

wwPDB X-ray Structure Validation Summary Report (i)

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:	1UAA
:	E. COLI REP HELICASE/DNA COMPLEX
:	Korolev, S.; Waksman, G.
:	1997-06-30
:	3.00 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) 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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.00 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	С	16	6%	94%				
2	А	673	24%	51%	18%	• 5%		
2	В	673	24%	51%	17%	• 6%		



 $\mathbf{2}$

Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10404 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	С	16	Total 317	C 160	N 32	0 110	Р 15	0	0	0

• Molecule 2 is a protein called PROTEIN (ATP-DEPENDENT DNA HELICASE REP.).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	А	636	Total 5032	C 3186	N 881	0 942	S 23	0	0	0
2	В	633	Total 5055	C 3203	N 886	0 945	S 21	0	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.







9581 9582 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 9583 8583 8583 8583 8583 8583 8583 8583 8583 8583 8594 8594 8595 8595 8505 <li

• Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 43 21 2	Depositor	
Cell constants	141.80Å 141.80Å 284.80Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	15.00 - 3.00	Depositor	
% Data completeness	88.0 (15.00-3.00)	Depositor	
(in resolution range)	00.0 (10.00-0.00)	Depositor	
R_{merge}	0.05	Depositor	
R_{sym}	(Not available)	Depositor	
Refinement program	X-PLOR 3.1	Depositor	
R, R_{free}	0.228 , 0.328	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	10404	wwPDB-VP	
Average B, all atoms $(Å^2)$	43.0	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).

Mal	Chain	Bo	nd lengths	Bond angles		
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	С	1.08	0/348	1.07	0/536	
2	А	0.83	0/5127	0.96	7/6932~(0.1%)	
2	В	0.92	4/5151~(0.1%)	0.97	7/6961~(0.1%)	
All	All	0.88	4/10626~(0.0%)	0.97	14/14429~(0.1%)	

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	А	0	2

Ζ Mol Chain Res Type Atoms Observed(Å) Ideal(Å) 2В 18CYS CB-SG -6.211.711.822В 612 CYS CB-SG -6.151.711.82 $\mathbf{2}$ В 337 VAL CB-CG1 -6.131.40 1.52 $\mathbf{2}$ В 65GLU CG-CD 5.241.591.51

All (4) bond length outliers are listed below:

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	410	LYS	N-CA-C	8.50	133.94	111.00
2	В	411	ARG	NE-CZ-NH2	7.69	124.14	120.30
2	А	3	LEU	N-CA-C	-5.65	95.74	111.00
2	В	266	PRO	CB-CA-C	-5.52	98.21	112.00
2	В	149	PRO	N-CA-CB	5.52	109.92	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	А	308	TYR	Sidechain
2	А	569	TYR	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	С	317	0	194	68	0
2	А	5032	0	4953	650	0
2	В	5055	0	5014	660	0
All	All	10404	0	10161	1353	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 66.

The worst 5 of 1353 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:C:10:DT:H5'	1:C:10:DT:C6	1.73	1.24
1:C:10:DT:OP1	1:C:10:DT:H3'	1.41	1.20
1:C:4:DT:H2"	1:C:5:DT:C5'	1.79	1.12
1:C:11:DT:H2'	1:C:11:DT:OP2	1.49	1.11
1:C:10:DT:H6	1:C:10:DT:C5'	1.66	1.09

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
2	А	632/673~(94%)	449 (71%)	142 (22%)	41 (6%)	1 7
2	В	629/673~(94%)	443 (70%)	148 (24%)	38 (6%)	1 9
All	All	1261/1346~(94%)	892 (71%)	290 (23%)	79(6%)	1 7

5 of 79 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	А	127	ASP
2	А	341	GLN
2	А	357	VAL
2	А	372	SER
2	А	375	THR

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
2	А	528/580~(91%)	402 (76%)	126 (24%)	0 3
2	В	536/580~(92%)	403 (75%)	133 (25%)	0 3
All	All	1064/1160~(92%)	805 (76%)	259 (24%)	0 3

5 of 259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	499	GLU
2	В	529	GLN
2	А	472	ILE
2	А	445	LEU
2	В	578	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such side chains are listed below:

2 B 206 ASN	Mol	Chain	Res	Type
	2	В	206	ASN

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Mol	Chain	Res	Type
2	В	354	GLN
2	В	217	GLN
2	В	263	GLN
2	В	365	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 monosaccharides 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.

