



# wwPDB X-ray Structure Validation Summary Report

Aug 22, 2023 – 07:13 AM EDT

PDB ID : 2R1A  
Title : Crystal structure of the periplasmic lipopolysaccharide transport protein LptA (YhbN), trigonal form  
Authors : Suits, M.D.L.; Polissi, A.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)  
Deposited on : 2007-08-22  
Resolution : 3.26 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](mailto: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 : 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

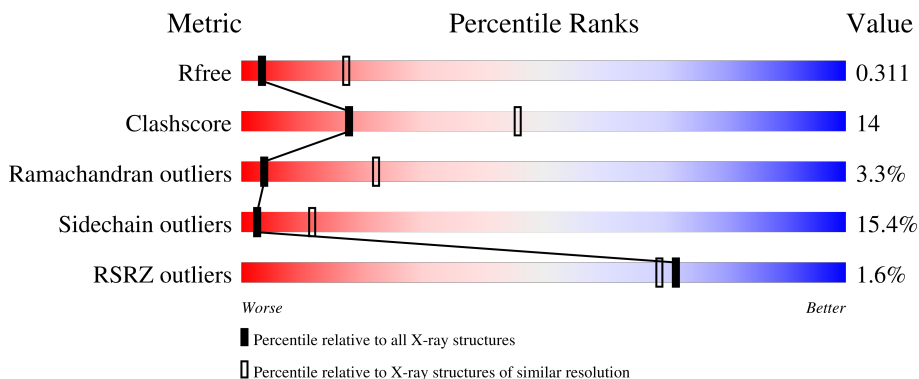
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 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.



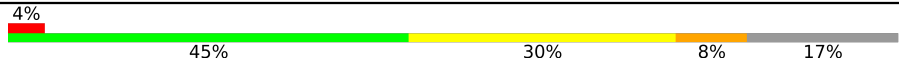


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	159	 58% 22% 18% 2%
1	B	159	 47% 34% 16% 2%
1	C	159	 60% 20% 15% 5%
1	D	159	 61% 21% 14% 4%
1	E	159	 55% 24% 17% 4%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	159	 4% 45% 30% 8% 17%
1	G	159	 67% 13% 5% 15%
1	H	159	 2% 60% 18% • 18%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7620 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 Protein yhbN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	131	Total 927	C 578	N 154	O 191	S 4	0	0	0
1	B	134	Total 956	C 594	N 160	O 198	S 4	0	0	0
1	C	135	Total 989	C 617	N 163	O 206	S 3	0	0	0
1	D	136	Total 923	C 572	N 156	O 193	S 2	0	0	0
1	E	132	Total 918	C 569	N 155	O 192	S 2	0	0	0
1	F	132	Total 938	C 584	N 155	O 196	S 3	0	0	0
1	G	135	Total 980	C 609	N 165	O 203	S 3	0	0	0
1	H	131	Total 921	C 572	N 152	O 195	S 2	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	9	Total 9	O 9	0	0
2	B	8	Total 8	O 8	0	0
2	C	2	Total 2	O 2	0	0
2	D	8	Total 8	O 8	0	0
2	E	14	Total 14	O 14	0	0
2	F	9	Total 9	O 9	0	0

*Continued on next page...*

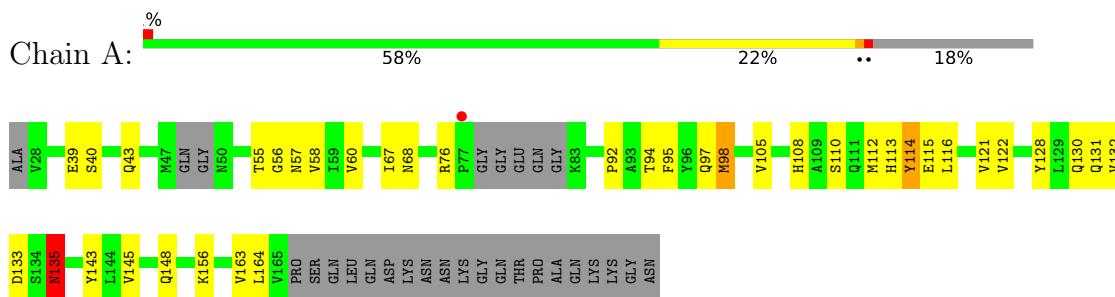
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	G	14	Total	O	0	0
			14	14		
2	H	4	Total	O	0	0
			4	4		

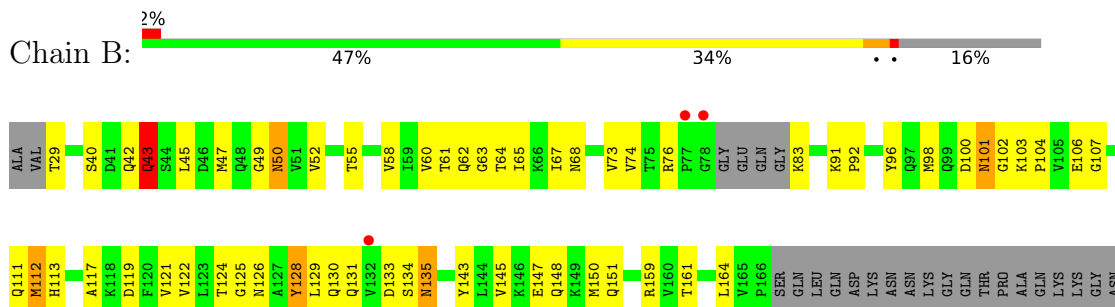
### 3 Residue-property plots [i](#)

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.

