wwPDB X-ray Structure Validation Summary Report (i)

Aug 26, 2021 – 12:33 am BST

PDB ID	:	7AQS
Title	:	Crystal structure of E. coli DPS in space group P1
Authors	:	Jakob, R.P.; Pipercevic, J.; Righetto, R.; Goldie, K.; Stahlberg, H.; Maier, T.; Hiller, S.
Deposited on	:	2020-10-22
Resolution	:	2.80 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 following versions of software and data (see references (1)) were used in the production of this report:

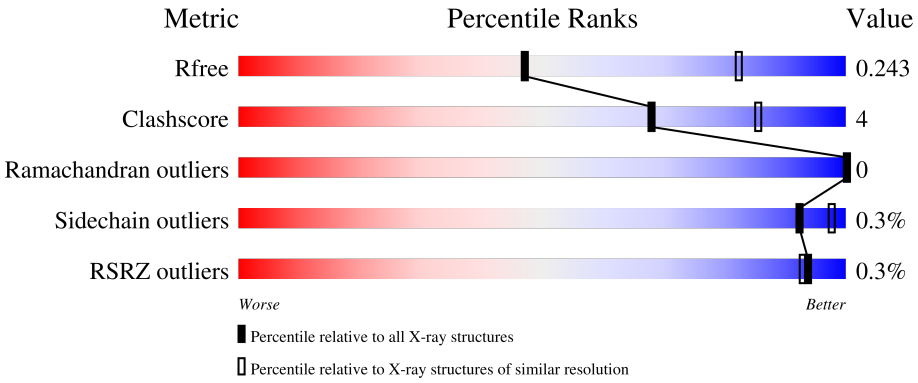
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	A	167	86% 8% 7%
1	B	167	84% 8% 7%
1	C	167	87% 7% 6%
1	D	167	80% 13% 7%
1	E	167	86% 9% 5%

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Mol	Chain	Length	Quality of chain
1	F	167	81% 11% 7%
1	G	167	84% 11% 5%
1	H	167	84% 10% 7%
1	I	167	79% 14% 7%
1	J	167	83% 10% 7%
1	K	167	84% 10% 7%
1	L	167	84% 11% 5%
1	M	167	87% 6% 7%
1	N	167	81% 11% 7%
1	O	167	88% 6% 6%
1	P	167	81% 11% 7%
1	Q	167	89% 6% 5%
1	R	167	80% 13% 7%
1	S	167	85% 8% 7%
1	T	167	84% 9% 7%
1	U	167	81% 12% 7%
1	V	167	83% 10% 7%
1	W	167	89% 5% 7%
1	X	167	85% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 59906 atoms, of which 29660 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 DNA protection during starvation protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	B	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	C	157	Total	C	H	N	O	Se	0	0	0
			2478	779	1237	217	242	3			
1	D	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	E	159	Total	C	H	N	O	Se	0	0	0
			2511	788	1255	220	245	3			
1	F	155	Total	C	H	N	O	Se	0	0	0
			2454	772	1225	215	239	3			
1	G	159	Total	C	H	N	O	Se	0	0	0
			2511	788	1255	220	245	3			
1	H	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	I	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	J	155	Total	C	H	N	O	Se	0	0	0
			2454	772	1225	215	239	3			
1	K	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	L	159	Total	C	H	N	O	Se	0	0	0
			2511	788	1255	220	245	3			
1	M	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	N	155	Total	C	H	N	O	Se	0	0	0
			2454	772	1225	215	239	3			
1	O	157	Total	C	H	N	O	Se	0	0	0
			2478	779	1237	217	242	3			
1	P	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	159	Total	C	H	N	O	Se	0	0	0
			2511	788	1255	220	245	3			
1	R	155	Total	C	H	N	O	Se	0	0	0
			2454	772	1225	215	239	3			
1	S	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	T	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	U	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	V	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	W	156	Total	C	H	N	O	Se	0	0	0
			2468	776	1232	216	241	3			
1	X	158	Total	C	H	N	O	Se	0	0	0
			2500	785	1250	219	243	3			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		
2	G	1	Total	Fe	0	0
			1	1		
2	H	1	Total	Fe	0	0
			1	1		
2	I	1	Total	Fe	0	0
			1	1		
2	J	1	Total	Fe	0	0
			1	1		
2	K	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	P	1	Total Fe 1 1	0	0
2	Q	1	Total Fe 1 1	0	0
2	R	1	Total Fe 1 1	0	0
2	S	1	Total Fe 1 1	0	0
2	T	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	V	1	Total Fe 1 1	0	0
2	W	1	Total Fe 1 1	0	0
2	X	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	35	Total O 35 35	0	0
3	C	21	Total O 21 21	0	0
3	D	11	Total O 11 11	0	0
3	E	27	Total O 27 27	0	0
3	F	9	Total O 9 9	0	0

