



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:08 PM GMT

PDB ID : 1IVS
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-
TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-
ADENYLATE ANALOGUE
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S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-03-29
Resolution : 2.90 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

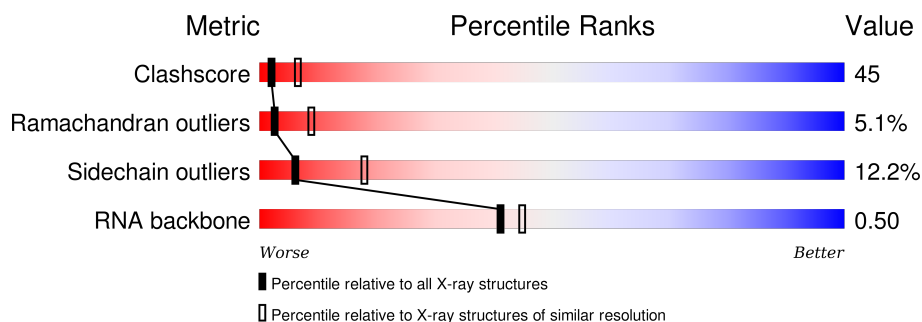
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	75	
1	D	75	
2	A	862	
2	B	862	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17424 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.

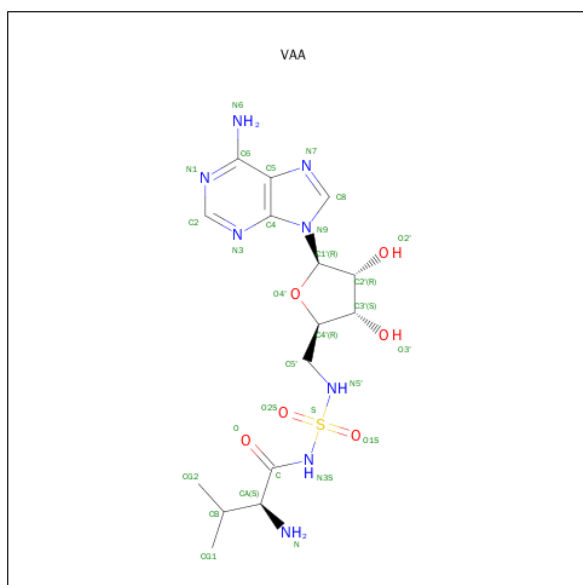
- Molecule 1 is a RNA chain called tRNA (Val).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			
1	D	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			

- Molecule 2 is a protein called Valyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			
2	B	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			

