WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 4, 2024 – 09:43 PM EST

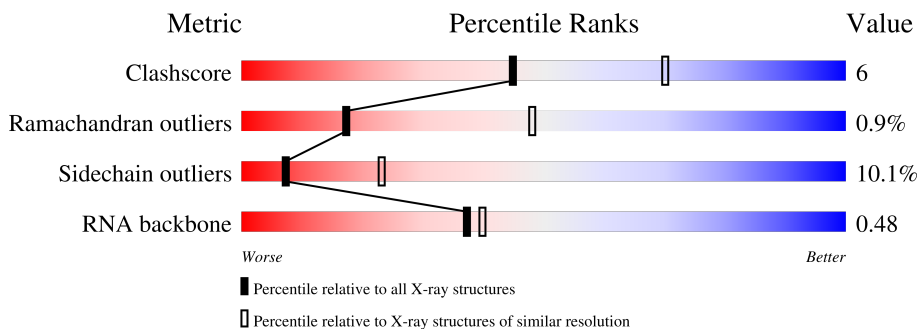|		
PDB ID	:	1SER
Title	:	THE 2.9 ANGSTROMS CRYSTAL STRUCTURE OF T. THERMOPHILUS SERYL-TRNA SYNTHETASE COMPLEXED WITH TRNA SER
Authors	:	Biou, S.; Cusack, V.; Yaremchuk, A.; Tukalo, M.
Deposited on	:	1994-02-21
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Clashscore		6
Ramachandran outliers		0.9%
Sidechain outliers		10.1%
RNA backbone		0.48

Worse   *Better*

▌ Percentile relative to all X-ray structures

❚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	94	9% 45% 13% • 31%
2	A	421	60% 23% 5% • 12%
2	B	421	70% 25% • •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7780 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 TRNASER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	65	Total 1381	C 613	N 247	O 456	P 65	60	0	0

- Molecule 2 is a protein called PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	372	Total 2982	C 1901	N 531	O 539	S 11	30	0	0
2	B	421	Total 3373	C 2143	N 606	O 613	S 11	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	TYR	THR	conflict	UNP P34945
B	708	TYR	THR	conflict	UNP P34945

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total 1	O 1	0	0
3	A	14	Total 14	O 14	0	0
3	B	29	Total 29	O 29	0	0

3 Residue-property plots ⓘ

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.
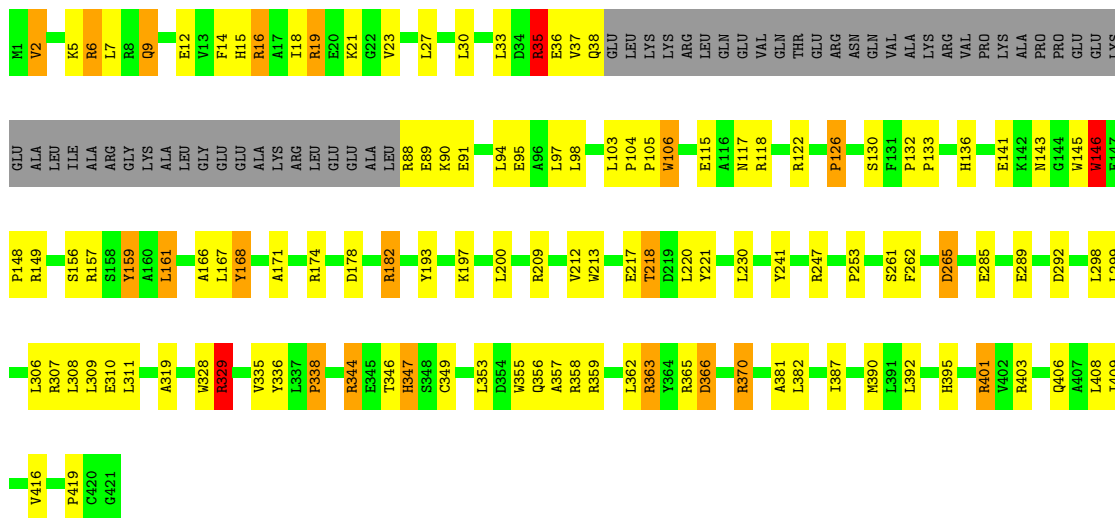
Note EDS was not executed.

- Molecule 1: TRNASER

Chain T:
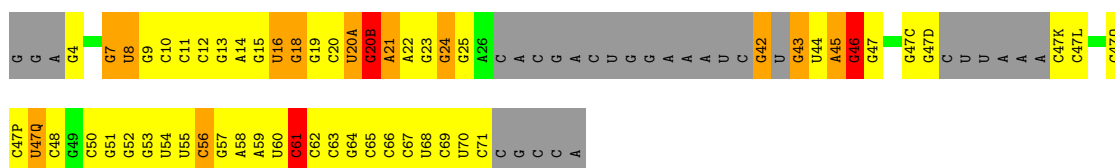
- Molecule 2: PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11))

Chain A:

- Molecule 2: PROTEIN (SERYL-TRNA SYNTHETASE (E.C.6.1.1.11))

