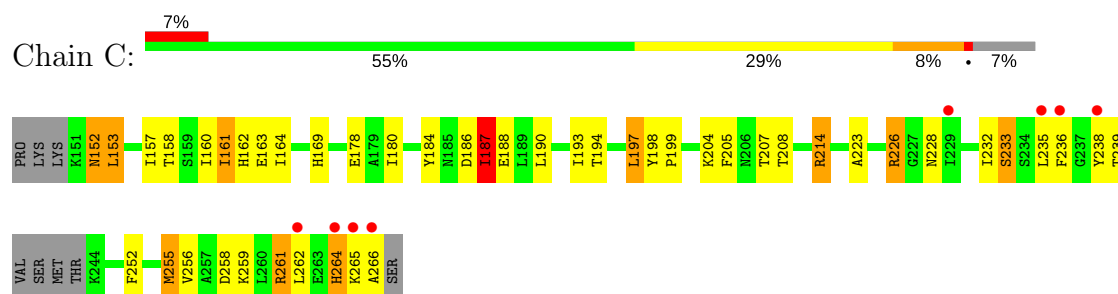
Chain A: 



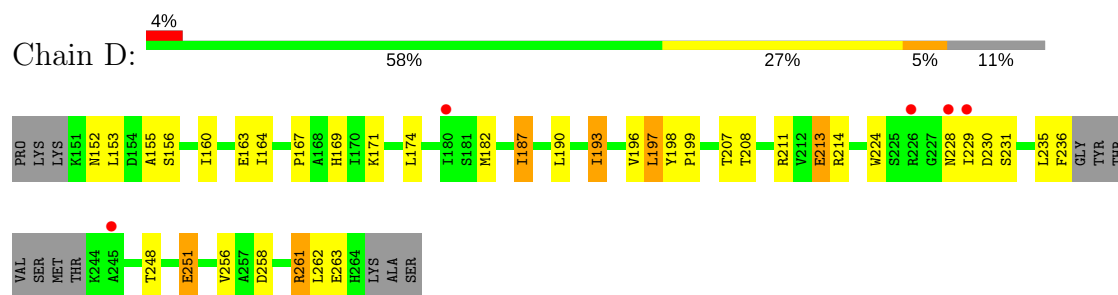
- Molecule 3: Stage 0 sporulation protein A



- Molecule 3: Stage 0 sporulation protein A



- Molecule 3: Stage 0 sporulation protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.92Å 83.30Å 91.24Å 90.00° 94.18° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 45.50 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.30) 89.6 (45.50-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.16Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.258 0.225 , 0.260	Depositor DCC
R_{free} test set	1653 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4909	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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, 0.333 respectively for untwinned datasets, and 0.375, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.98	3/362 (0.8%)	1.25	6/558 (1.1%)
1	G	0.85	1/362 (0.3%)	1.06	3/558 (0.5%)
2	F	0.57	0/366	0.95	0/562
2	H	0.52	0/366	0.84	0/562
3	A	0.47	0/859	0.69	2/1159 (0.2%)
3	B	0.34	0/818	0.56	0/1106
3	C	0.52	0/884	0.69	2/1192 (0.2%)
3	D	0.52	0/859	0.65	0/1159
All	All	0.57	4/4876 (0.1%)	0.80	13/6856 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	15	DT	C5-C7	8.45	1.55	1.50
1	E	15	DT	C5-C7	8.42	1.55	1.50
1	E	13	DT	C5-C7	7.11	1.54	1.50
1	E	14	DT	C5-C7	6.80	1.54	1.50

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	247	PRO	CA-N-CD	-9.37	98.38	111.50
1	E	15	DT	O4'-C4'-C3'	-8.11	101.13	106.00
1	G	15	DT	C4-C5-C6	7.45	122.47	118.00
1	G	15	DT	OP1-P-OP2	-6.47	109.89	119.60
1	E	13	DT	C6-C5-C7	-6.14	119.22	122.90

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	325	0	186	11	0
1	G	325	0	186	14	0
2	F	325	0	180	12	0
2	H	325	0	180	14	0
3	A	845	0	871	37	0
3	B	805	0	828	56	0
3	C	870	0	894	49	0
3	D	845	0	871	41	0
4	A	26	0	0	1	0
4	B	9	0	0	0	0
4	C	51	0	0	2	0
4	D	51	0	0	7	0
4	E	39	0	0	0	0
4	F	20	0	0	2	0
4	G	18	0	0	2	0
4	H	30	0	0	2	0
All	All	4909	0	4196	224	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 25.

The worst 5 of 224 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:G:7:DT:H2''	1:G:8:DC:H5'	1.26	1.17
3:C:235:LEU:HD21	3:C:259:LYS:HD2	1.16	1.13
3:C:158:THR:HG22	3:C:162:HIS:CD2	1.95	1.01
3:A:180:ILE:HD13	3:A:256:VAL:HG21	1.42	0.96
3:C:259:LYS:HE3	3:C:265:LYS:HA	1.49	0.93

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	A	103/120 (86%)	96 (93%)	6 (6%)	1 (1%)	18	20
3	B	99/120 (82%)	81 (82%)	16 (16%)	2 (2%)	9	7
3	C	108/120 (90%)	96 (89%)	10 (9%)	2 (2%)	9	8
3	D	103/120 (86%)	95 (92%)	7 (7%)	1 (1%)	18	20
All	All	413/480 (86%)	368 (89%)	39 (9%)	6 (2%)	12	11

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	206	ASN
3	B	228	ASN
3	A	197	LEU
3	D	263	GLU
3	C	187	ILE

5.3.2 Protein sidechains ⓘ

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	A	92/103 (89%)	83 (90%)	9 (10%)	9	11
3	B	87/103 (84%)	81 (93%)	6 (7%)	18	23
3	C	92/103 (89%)	81 (88%)	11 (12%)	6	6
3	D	92/103 (89%)	80 (87%)	12 (13%)	5	5
All	All	363/412 (88%)	325 (90%)	38 (10%)	8	9

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	161	ILE
3	C	226	ARG
3	D	256	VAL
3	C	197	LEU
3	C	255	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	152	ASN
3	D	264	HIS
3	D	152	ASN
3	B	152	ASN
3	D	228	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	16/16 (100%)	0.02	0 100 100	34, 51, 58, 62	0
1	G	16/16 (100%)	0.25	1 (6%) 21 27	48, 55, 70, 118	0
2	F	16/16 (100%)	0.01	0 100 100	39, 54, 72, 107	0
2	H	16/16 (100%)	-0.09	0 100 100	49, 56, 73, 80	0
3	A	107/120 (89%)	0.71	16 (14%) 3 4	35, 58, 113, 128	0
3	B	103/120 (85%)	2.55	48 (46%) 0 0	52, 95, 139, 146	0
3	C	112/120 (93%)	0.49	8 (7%) 17 22	26, 54, 111, 134	0
3	D	107/120 (89%)	0.51	5 (4%) 32 39	27, 45, 101, 122	0
All	All	493/544 (90%)	0.91	78 (15%) 2 3	26, 58, 122, 146	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	235	LEU	13.1
3	C	264	HIS	8.9
3	B	232	ILE	8.9
3	B	260	LEU	8.9
3	B	236	PHE	8.8

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.