



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:56 PM GMT

PDB ID : 1FG0  
Title : LARGE RIBOSOMAL SUBUNIT COMPLEXED WITH A 13 BP  
MINIHELIX-PUROMYCIN COMPOUND  
Authors : Nissen, P.; Hansen, J.; Ban, N.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2000-07-26  
Resolution : 3.00 Å(reported)

This is a wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

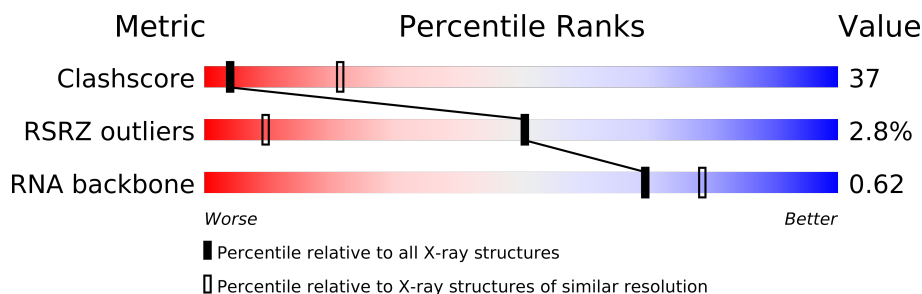
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1594 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	602	
2	B	34	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10704 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	P	0	0	0
			10627	4738	1937	3456	496			

- Molecule 2 is a RNA chain called 5'-R(CCGGCGGGCUGGUCAAACCGGCCCGCCGG ACC)-3'-5'-R(P-PUROMYCIN)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	P	0	0	0
			77	40	13	21	3			



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.00Å 300.00Å 574.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.00 53.54 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.6 (70.00-3.00) 90.5 (53.54-2.79)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.77Å)	Xtriage
Refinement program	O	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.512 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 24.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 446978 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.41	EDS
Total number of atoms	10704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	2.39	63/11888 (0.5%)	1.73	213/18532 (1.1%)
2	B	2.75	1/43 (2.3%)	1.62	1/64 (1.6%)
All	All	2.40	64/11931 (0.5%)	1.73	214/18596 (1.2%)

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	A	2	7

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2533	C	O3'-P	-78.40	0.67	1.61
1	A	2615	U	O3'-P	-77.47	0.68	1.61
1	A	2539	U	O3'-P	-62.78	0.85	1.61
1	A	2537	G	O3'-P	-51.18	0.99	1.61
1	A	2618	G	O3'-P	-50.56	1.00	1.61

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2615	U	P-O3'-C3'	-64.04	42.85	119.70
1	A	2585	G	P-O3'-C3'	-38.78	73.16	119.70
1	A	2102	G	OP1-P-O3'	-36.59	24.71	105.20
1	A	2535	U	P-O3'-C3'	35.79	162.65	119.70
1	A	2633	A	P-O3'-C3'	-33.02	80.07	119.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2083	A	C3'
1	A	2427	C	C3'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2316	G	Sidechain
1	A	2463	A	Sidechain
1	A	2493	C	Sidechain
1	A	2506	A	Sidechain
1	A	2597	U	Sidechain

## 5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10627	0	5381	536	0
2	B	77	0	45	65	0
All	All	10704	0	5426	587	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

The worst 5 of 587 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2101:A:O3'	1:A:2102:G:P	1.16	1.54
1:A:2534:C:O3'	1:A:2535:U:P	1.13	1.52
1:A:2540:G:O3'	1:A:2541:U:P	1.12	1.51
1:A:2283:G:O3'	1:A:2284:G:P	1.14	1.50
1:A:2104:C:O3'	1:A:2105:C:P	1.10	1.49

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

### 5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	491/602 (81%)	77 (15%)	34 (6%)
2	B	1/34 (2%)	0	0
All	All	492/636 (77%)	77 (15%)	34 (6%)

5 of 77 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2075	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2290	U
1	A	2395	A
1	A	2634	G
1	A	2321	A
1	A	2104	C

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PPU	B	76	1	38,40,41	1.52	4 (10%)	54,57,60	1.99	10 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPU	B	76	1	-	0/26/43/44	0/2/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	76	PPU	C-N3'	5.52	1.47	1.34
2	B	76	PPU	C8-N7	-3.67	1.27	1.34
2	B	76	PPU	C2'-C1'	-2.54	1.49	1.53
2	B	76	PPU	CE1-CZ	2.03	1.42	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	76	PPU	C4'-C3'-N3'	-6.66	99.18	113.69
2	B	76	PPU	C2-N1-C6	5.33	123.08	111.53
2	B	76	PPU	N1-C6-N6	4.66	121.96	117.04
2	B	76	PPU	CA-C-N3'	-4.10	110.86	116.31
2	B	76	PPU	P-O5'-C5'	-3.84	108.21	123.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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<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	496/602 (82%)	0.57	13 (2%) 53 10	15, 26, 55, 84	0
2	B	3/34 (8%)	1.57	1 (33%) 1 0	0, 0, 0, 5	0
All	All	499/636 (78%)	0.58	14 (2%) 50 10	0, 26, 55, 84	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	76	PPU	4.4
1	A	2344	G	4.4
1	A	2136	G	3.5
1	A	2345	A	3.2
1	A	2508	C	3.1

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PPU	B	76	37/38	0.22	-0.61	0,0,26,29	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates 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.