



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:24 PM GMT

PDB ID : 1OND
Title : THE CRYSTAL STRUCTURE OF THE 50S LARGE RIBOSOMAL SUB-UNIT FROM DEINOCOCCUS RADIODURANS COMPLEXED WITH TROLEANDOMYCIN MACROLIDE ANTIBIOTIC
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Deposited on : 2003-02-27
Resolution : 3.40 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

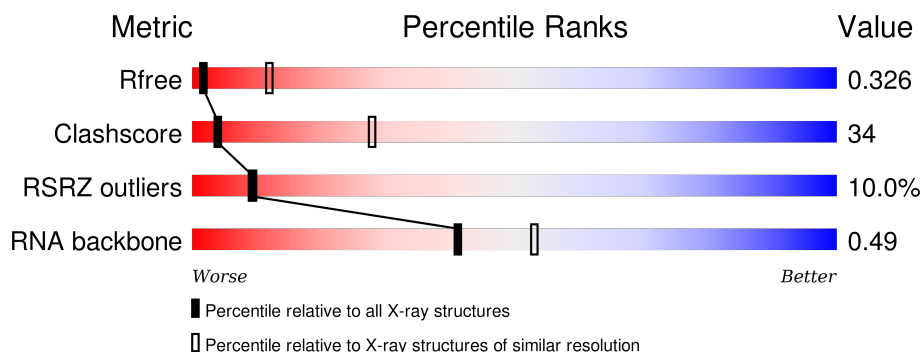
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	0	2880	
2	Q	134	
3	Z	60	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TAO	0	2881	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59581 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 RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2765	Total	C	N	O	P	0	0	0
			59336	26469	10944	19159	2764			

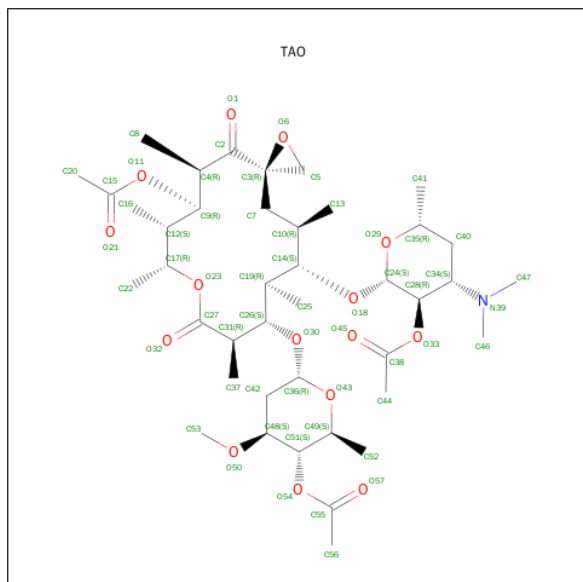
- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
2	Q	130	Total	C	0	0	130
			130	130			

- Molecule 3 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
3	Z	58	Total	C	0	0	58
			58	58			

- Molecule 4 is TROLEANDOMYCIN (three-letter code: TAO) (formula: $C_{41}H_{67}NO_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	0	1	Total	C	N	O	0	0
			57	41	1	15		





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	170.25Å 411.09Å 695.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40 20.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.40) 88.0 (20.02-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 3.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.310 0.325 , 0.326	Depositor DCC
R_{free} test set	8414 reflections (2.89%)	DCC
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , 23.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 291031 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	59581	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: TAO

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	0	0.83	17/66440 (0.0%)	0.75	34/103628 (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	0	0	47

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	1549	C	N1-C2	11.30	1.51	1.40
1	0	1549	C	N3-C4	9.79	1.40	1.33
1	0	929	A	N1-C2	8.60	1.42	1.34
1	0	1149	G	C6-O6	-8.38	1.16	1.24
1	0	1549	C	C2-O2	7.25	1.30	1.24

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2590	U	P-O3'-C3'	-9.16	108.70	119.70
1	0	633	G	N3-C2-N2	7.30	125.01	119.90
1	0	2591	C	OP1-P-OP2	-6.77	109.45	119.60
1	0	2428	U	N1-C1'-C2'	6.61	122.60	114.00
1	0	459	A	N9-C1'-C2'	6.53	122.49	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	211	U	Sidechain
1	0	343	A	Sidechain
1	0	470	U	Sidechain
1	0	491	A	Sidechain
1	0	82	G	Sidechain

5.2 Too-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 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	0	59336	0	29907	3024	0
2	Q	130	0	0	0	0
3	Z	58	0	0	4	0
4	0	57	0	67	22	0
All	All	59581	0	29974	3039	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 3039 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)
4:0:2881:TAO:C31	4:0:2881:TAO:C26	1.82	1.56
4:0:2881:TAO:C24	4:0:2881:TAO:O18	1.65	1.41
1:0:2058:U:H1'	1:0:2576:G:H21	1.09	1.17
1:0:1458:A:H3'	1:0:1459:U:C5'	1.74	1.17
1:0:2548:G:H2'	1:0:2549:G:H5''	1.17	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2755/2880 (95%)	523 (18%)	52 (1%)

5 of 523 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	13	A
1	0	35	G
1	0	45	C
1	0	48	A
1	0	49	U

5 of 52 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1338	G
1	0	1651	U
1	0	2592	U
1	0	1354	A
1	0	1410	U

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](#)

1 ligand 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	$\# Z > 2$
4	TAO	0	2881	-	58,60,60	4.18	33 (56%)	77,89,89	3.96	43 (55%)

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
4	TAO	0	2881	-	-	2/77/113/113	1/3/4/4

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	0	2881	TAO	O23-C17	-6.28	1.35	1.46
4	0	2881	TAO	C7-C10	-4.78	1.47	1.54
4	0	2881	TAO	C10-C14	-3.56	1.47	1.53
4	0	2881	TAO	C25-C19	2.09	1.58	1.53
4	0	2881	TAO	O1-C2	2.15	1.26	1.21

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	0	2881	TAO	C16-C12-C9	-7.91	96.58	111.38
4	0	2881	TAO	C13-C10-C14	-6.84	99.22	111.27
4	0	2881	TAO	O23-C27-O32	-6.74	110.01	123.89
4	0	2881	TAO	O43-C36-C42	-5.92	101.82	110.85
4	0	2881	TAO	C14-C19-C26	-5.00	101.81	113.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	C17-O23-C27-O32
4	0	2881	TAO	C17-O23-C27-C31

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	0	2881	TAO	C10-C12-C14-C17-C19-C2-C26-C27-C3-C31-C4-C7-C9-O23

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	0	2881	TAO	22	0

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	0	2765/2880 (96%)	0.46	186 (6%)	21 20	10, 30, 100, 100	0
2	Q	130/134 (97%)	2.57	69 (53%)	0 0	10, 28, 83, 167	0
3	Z	58/60 (96%)	3.46	40 (68%)	0 0	10, 18, 60, 89	0
All	All	2953/3074 (96%)	0.61	295 (9%)	9 9	10, 30, 100, 167	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	11	THR	11.9
3	Z	8	LYS	11.4
3	Z	6	VAL	11.1
2	Q	76	LYS	10.9
3	Z	42	SER	9.7

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](#)

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	TAO	0	2881	57/57	0.85	0.30	1.88	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.