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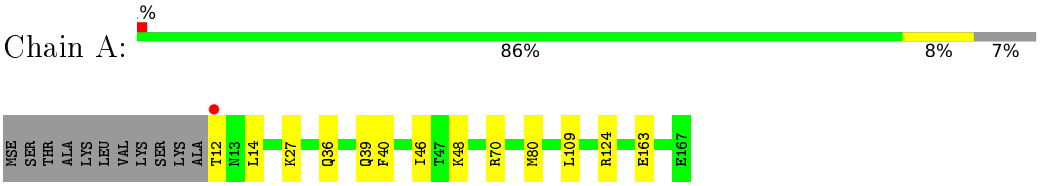
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	25	Total O 25 25	0	0
3	H	22	Total O 22 22	0	0
3	I	31	Total O 31 31	0	0
3	J	34	Total O 34 34	0	0
3	K	19	Total O 19 19	0	0
3	L	20	Total O 20 20	0	0
3	M	11	Total O 11 11	0	0
3	N	16	Total O 16 16	0	0
3	O	16	Total O 16 16	0	0
3	P	7	Total O 7 7	0	0
3	Q	22	Total O 22 22	0	0
3	R	15	Total O 15 15	0	0
3	S	20	Total O 20 20	0	0
3	T	19	Total O 19 19	0	0
3	U	28	Total O 28 28	0	0
3	V	22	Total O 22 22	0	0
3	W	14	Total O 14 14	0	0
3	X	14	Total O 14 14	0	0

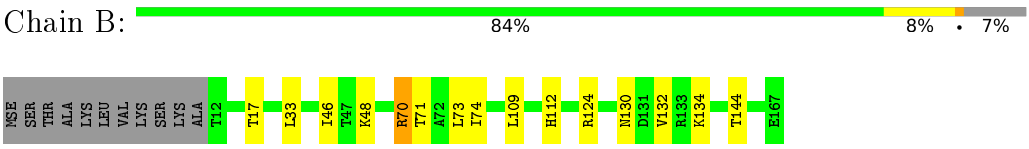
3 Residue-property plots (i)

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 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.

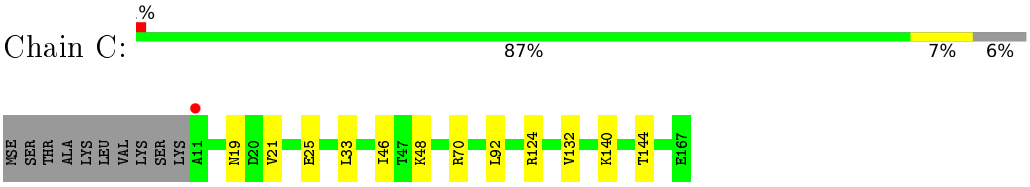
- Molecule 1: DNA protection during starvation protein



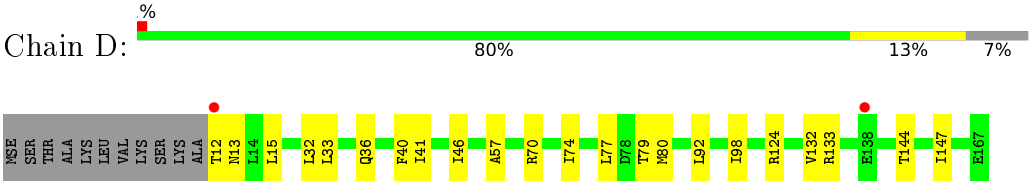
- Molecule 1: DNA protection during starvation protein



