wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 01:11 am BST

PDB ID	:	2D7E
Title	:	Crystal structure of N-terminal domain of PriA from E.coli
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Deposited on	:	2005-11-18
Resolution	:	2.50 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:

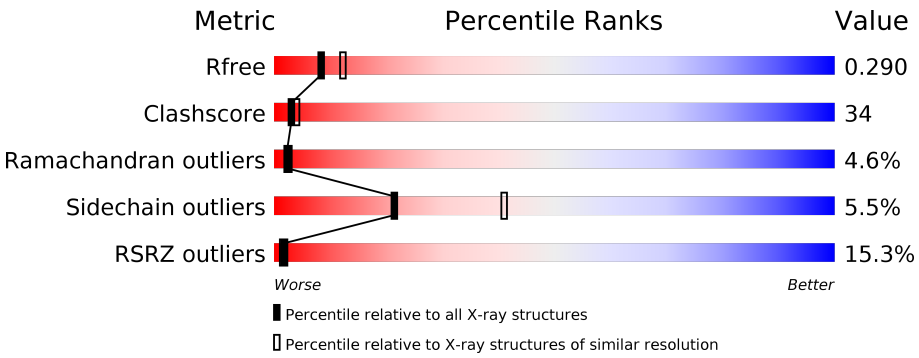
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	105	9% 53% 43% •
1	B	105	30% 38% 53% 7% • •
1	C	105	14% 57% 36% 5% •
1	D	105	9% 52% 34% 10% • •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3352 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 Primosomal protein N'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	105	832	546	141	142	3	0	0	0
1	B	104	820	540	137	140	3	0	0	0
1	C	105	832	546	141	142	3	0	0	0
1	D	103	812	535	136	139	2	0	0	0

- Molecule 2 is water.

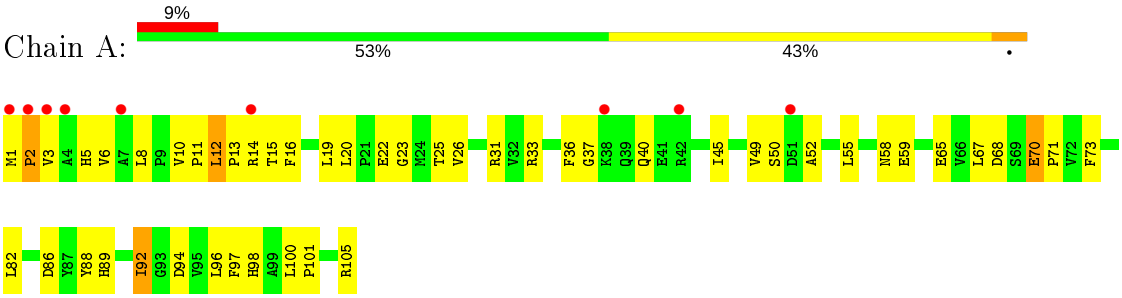
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	12	12	12	0	0
2	B	11	11	11	0	0
2	C	14	14	14	0	0
2	D	19	19	19	0	0

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.

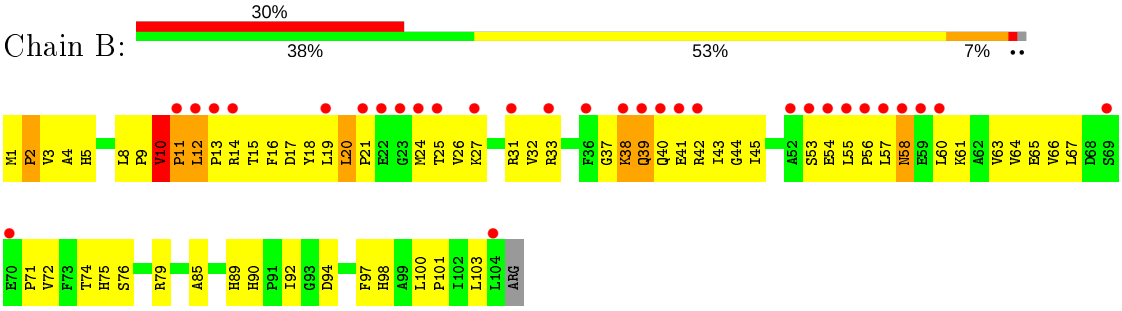
- Molecule 1: Primosomal protein N'

Chain A:



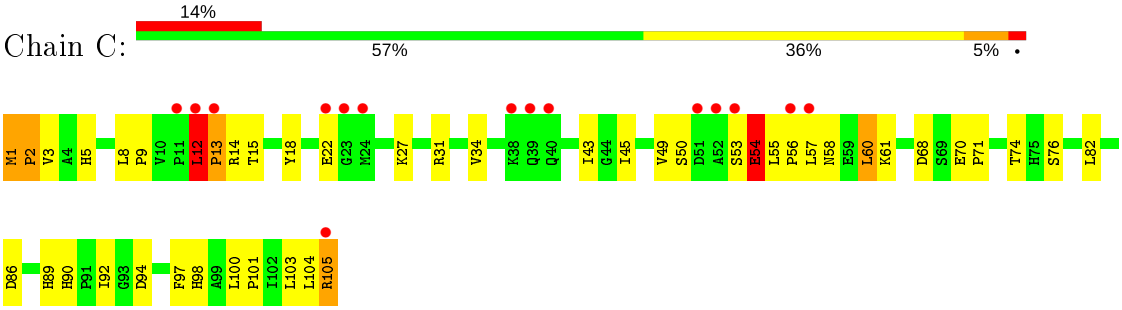
- Molecule 1: Primosomal protein N'

