

wwPDB X-ray Structure Validation Summary Report (i)

Aug 23, 2023 – 09:49 AM EDT

PDB ID : 3D3C

Title : Structural and functional analysis of the E. coli NusB-S10 transcription an-

titermination complex.

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Deposited on : 2008-05-09

Resolution : 2.60 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:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS : 2.35

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)

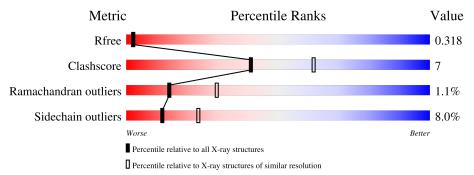
Validation Pipeline (wwPDB-VP) : 2.35

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 2.60 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	Similar resolution
Metric	$(\# { m Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Mol	Chain	Length	Quality of chain		
1	A	141	80%	12%	5% • •
1	В	141	87%	9%	, 6 ••
1	С	141	71%	23%	• •
2	J	87	83%	14%	•••
2	K	87	80%	17%	•
2	L	87	78%	21%	



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5505 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 N utilization substance protein B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	138	Total	С	N	О	S	0	0	0
1	A	130	1097	699	189	207	2	0	0	0
1	D	138	Total	С	N	О	S	0	0	0
1	Б	130	1097	699	189	207	2	0	0	0
1	С	138	Total	С	N	О	S	0	0	0
1		130	1097	699	189	207	2			U

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P0A780
A	0	ALA	-	expression tag	UNP P0A780
A	2	GLU	LYS	engineered mutation	UNP P0A780
В	-1	GLY	-	expression tag	UNP P0A780
В	0	ALA	-	expression tag	UNP P0A780
В	2	GLU	LYS	engineered mutation	UNP P0A780
С	-1	GLY	-	expression tag	UNP P0A780
С	0	ALA	-	expression tag	UNP P0A780
С	2	GLU	LYS	engineered mutation	UNP P0A780

• Molecule 2 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	Ţ	85	Total	С	N	О	S	0	0	0
2	J	0.0	665	411	128	124	2	0	U	U
2	V	87	Total	С	N	О	S	0	0	0
	IX	01	676	418	130	126	2	0	U	U
2	т	87	Total	С	N	О	S	0	0	0
	ь	01	676	418	130	126	2		U	U

There are 21 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	expression tag	UNP P0A7R5
J	-3	PRO	-	expression tag	UNP P0A7R5
J	-2	LEU	-	expression tag	UNP P0A7R5
J	-1	GLY	-	expression tag	UNP P0A7R5
J	0	SER	-	expression tag	UNP P0A7R5
J	46	SER	-	SEE REMARK 999	UNP P0A7R5
J	65	ASP	ALA	engineered mutation	UNP P0A7R5
K	-4	GLY	-	expression tag	UNP P0A7R5
K	-3	PRO	-	expression tag	UNP P0A7R5
K	-2	LEU	-	expression tag	UNP P0A7R5
K	-1	GLY	-	expression tag	UNP P0A7R5
K	0	SER	-	expression tag	UNP P0A7R5
K	46	SER	-	SEE REMARK 999	UNP P0A7R5
K	65	ASP	ALA	engineered mutation	UNP P0A7R5
L	-4	GLY	-	expression tag	UNP P0A7R5
L	-3	PRO	-	expression tag	UNP P0A7R5
L	-2	LEU	-	expression tag	UNP P0A7R5
L	-1	GLY	-	expression tag	UNP P0A7R5
L	0	SER	-	expression tag	UNP P0A7R5
L	46	SER	-	SEE REMARK 999	UNP P0A7R5
L	65	ASP	ALA	engineered mutation	UNP P0A7R5

• Molecule 3 is water.

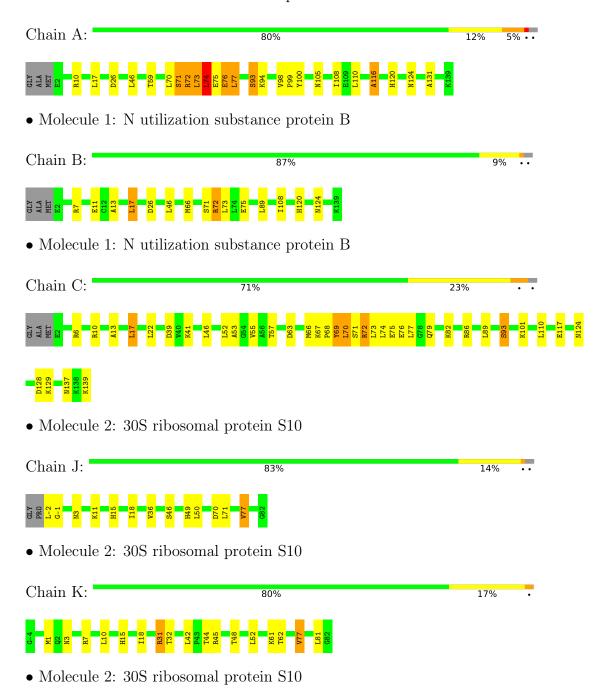
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	32	Total O 32 32	0	0
3	J	21	Total O 21 21	0	0
3	В	55	Total O 55 55	0	0
3	K	28	Total O 28 28	0	0
3	С	28	Total O 28 28	0	0
3	L	33	Total O 33 33	0	0