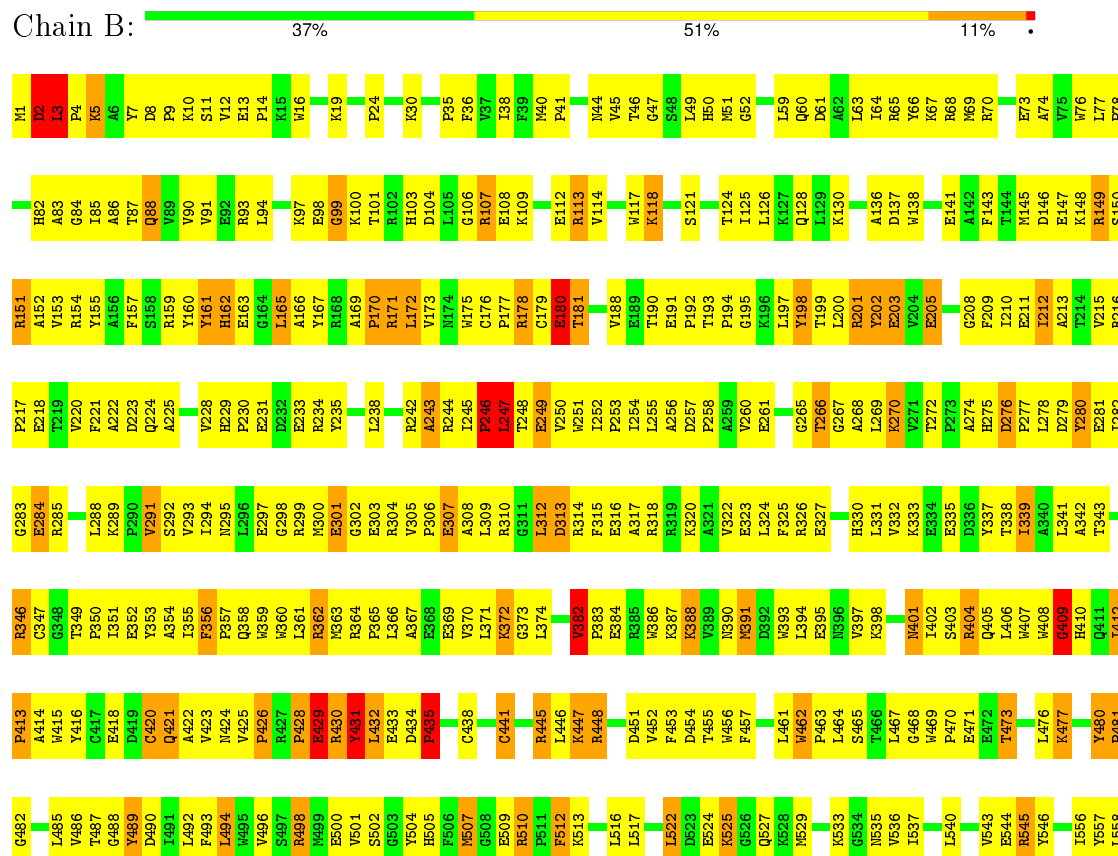
- Molecule 3 is N-[VALINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (three-letter code: VAA) (formula: C₁₅H₂₄N₈O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	15	8	6	1		
3	B	1	Total	C	N	O	S	0	0
			30	15	8	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	75	Total	O	0	0
			75	75		
4	C	29	Total	O	0	0
			29	29		
4	D	13	Total	O	0	0
			13	13		



W801	R802	R803	R804	Q805	E806	K807	R808	L809	K810	E811	L812	L813	A814	R818	S819	Q820	R821	K822	L823	G827	F828	R829	E830	R831	A832	P833	K834	P835	V836	V837	E838	A839	E840	E841	A842	R843	L844	K845	E846	N847	L848	E849	I854	R855	L858	S859	Q860	I861	G862	L859	E851	K854	P855	K856	L857	D858	L859	E863	T864	R866	A873	K877	L878	L879	H880	P881	M882	M883	P884	F885	L886	T887	L890	Y891	Q892	T895	G896	K897	E898	E899	L900	E903	A904	W905	P906	F907	P908	G909	G910	R911	R912	D917	E913	E914	A915	E916	R917	F918	F919	E920	A921	L922	K923	Q924	A925	V926	L959	T960	D964	I965	R966	R970	E973	A979	N980	L981	Y983	N984	L985	A986	R987	Y989	L990	L991	S992	R993	E994	G999	D901	T902	P903	T904	L905	A906	P907	R908	F909	N910	N911	S912	R913	G917	V918	L924	A927	L928	A933	A934	R935	L940	Y949	T977	A731	L732	K733	A734	E735	A736	L737	L738	P739	V744	R745	V746	L747	L748	E751	T752	A753	P754	V755	L759	F762	R763	F764	L765	S766	R767	A768	D769	L770	L771	P772	E773	R774	K777	A778	L779	V780	M783	P784	R785	V786	T787	A788	R789	M790	P791	L792	L795	L796	L659	T660	D601	T602	P603	T604	L605	A606	P607	R608	F609	N610	N611	S612	R613	G617	V618	L624	A627	L628	A633	A634	R635	L640	Y649
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	411.81Å 411.81Å 81.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17424	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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: VAA