Chain B:
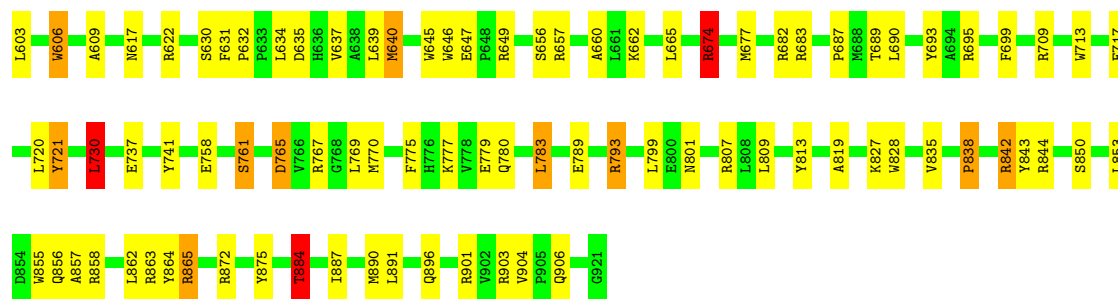
4   Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.50Å 128.90Å 121.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	92.9 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, PSU

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	T	1.54	6/1472 (0.4%)	2.24	96/2290 (4.2%)
2	A	0.86	0/3053	1.60	53/4138 (1.3%)
2	B	0.90	0/3448	1.73	75/4667 (1.6%)
All	All	1.03	6/7973 (0.1%)	1.80	224/11095 (2.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	58	A	C5'-C4'	6.34	1.58	1.51
1	T	18	G	P-O5'	6.24	1.66	1.59
1	T	18	G	C2'-C1'	-6.12	1.46	1.53
1	T	50	C	P-O5'	6.07	1.65	1.59
1	T	18	G	N9-C8	-5.48	1.34	1.37

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	16	U	O4'-C1'-N1	-14.53	96.58	108.20
2	B	903	ARG	NE-CZ-NH2	-14.46	113.07	120.30
1	T	18	G	O4'-C1'-N9	13.52	119.02	108.20
2	B	657	ARG	NE-CZ-NH2	-12.82	113.89	120.30
2	B	657	ARG	NE-CZ-NH1	11.41	126.00	120.30

There are no chirality outliers.

There are no planarity outliers.

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	T	1381	0	701	7	0
2	A	2982	0	2974	44	0
2	B	3373	0	3391	48	0
3	A	14	0	0	0	0
3	B	29	0	0	0	0
3	T	1	0	0	0	0
All	All	7780	0	7066	95	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 6.

The worst 5 of 95 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)
2:A:21:LYS:HE3	2:A:105:PRO:HD3	1.51	0.92
2:A:36:GLU:HB3	2:A:90:LYS:HG2	1.74	0.70
2:B:550:GLU:HB3	2:B:576:LEU:HD21	1.75	0.67
2:A:382:LEU:HD21	2:A:387:ILE:HG21	1.80	0.64
2:B:558:VAL:N	2:B:559:PRO:HD2	2.13	0.64

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	A	368/421 (87%)	345 (94%)	20 (5%)	3 (1%)	19	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	419/421 (100%)	405 (97%)	10 (2%)	4 (1%)	15	45
All	All	787/842 (94%)	750 (95%)	30 (4%)	7 (1%)	17	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	765	ASP
2	A	35	ARG
2	B	564	GLU
2	A	126	PRO
2	A	338	PRO

5.3.2 Protein sidechains ⓘ

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	
2	A	307/347 (88%)	269 (88%)	38 (12%)	4	14
2	B	347/347 (100%)	319 (92%)	28 (8%)	11	33
All	All	654/694 (94%)	588 (90%)	66 (10%)	7	23

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	783	LEU
2	B	799	LEU
2	B	906	GLN
2	A	262	PHE
2	A	261	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	780	GLN
2	B	879	ASN

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Mol	Chain	Res	Type
2	A	347	HIS
2	A	395	HIS
2	B	538	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	61/94 (64%)	11 (18%)	5 (8%)

5 of 11 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	8	U
1	T	9	G
1	T	16	U
1	T	18	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	16	U
1	T	20(A)	H2U
1	T	24	G
1	T	45	A

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

3 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	H2U	T	20(A)	1	18,21,22	1.02	2 (11%)	21,30,33	1.09	2 (9%)
1	5MU	T	54	1	19,22,23	0.69	0	28,32,35	1.60	5 (17%)
1	PSU	T	55	1	18,21,22	0.84	0	22,30,33	2.15	6 (27%)

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
1	H2U	T	20(A)	1	-	0/7/38/39	0/2/2/2
1	5MU	T	54	1	-	0/7/25/26	0/2/2/2
1	PSU	T	55	1	-	1/7/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	20(A)	H2U	C5-C4	-2.68	1.43	1.50
1	T	20(A)	H2U	C2-N1	2.29	1.38	1.35

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	55	PSU	C6-C5-C4	7.21	123.24	118.20
1	T	54	5MU	C5M-C5-C6	-4.08	117.40	122.85
1	T	54	5MU	C6-C5-C4	3.42	120.89	118.03
1	T	55	PSU	N1-C2-N3	2.75	118.24	115.13
1	T	54	5MU	C5M-C5-C4	2.68	121.72	118.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	T	55	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3   Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4   Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5   Other polymers ⓘ

EDS was not executed - this section is therefore empty.