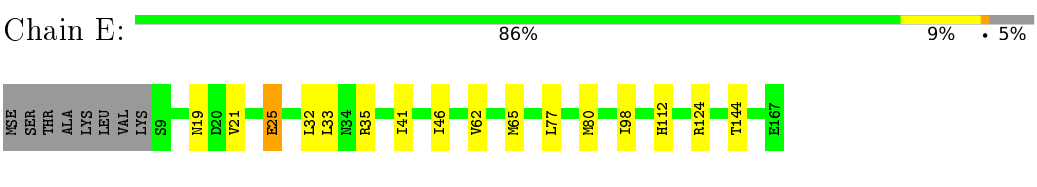
- Molecule 1: DNA protection during starvation protein



- Molecule 1: DNA protection during starvation protein

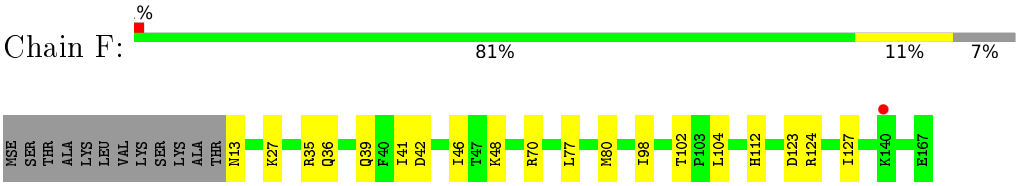


- Molecule 1: DNA protection during starvation protein



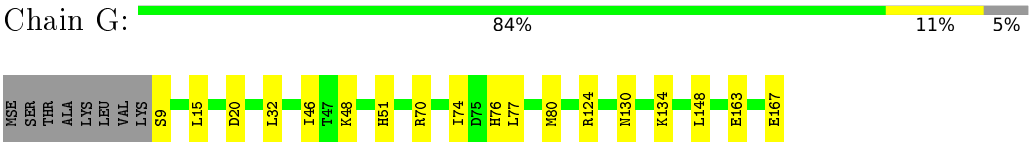
- Molecule 1: DNA protection during starvation protein

Chain F:



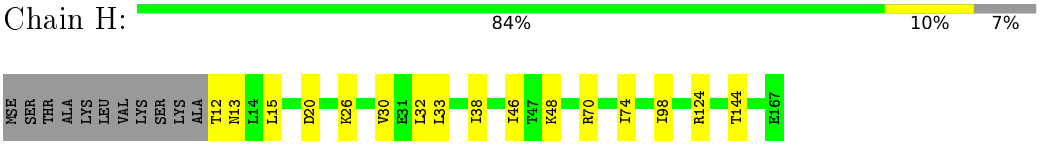
• Molecule 1: DNA protection during starvation protein

Chain G:



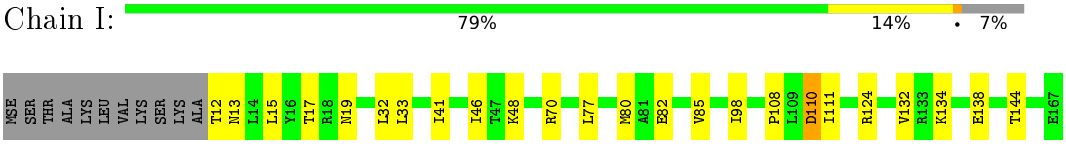
• Molecule 1: DNA protection during starvation protein

Chain H:



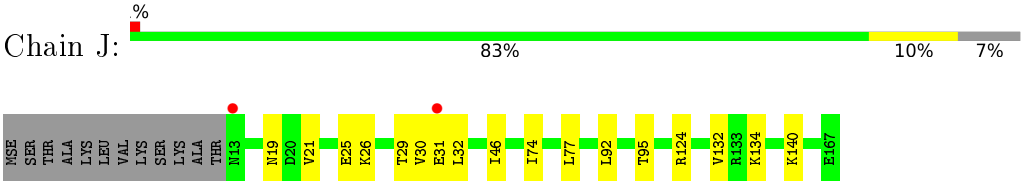
• Molecule 1: DNA protection during starvation protein

Chain I:



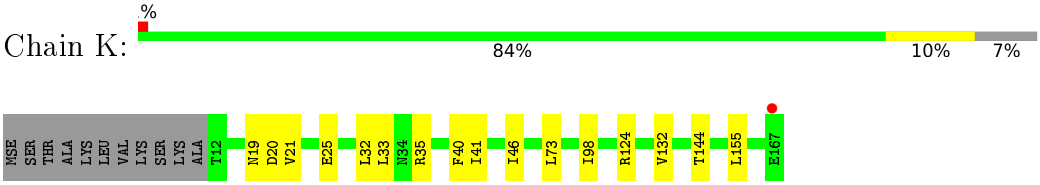
• Molecule 1: DNA protection during starvation protein

Chain J:



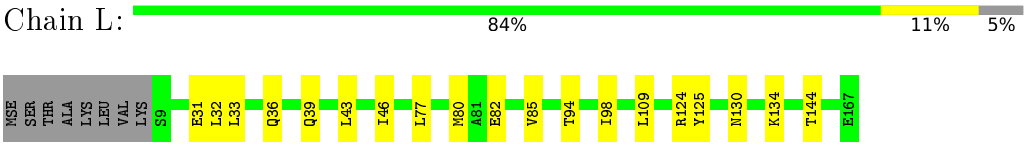
• Molecule 1: DNA protection during starvation protein

Chain K:



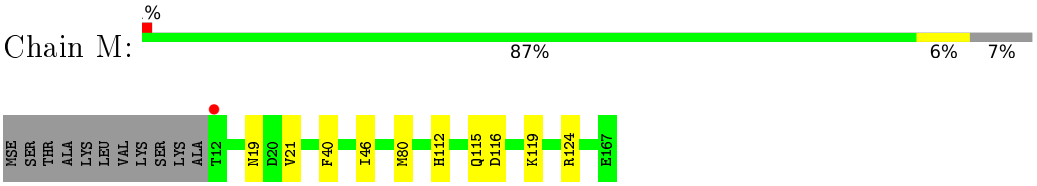
• Molecule 1: DNA protection during starvation protein

Chain L:



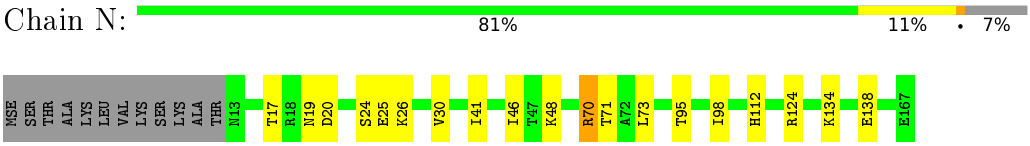
• Molecule 1: DNA protection during starvation protein

Chain M:



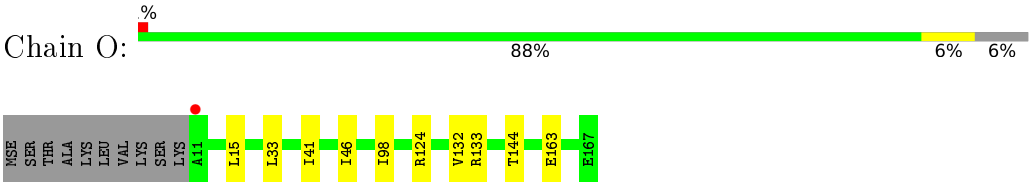
• Molecule 1: DNA protection during starvation protein

Chain N:



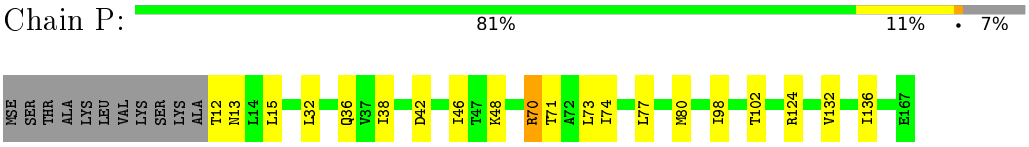
• Molecule 1: DNA protection during starvation protein

Chain O:



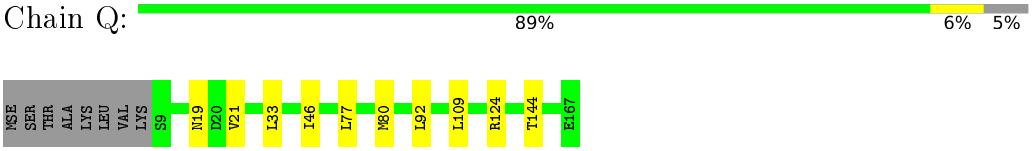
• Molecule 1: DNA protection during starvation protein