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	C	0.49	1/1791 (0.1%)	0.82	4/2789 (0.1%)
1	D	0.49	1/1791 (0.1%)	0.79	1/2789 (0.0%)
2	A	0.45	0/7143	0.68	2/9678 (0.0%)
2	B	0.46	0/7143	0.70	3/9678 (0.0%)
All	All	0.46	2/17868 (0.0%)	0.72	10/24934 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	901	G	OP3-P	-7.20	1.52	1.61
1	C	901	G	OP3-P	-7.03	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	975	A	C4'-C3'-O3'	7.18	127.36	113.00
1	C	947	C	N1-C1'-C2'	6.45	122.38	114.00
2	B	382	VAL	C-N-CD	6.04	141.09	128.40
1	D	937	C	C2'-C3'-O3'	5.90	123.14	113.70
2	B	409	GLY	N-CA-C	5.43	126.67	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	918	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	C	1603	0	816	63	0
1	D	1603	0	816	56	0
2	A	6970	0	6949	682	1
2	B	6970	0	6949	725	0
3	A	30	0	24	5	0
3	B	30	0	24	1	0
4	A	101	0	0	16	0
4	B	75	0	0	12	0
4	C	29	0	0	0	0
4	D	13	0	0	1	0
All	All	17424	0	15578	1490	1

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 45.

The worst 5 of 1490 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:B:382:VAL:HG23	2:B:383:PRO:CD	1.71	1.20
2:B:448:ARG:HD3	2:B:448:ARG:H	1.05	1.18
2:A:282:ILE:HA	2:A:285:ARG:HD3	1.31	1.13
2:B:382:VAL:HG23	2:B:383:PRO:HD3	1.29	1.12
2:A:777:LYS:H	2:A:777:LYS:HD3	0.98	1.12

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:742:GLN:OE1	2:A:742:GLN:OE1[7_555]	2.19	0.01

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	
2	A	860/862 (100%)	683 (79%)	141 (16%)	36 (4%)	3	13
2	B	860/862 (100%)	670 (78%)	139 (16%)	51 (6%)	2	6
All	All	1720/1724 (100%)	1353 (79%)	280 (16%)	87 (5%)	2	9

5 of 87 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	106	GLY
2	A	171	ARG
2	A	243	ALA
2	A	257	ASP
2	A	312	LEU

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	
2	A	724/724 (100%)	640 (88%)	84 (12%)	7	20
2	B	724/724 (100%)	632 (87%)	92 (13%)	5	16
All	All	1448/1448 (100%)	1272 (88%)	176 (12%)	6	18

5 of 176 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	783	MET
2	B	181	THR
2	B	767	ARG
2	A	805	GLN
2	B	107	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	692	GLN
2	B	60	GLN
2	B	724	GLN
2	A	724	GLN
2	A	860	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	22 (29%)	9 (12%)
1	D	74/75 (98%)	28 (37%)	9 (12%)
All	All	148/150 (98%)	50 (33%)	18 (12%)

5 of 50 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	908	U
1	C	910	G
1	C	916	C
1	C	917	G

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	959	U
1	D	907	C
1	D	937	C
1	C	947	C
1	C	957	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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$
3	VAA	A	990	-	25,32,32	3.59	11 (44%)	27,48,48	1.88	6 (22%)
3	VAA	B	991	-	25,32,32	3.71	9 (36%)	27,48,48	2.10	5 (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
3	VAA	A	990	-	-	0/17/39/39	0/3/3/3
3	VAA	B	991	-	-	0/17/39/39	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	990	VAA	C5'-N5'	-7.61	1.32	1.47
3	B	991	VAA	C5'-N5'	-7.39	1.33	1.47
3	A	990	VAA	C5'-C4'	-4.36	1.41	1.51
3	A	990	VAA	C8-N7	-3.15	1.28	1.34
3	B	991	VAA	C8-N7	-2.62	1.29	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	991	VAA	O2S-S-O1S	-6.31	109.75	120.04
3	A	990	VAA	O2S-S-O1S	-5.33	111.34	120.04
3	B	991	VAA	C1'-N9-C4	-4.37	120.36	126.94
3	A	990	VAA	C-N3S-S	-3.45	119.22	124.05
3	B	991	VAA	C-N3S-S	-3.28	119.45	124.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	990	VAA	5	0
3	B	991	VAA	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.