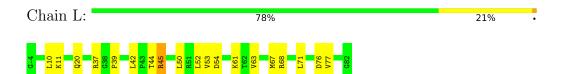
3 Residue-property plots (i)

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.

• Molecule 1: N utilization substance protein B









4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants	113.00Å 113.00Å 267.20Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.60	Depositor
Resolution (A)	49.65 - 2.61	EDS
% Data completeness	100.0 (30.00-2.60)	Depositor
(in resolution range)	98.5 (49.65-2.61)	EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) > 1$	3.66 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
D D	0.218 , 0.280	Depositor
R, R_{free}	0.280 , 0.318	DCC
R_{free} test set	1318 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.30 , 44.6	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5505	wwPDB-VP
Average B, all atoms $(Å^2)$	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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		
WIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.36	0/1115	0.58	1/1508 (0.1%)	
1	В	0.31	0/1115	0.51	0/1508	
1	С	0.33	0/1115	0.52	0/1508	
2	J	0.31	0/671	0.58	0/905	
2	K	0.32	0/683	0.57	0/922	
2	L	0.31	0/683	0.52	0/922	
All	All	0.33	0/5382	0.55	$1/7273 \ (0.0\%)$	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	74	LEU	CB-CG-CD2	6.85	122.65	111.00

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	1097	0	1110	16	0
1	В	1097	0	1110	6	0
1	С	1097	0	1110	32	0
2	J	665	0	702	5	0
2	K	676	0	712	8	0
2	L	676	0	712	11	0

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Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	32	0	0	0	0
3	В	55	0	0	0	0
3	С	28	0	0	0	0
3	J	21	0	0	0	0
3	K	28	0	0	1	0
3	L	33	0	0	0	0
All	All	5505	0	5456	76	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 7.

The worst 5 of 76 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
1:C:70:LEU:HD12	1:C:74:LEU:HA	1.40	1.02
1:C:72:ARG:H	1:C:72:ARG:CD	1.68	1.01
1:C:72:ARG:H	1:C:72:ARG:HD2	1.36	0.88
1:C:72:ARG:HH21	1:C:72:ARG:CG	1.98	0.76
1:C:66:MET:HG3	1:C:89:LEU:HD11	1.68	0.75

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	Percentile	s
1	A	$136/141 \ (96\%)$	126 (93%)	6 (4%)	4 (3%)	4 7	
1	В	$136/141\ (96\%)$	134 (98%)	2 (2%)	0	100 100	,
1	С	$136/141 \ (96\%)$	128 (94%)	7 (5%)	1 (1%)	22 43	
2	J	83/87~(95%)	79 (95%)	2 (2%)	2 (2%)	6 10	
2	K	85/87~(98%)	84 (99%)	1 (1%)	0	100 100	

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
2	L	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
All	All	661/684 (97%)	632 (96%)	22 (3%)	7 (1%)	14	30

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	76	GLU
1	A	77	LEU
1	С	76	GLU
2	J	-1	GLY

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	115/116 (99%)	105 (91%)	10 (9%)	10 20
1	В	115/116 (99%)	108 (94%)	7 (6%)	18 38
1	С	115/116 (99%)	104 (90%)	11 (10%)	8 16
2	J	73/74 (99%)	68 (93%)	5 (7%)	16 32
2	K	74/74 (100%)	67 (90%)	7 (10%)	8 16
2	L	74/74 (100%)	69 (93%)	5 (7%)	16 32
All	All	566/570 (99%)	521 (92%)	45 (8%)	12 24

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	K	77	VAL
1	С	93	SER
1	С	6	ARG
1	С	69	TYR
1	С	117	GLU



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

Mol	Chain	Res	Type
1	С	21	GLN
1	С	33	GLN
2	L	49	HIS
1	С	79	GLN
2	J	35	GLN

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