Chain P:



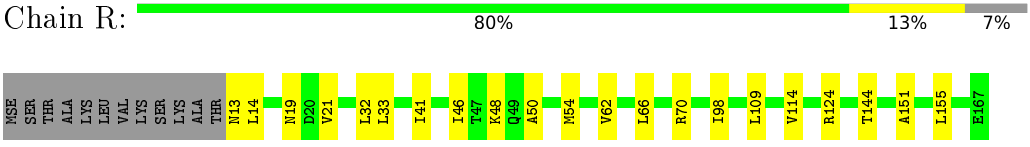
• Molecule 1: DNA protection during starvation protein

Chain Q:



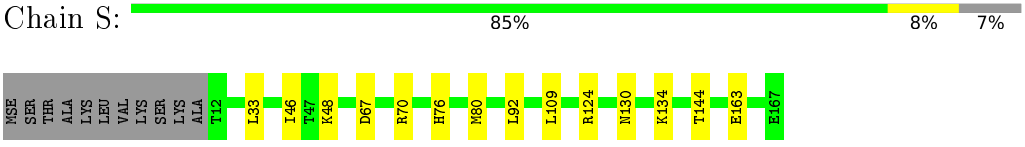
• Molecule 1: DNA protection during starvation protein

Chain R:



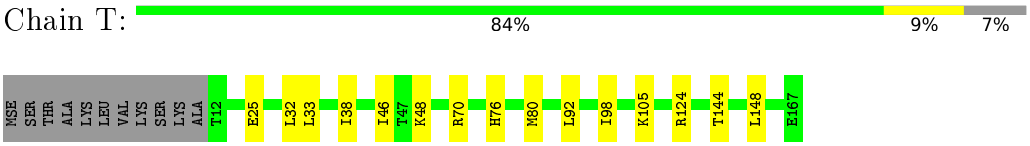
• Molecule 1: DNA protection during starvation protein

Chain S:



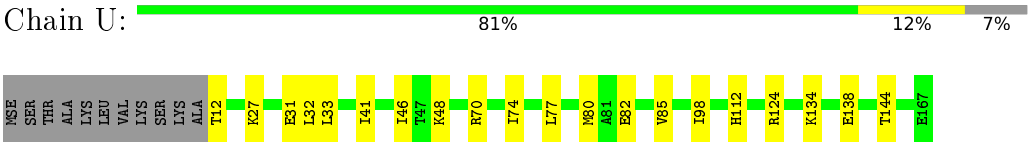
• Molecule 1: DNA protection during starvation protein

Chain T:



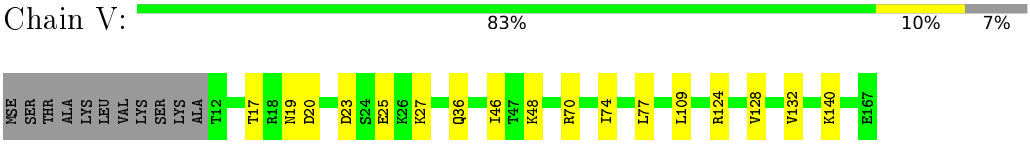
• Molecule 1: DNA protection during starvation protein

Chain U:



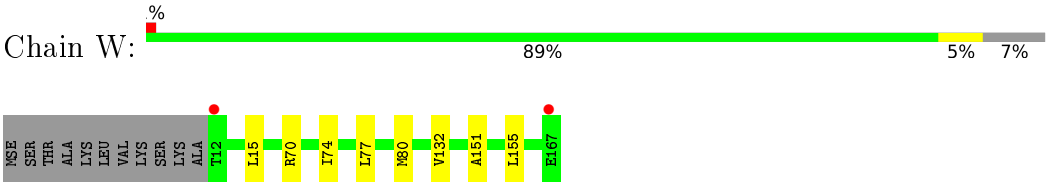
• Molecule 1: DNA protection during starvation protein

Chain V:



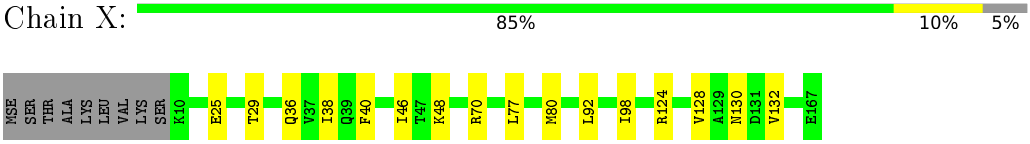
• Molecule 1: DNA protection during starvation protein

Chain W:



• Molecule 1: DNA protection during starvation protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	91.55Å 91.81Å 172.64Å 91.17° 100.52° 119.92°	Depositor
Resolution (Å)	45.90 – 2.80 45.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.90-2.80) 88.0 (45.90-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.202 , 0.243 0.202 , 0.243	Depositor DCC
R_{free} test set	3518 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.858	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	59906	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.96 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.0024e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.33	0/1251	0.49	0/1689
1	B	0.36	0/1251	0.55	0/1689
1	C	0.31	0/1256	0.52	0/1696
1	D	0.33	0/1251	0.52	0/1689
1	E	0.38	1/1271 (0.1%)	0.55	1/1715 (0.1%)
1	F	0.37	1/1244 (0.1%)	0.54	0/1679
1	G	0.37	0/1271	0.53	0/1715
1	H	0.32	0/1251	0.50	0/1689
1	I	0.32	0/1251	0.52	1/1689 (0.1%)
1	J	0.30	0/1244	0.48	0/1679
1	K	0.33	0/1251	0.54	1/1689 (0.1%)
1	L	0.33	0/1271	0.48	0/1715
1	M	0.32	0/1251	0.46	0/1689
1	N	0.37	0/1244	0.50	0/1679
1	O	0.36	0/1256	0.52	0/1696
1	P	0.38	1/1251 (0.1%)	0.52	0/1689
1	Q	0.32	0/1271	0.47	0/1715
1	R	0.34	0/1244	0.57	0/1679
1	S	0.33	0/1251	0.52	0/1689
1	T	0.35	0/1251	0.52	0/1689
1	U	0.33	0/1251	0.49	0/1689
1	V	0.33	0/1251	0.53	0/1689
1	W	0.33	0/1251	0.53	0/1689
1	X	0.33	0/1265	0.48	0/1707
All	All	0.34	3/30100 (0.0%)	0.52	3/40632 (0.0%)

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
1	B	0	1
1	N	0	1
1	P	0	1
1	X	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	35	ARG	CG-CD	6.74	1.68	1.51
1	F	35	ARG	CG-CD	5.42	1.65	1.51
1	P	74	ILE	CG1-CD1	-5.12	1.15	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	35	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	I	110	ASP	CB-CG-OD2	5.56	123.31	118.30
1	K	35	ARG	NE-CZ-NH1	-5.37	117.62	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	70	ARG	Mainchain
1	N	70	ARG	Mainchain
1	P	70	ARG	Mainchain
1	X	130	ASN	Mainchain

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	1236	1232	1232	8	0
1	B	1236	1232	1232	11	0
1	C	1241	1237	1237	6	0
1	D	1236	1232	1232	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1256	1255	1255	9	0
1	F	1229	1225	1225	10	0
1	G	1256	1255	1255	13	0
1	H	1236	1232	1232	10	0
1	I	1236	1232	1232	15	0
1	J	1229	1225	1225	12	0
1	K	1236	1232	1232	12	0
1	L	1256	1255	1255	15	0
1	M	1236	1232	1232	5	1
1	N	1229	1225	1225	15	1
1	O	1241	1237	1237	6	0
1	P	1236	1232	1232	14	0
1	Q	1256	1255	1255	6	0
1	R	1229	1225	1225	13	0
1	S	1236	1232	1232	12	0
1	T	1236	1232	1232	10	0
1	U	1236	1232	1232	12	0
1	V	1236	1232	1232	11	0
1	W	1236	1232	1232	4	0
1	X	1250	1250	1250	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	1	0	0	0	0
2	X	1	0	0	0	0
3	A	24	0	0	0	0
3	B	35	0	0	0	0
3	C	21	0	0	0	0
3	D	11	0	0	0	0
3	E	27	0	0	0	0
3	F	9	0	0	0	0
3	G	25	0	0	0	0
3	H	22	0	0	0	0
3	I	31	0	0	0	0
3	J	34	0	0	1	0
3	K	19	0	0	0	0
3	L	20	0	0	1	0
3	M	11	0	0	0	0
3	N	16	0	0	1	0
3	O	16	0	0	0	0
3	P	7	0	0	0	0
3	Q	22	0	0	0	0
3	R	15	0	0	0	0
3	S	20	0	0	0	0
3	T	19	0	0	1	0
3	U	28	0	0	0	0
3	V	22	0	0	0	0
3	W	14	0	0	0	0
3	X	14	0	0	1	0
All	All	30246	29660	29660	227	1

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 4.