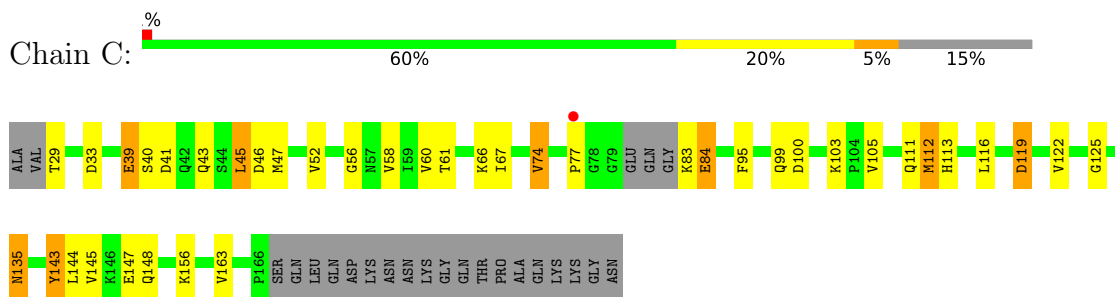
- Molecule 1: Protein yhbN



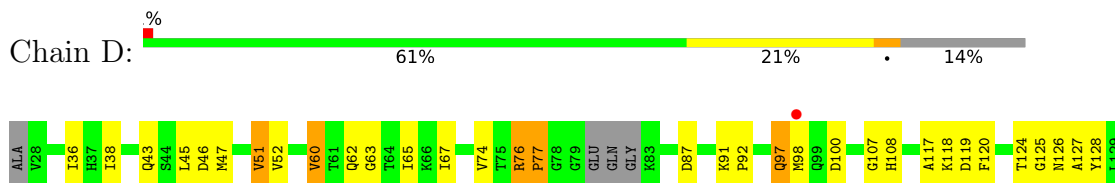
- Molecule 1: Protein yhbN

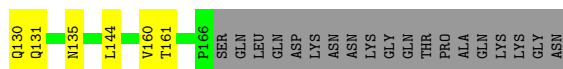


- Molecule 1: Protein yhbN

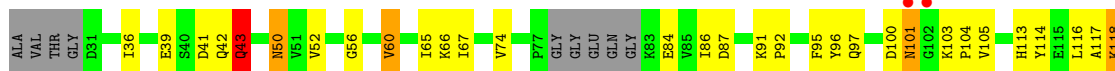


- Molecule 1: Protein yhbN

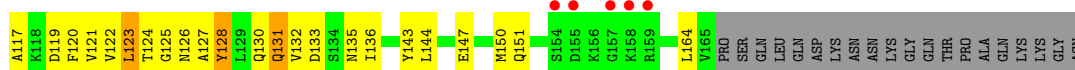
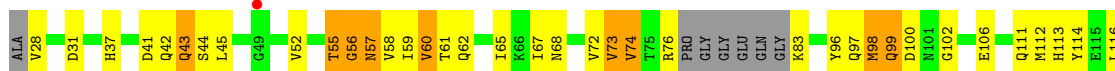
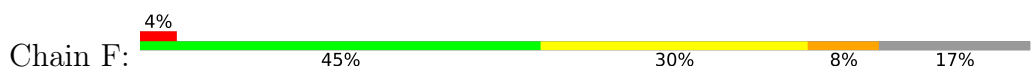




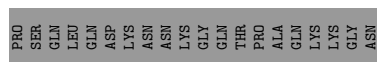
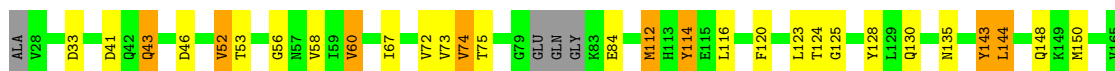
- Molecule 1: Protein yhbN



