Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 07:13 PM EDT

PDB ID	:	6PTG
Title	:	Structure of RNA polymerase binding protein and transcriptional regulator Dks from Chlamydia trachomatis L2 (LGV434)
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2019-07-15
Resolution	:	2.95 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:

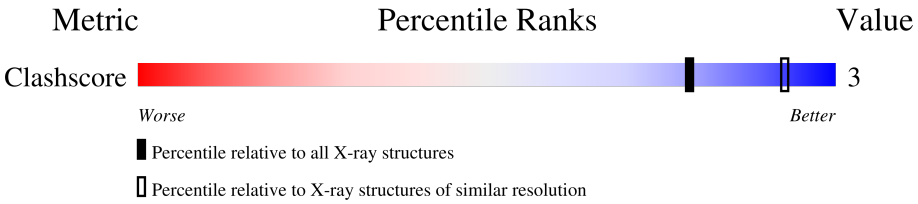
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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	3462 (3.00-2.92)

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1293 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 DnaK Suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			632	401	103	124	4			
1	B	86	Total	C	N	O	S	0	0	0
			638	405	105	124	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	13	Total	O	0	0
			13	13		

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.42Å 83.42Å 99.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.02 – 2.95	Depositor
% Data completeness (in resolution range)	99.0 (30.02-2.95)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.95Å)	Xtriage
Refinement program	PHENIX (dev_3500)	Depositor
R, R_{free}	0.182 , 0.226	Depositor
Wilson B-factor (Å^2)	67.9	Xtriage
Anisotropy	0.505	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
Total number of atoms	1293	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality (i)

4.1 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	0.27	0/637	0.41	0/858
1	B	0.27	0/643	0.42	0/863
All	All	0.27	0/1280	0.41	0/1721

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	632	0	626	3	0
1	B	638	0	633	5	0
2	A	10	0	0	0	0
2	B	13	0	0	0	0
All	All	1293	0	1259	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 3.

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:A:99:ARG:NH2	1:A:113:GLN:OE1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:HG11	1:B:92:GLY:HA3	1.95	0.49
1:B:18:MET:HE2	1:B:73:ILE:HD11	1.95	0.48
1:B:90:VAL:HB	1:B:112:SER:HB3	2.00	0.44
1:A:88:CYS:HB2	1:A:109:THR:HG23	2.00	0.43
1:B:88:CYS:HB2	1:B:109:THR:HG23	2.01	0.43
1:B:22:LEU:HD21	1:B:69:LEU:HD23	1.99	0.43

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

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5.3 Carbohydrates

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5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.