The worst 5 of 227 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:N:134:LYS:NZ	1:N:138:GLU:OE2	2.01	0.94
1:N:25:GLU:OE2	3:N:301:HOH:O	1.91	0.88
1:L:31:GLU:OE2	3:L:301:HOH:O	2.01	0.79
1:I:134:LYS:NZ	1:I:138:GLU:OE2	2.18	0.75
1:T:25:GLU:OE2	3:T:301:HOH:O	2.02	0.75

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:ASP:OD2	1:N:24:SER:OG[1_455]	2.04	0.16

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	
1	A	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	B	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	C	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
1	D	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	E	157/167 (94%)	155 (99%)	2 (1%)	0	100	100
1	F	153/167 (92%)	151 (99%)	2 (1%)	0	100	100
1	G	157/167 (94%)	155 (99%)	2 (1%)	0	100	100
1	H	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
1	I	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
1	J	153/167 (92%)	150 (98%)	3 (2%)	0	100	100
1	K	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	L	157/167 (94%)	155 (99%)	2 (1%)	0	100	100
1	M	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
1	N	153/167 (92%)	151 (99%)	2 (1%)	0	100	100
1	O	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
1	P	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
1	Q	157/167 (94%)	154 (98%)	3 (2%)	0	100	100
1	R	153/167 (92%)	150 (98%)	3 (2%)	0	100	100
1	S	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	T	154/167 (92%)	152 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	V	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	W	154/167 (92%)	152 (99%)	2 (1%)	0	100	100
1	X	156/167 (93%)	154 (99%)	2 (1%)	0	100	100
All	All	3708/4008 (92%)	3650 (98%)	58 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	134/139 (96%)	134 (100%)	0	100	100
1	B	134/139 (96%)	133 (99%)	1 (1%)	84	95
1	C	134/139 (96%)	133 (99%)	1 (1%)	84	95
1	D	134/139 (96%)	134 (100%)	0	100	100
1	E	136/139 (98%)	135 (99%)	1 (1%)	84	95
1	F	133/139 (96%)	133 (100%)	0	100	100
1	G	136/139 (98%)	135 (99%)	1 (1%)	84	95
1	H	134/139 (96%)	134 (100%)	0	100	100
1	I	134/139 (96%)	133 (99%)	1 (1%)	84	95
1	J	133/139 (96%)	132 (99%)	1 (1%)	81	94
1	K	134/139 (96%)	133 (99%)	1 (1%)	84	95
1	L	136/139 (98%)	136 (100%)	0	100	100
1	M	134/139 (96%)	134 (100%)	0	100	100
1	N	133/139 (96%)	133 (100%)	0	100	100
1	O	134/139 (96%)	133 (99%)	1 (1%)	84	95
1	P	134/139 (96%)	134 (100%)	0	100	100
1	Q	136/139 (98%)	136 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	133/139 (96%)	133 (100%)	0	100 100
1	S	134/139 (96%)	134 (100%)	0	100 100
1	T	134/139 (96%)	134 (100%)	0	100 100
1	U	134/139 (96%)	134 (100%)	0	100 100
1	V	134/139 (96%)	134 (100%)	0	100 100
1	W	134/139 (96%)	133 (99%)	1 (1%)	84 95
1	X	135/139 (97%)	135 (100%)	0	100 100
All	All	3221/3336 (97%)	3212 (100%)	9 (0%)	92 98

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	132	VAL
1	W	132	VAL
1	G	9	SER
1	I	132	VAL
1	J	132	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	113	ASN
1	G	13	ASN
1	T	99	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