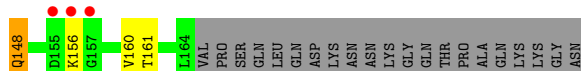
- Molecule 1: Protein yhbN



- Molecule 1: Protein yhbN



- Molecule 1: Protein yhbN



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.21Å 146.21Å 186.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 3.26 29.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	83.6 (29.98-3.26) 97.3 (29.98-3.25)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.55 (at 3.24Å)	Xtrriage
Refinement program	REFMAC 5.4.0065, PHENIX	Depositor
R, $R_{free}$	0.298 , 0.361 0.306 , 0.311	Depositor DCC
$R_{free}$ test set	1794 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.8	Xtrriage
Anisotropy	0.935	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.033 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	7620	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.40 % 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 9.4591e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.34	0/940	0.52	0/1283
1	B	0.38	0/971	0.54	0/1327
1	C	0.36	0/1004	0.53	0/1371
1	D	0.36	0/937	0.51	0/1285
1	E	0.36	0/932	0.57	0/1280
1	F	0.39	1/951 (0.1%)	0.58	0/1301
1	G	0.34	0/994	0.52	0/1356
1	H	0.34	0/934	0.50	0/1281
All	All	0.36	1/7663 (0.0%)	0.53	0/10484

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	132	VAL	CB-CG1	-5.18	1.42	1.52

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	927	0	798	25	0
1	B	956	0	831	35	0
1	C	989	0	899	28	0
1	D	923	0	762	20	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	918	0	758	25	0
1	F	938	0	817	36	0
1	G	980	0	882	16	0
1	H	921	0	783	17	0
2	A	9	0	0	1	0
2	B	8	0	0	1	0
2	C	2	0	0	0	0
2	D	8	0	0	0	0
2	E	14	0	0	1	0
2	F	9	0	0	1	0
2	G	14	0	0	1	0
2	H	4	0	0	2	0
All	All	7620	0	6530	191	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 14.

The worst 5 of 191 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:148:GLN:HG3	1:B:47:MET:HB2	1.48	0.95
1:F:98:MET:HA	1:F:99:GLN:CB	1.98	0.93
1:F:97:GLN:HG2	1:F:98:MET:H	1.43	0.83
1:B:148:GLN:HB3	1:C:47:MET:HB2	1.60	0.81
1:C:143:TYR:CE1	1:C:145:VAL:HA	2.15	0.81

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	125/159 (79%)	98 (78%)	23 (18%)	4 (3%)	4	23
1	B	130/159 (82%)	95 (73%)	31 (24%)	4 (3%)	4	24
1	C	131/159 (82%)	117 (89%)	12 (9%)	2 (2%)	10	39
1	D	132/159 (83%)	105 (80%)	19 (14%)	8 (6%)	1	10
1	E	128/159 (80%)	101 (79%)	19 (15%)	8 (6%)	1	9
1	F	128/159 (80%)	100 (78%)	24 (19%)	4 (3%)	4	24
1	G	131/159 (82%)	116 (88%)	14 (11%)	1 (1%)	19	52
1	H	127/159 (80%)	109 (86%)	15 (12%)	3 (2%)	6	28
All	All	1032/1272 (81%)	841 (82%)	157 (15%)	34 (3%)	4	22

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	156	LYS
1	D	77	PRO
1	D	119	ASP
1	E	118	LYS
1	F	99	GLN

### 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	88/135 (65%)	77 (88%)	11 (12%)	4	19
1	B	91/135 (67%)	73 (80%)	18 (20%)	1	5
1	C	101/135 (75%)	89 (88%)	12 (12%)	5	20
1	D	82/135 (61%)	72 (88%)	10 (12%)	5	20
1	E	82/135 (61%)	71 (87%)	11 (13%)	4	16
1	F	91/135 (67%)	65 (71%)	26 (29%)	0	1
1	G	98/135 (73%)	85 (87%)	13 (13%)	4	16
1	H	87/135 (64%)	77 (88%)	10 (12%)	5	22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	720/1080 (67%)	609 (85%)	111 (15%)	<b>2</b> <b>12</b>

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	100	ASP
1	H	144	LEU
1	F	73	VAL
1	H	135	ASN
1	G	143	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	108	HIS
1	H	68	ASN
1	G	42	GLN
1	G	135	ASN
1	H	131	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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	131/159 (82%)	-0.06	1 (0%) 86 86	44, 64, 75, 77	0
1	B	134/159 (84%)	0.08	3 (2%) 62 59	54, 63, 74, 80	0
1	C	135/159 (84%)	-0.21	1 (0%) 87 88	32, 41, 61, 65	0
1	D	136/159 (85%)	-0.03	1 (0%) 87 88	46, 69, 76, 78	0
1	E	132/159 (83%)	0.11	2 (1%) 73 71	63, 71, 77, 80	0
1	F	132/159 (83%)	0.03	6 (4%) 33 31	46, 58, 68, 70	0
1	G	135/159 (84%)	-0.20	0 100 100	34, 46, 58, 60	0
1	H	131/159 (82%)	-0.09	3 (2%) 60 58	35, 54, 68, 71	0
All	All	1066/1272 (83%)	-0.05	17 (1%) 72 69	32, 60, 75, 80	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	77	PRO	3.6
1	F	49	GLY	2.6
1	H	155	ASP	2.6
1	F	155	ASP	2.5
1	B	77	PRO	2.4

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.