



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:16 AM UTC

PDB ID : 2AAR / pdb_00002aar
Title : Structure of trigger factor binding domain in biologically homologous complex with eubacterial ribosome.
Authors : Baram, D.; Pyetan, E.; Sittner, A.; Auerbach-Nevo, T.; Bashan, A.; Yonath, A.
Deposited on : 2005-07-14
Resolution : 3.50 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 ⓘ 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 : **FAILED**
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

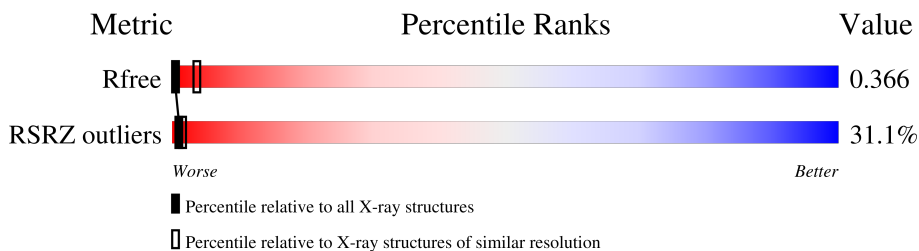
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	180053	1085 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59630 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
			Total	C	N	O	P			
1	0	2766	59359	26479	10949	19166	2765	0	0	0

- Molecule 2 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
2	R	93	93	93	0	0	93

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
3	W	65	65	65	0	0	65

- Molecule 4 is a protein called Trigger Factor.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace
			Total	C			
4	7	113	113	113	0	0	113

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3 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.39Å 407.06Å 692.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 8.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-3.50) 91.3 (8.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.52Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.320 0.336 , 0.366	Depositor DCC
R_{free} test set	13451 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	98.5	Xtrriage
Anisotropy	0.659	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 70.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	59630	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 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	2766/2880 (96%)	1.44	728 (26%) 1 2	21, 75, 199, 205	0
2	R	93/95 (97%)	6.92	74 (79%) 0 0	16, 63, 157, 200	0
3	W	65/67 (97%)	4.22	44 (67%) 0 0	21, 86, 159, 200	0
4	7	113/113 (100%)	7.89	100 (88%) 0 0	16, 120, 200, 200	0
All	All	3037/3155 (96%)	1.91	946 (31%) 1 1	16, 76, 200, 205	0

The worst 5 of 946 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	7	53	GLU	76.8
2	R	92	ALA	47.3
4	7	102	GLU	46.9
4	7	89	THR	39.8
2	R	93	GLY	39.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

There are no ligands in this entry.

5.5 Other polymers [i](#)

There are no such residues in this entry.