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 95^{th} 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	A	153/167 (91%)	-0.41	1 (0%) 87 84	19, 32, 58, 93	0
1	B	153/167 (91%)	-0.48	0 100 100	15, 29, 50, 73	0
1	C	154/167 (92%)	-0.31	1 (0%) 89 86	21, 36, 56, 101	0
1	D	153/167 (91%)	-0.36	2 (1%) 77 72	21, 34, 61, 87	0
1	E	156/167 (93%)	-0.45	0 100 100	15, 27, 50, 72	0
1	F	152/167 (91%)	-0.30	1 (0%) 87 84	21, 38, 63, 81	0
1	G	156/167 (93%)	-0.47	0 100 100	15, 28, 53, 74	0
1	H	153/167 (91%)	-0.37	0 100 100	23, 35, 55, 81	0
1	I	153/167 (91%)	-0.47	0 100 100	14, 27, 49, 74	0
1	J	152/167 (91%)	-0.42	2 (1%) 77 72	17, 29, 56, 91	0
1	K	153/167 (91%)	-0.29	1 (0%) 87 84	20, 38, 59, 85	0
1	L	156/167 (93%)	-0.38	0 100 100	18, 30, 55, 75	0
1	M	153/167 (91%)	-0.28	1 (0%) 87 84	26, 36, 62, 91	0
1	N	152/167 (91%)	-0.27	0 100 100	30, 41, 62, 80	0
1	O	154/167 (92%)	-0.32	1 (0%) 89 86	24, 37, 58, 87	0
1	P	153/167 (91%)	-0.17	0 100 100	33, 43, 65, 93	0
1	Q	156/167 (93%)	-0.29	0 100 100	30, 38, 56, 73	0
1	R	152/167 (91%)	-0.27	0 100 100	27, 38, 62, 82	0
1	S	153/167 (91%)	-0.30	0 100 100	26, 40, 64, 85	0
1	T	153/167 (91%)	-0.34	0 100 100	24, 34, 61, 75	0
1	U	153/167 (91%)	-0.35	0 100 100	24, 35, 56, 91	0
1	V	153/167 (91%)	-0.40	0 100 100	23, 33, 53, 76	0
1	W	153/167 (91%)	-0.20	2 (1%) 77 72	29, 40, 59, 111	0
1	X	155/167 (92%)	-0.30	0 100 100	26, 39, 60, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	3684/4008 (91%)	-0.34	12 (0%)	94	93	14, 35, 59, 111	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	11	ALA	3.8
1	W	12	THR	3.7
1	M	12	THR	3.4
1	J	31	GLU	2.6
1	C	11	ALA	2.5

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	S	201	1/1	0.95	0.14	16,16,16,16	1
2	FE	C	201	1/1	0.96	0.11	16,16,16,16	1
2	FE	E	201	1/1	0.98	0.11	17,17,17,17	0
2	FE	F	201	1/1	0.98	0.13	20,20,20,20	1
2	FE	G	201	1/1	0.98	0.11	25,25,25,25	0
2	FE	J	201	1/1	0.98	0.13	17,17,17,17	1
2	FE	L	201	1/1	0.98	0.11	23,23,23,23	0
2	FE	N	201	1/1	0.98	0.07	14,14,14,14	1
2	FE	P	201	1/1	0.98	0.13	17,17,17,17	1
2	FE	B	201	1/1	0.98	0.11	23,23,23,23	1
2	FE	V	201	1/1	0.98	0.09	16,16,16,16	1
2	FE	W	201	1/1	0.98	0.14	20,20,20,20	1
2	FE	X	201	1/1	0.98	0.10	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	H	201	1/1	0.99	0.12	17,17,17,17	1
2	FE	O	201	1/1	0.99	0.08	23,23,23,23	1
2	FE	I	201	1/1	0.99	0.07	25,25,25,25	0
2	FE	Q	201	1/1	0.99	0.16	17,17,17,17	1
2	FE	R	201	1/1	0.99	0.10	18,18,18,18	1
2	FE	D	201	1/1	0.99	0.12	21,21,21,21	1
2	FE	T	201	1/1	0.99	0.11	19,19,19,19	1
2	FE	U	201	1/1	0.99	0.10	15,15,15,15	1
2	FE	K	201	1/1	0.99	0.08	23,23,23,23	0
2	FE	A	201	1/1	0.99	0.10	24,24,24,24	1
2	FE	M	201	1/1	0.99	0.14	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.