Chain B:



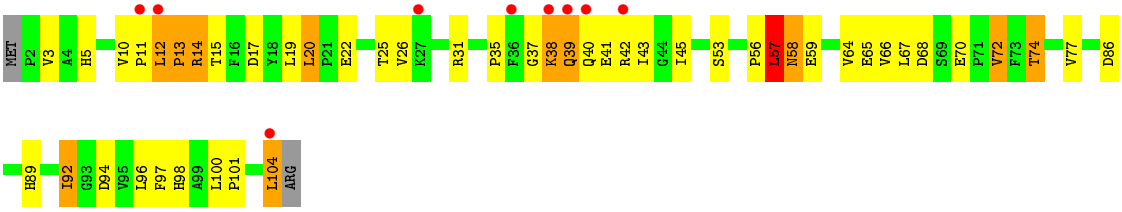
- Molecule 1: Primosomal protein N'

Chain C:



- Molecule 1: Primosomal protein N'

Chain D:


MET
P2
V3
A4
H5
V10
P11
L12
P13
R14
T15
F16
D17
Y18
L19
L20
P21
E22
T25
V26
K27
R31
P35
F36
G37
K38
Q39
Q40
E41
R42
I43
G44
I45
S53
P56
L57
N58
E59
V64
E65
V66
L67
D68
S69
E70
P71
V72
F73
T74
V77
D86
H89
I92
G93
D94
V95
L96
F97
H98
A99
L100
P101
L104
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	111.57Å 111.57Å 260.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 32.21 – 2.52	Depositor EDS
% Data completeness (in resolution range)	90.8 (20.00-2.50) 97.4 (32.21-2.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.28 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.292 0.247 , 0.290	Depositor DCC
R_{free} test set	1418 reflections (6.82%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.018 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.025 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	3352	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.42	0/857	0.68	0/1173
1	B	0.36	0/845	0.63	0/1159
1	C	0.46	0/857	0.70	0/1173
1	D	0.47	0/837	0.77	0/1148
All	All	0.43	0/3396	0.70	0/4653

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 (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	832	0	853	66	0
1	B	820	0	840	92	0
1	C	832	0	853	57	0
1	D	812	0	829	57	0
2	A	12	0	0	5	0
2	B	11	0	0	4	0
2	C	14	0	0	0	0
2	D	19	0	0	3	0
All	All	3352	0	3375	227	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 34.

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:A:3:VAL:HG21	1:B:53:SER:HB2	1.38	1.03
1:D:12:LEU:HG	1:D:13:PRO:HD3	1.43	0.98
1:C:12:LEU:HB3	1:C:13:PRO:HD3	1.46	0.97
1:B:12:LEU:HB3	1:B:13:PRO:HD3	1.44	0.96
1:D:57:LEU:HD23	1:D:57:LEU:H	1.40	0.87

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
1	A	103/105 (98%)	98 (95%)	3 (3%)	2 (2%)	8 13
1	B	102/105 (97%)	83 (81%)	14 (14%)	5 (5%)	2 2
1	C	103/105 (98%)	89 (86%)	9 (9%)	5 (5%)	2 2
1	D	101/105 (96%)	85 (84%)	9 (9%)	7 (7%)	1 1
All	All	409/420 (97%)	355 (87%)	35 (9%)	19 (5%)	2 2

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	12	LEU
1	C	12	LEU
1	C	58	ASN
1	D	12	LEU

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	92/92 (100%)	90 (98%)	2 (2%)	52	77
1	B	91/92 (99%)	87 (96%)	4 (4%)	28	52
1	C	92/92 (100%)	86 (94%)	6 (6%)	17	33
1	D	90/92 (98%)	82 (91%)	8 (9%)	9	19
All	All	365/368 (99%)	345 (94%)	20 (6%)	21	41

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	54	GLU
1	C	60	LEU
1	D	66	VAL
1	C	12	LEU
1	C	22	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	58	ASN
1	C	89	HIS
1	D	58	ASN
1	B	98	HIS
1	C	98	HIS

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 (i)

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	A	105/105 (100%)	0.50	9 (8%)	10	10	43, 62, 115, 136	0
1	B	104/105 (99%)	1.65	31 (29%)	0	0	42, 114, 140, 146	0
1	C	105/105 (100%)	0.68	15 (14%)	2	2	32, 62, 109, 120	0
1	D	103/105 (98%)	0.53	9 (8%)	10	10	34, 64, 89, 108	0
All	All	417/420 (99%)	0.84	64 (15%)	2	1	32, 67, 132, 146	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	12	LEU	9.7
1	B	60	LEU	9.2
1	B	11	PRO	7.6
1	A	1	MET	7.2
1	D	12	LEU	6.9

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.