



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 02:15 am GMT

PDB ID : 1GAX  
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-ADENYLATE ANALOGUE  
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Deposited on : 2000-06-23  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

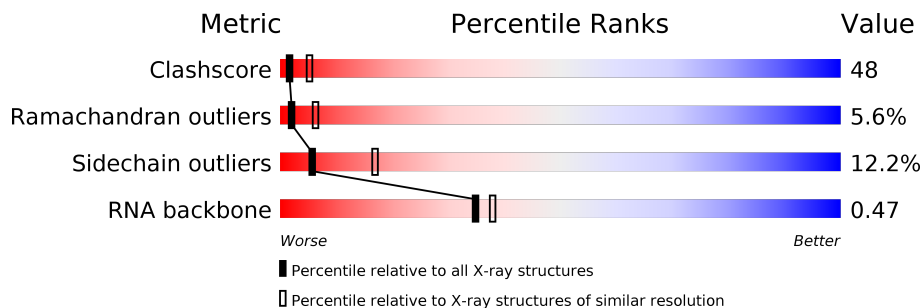
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

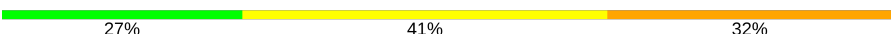
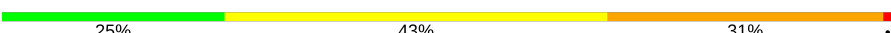

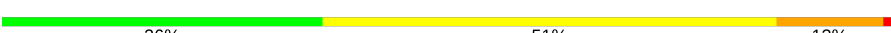
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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. 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	 27% 41% 32%
1	D	75	 25% 43% 31% .
2	A	862	 37% 52% 9% .
2	B	862	 36% 51% 12% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17368 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			

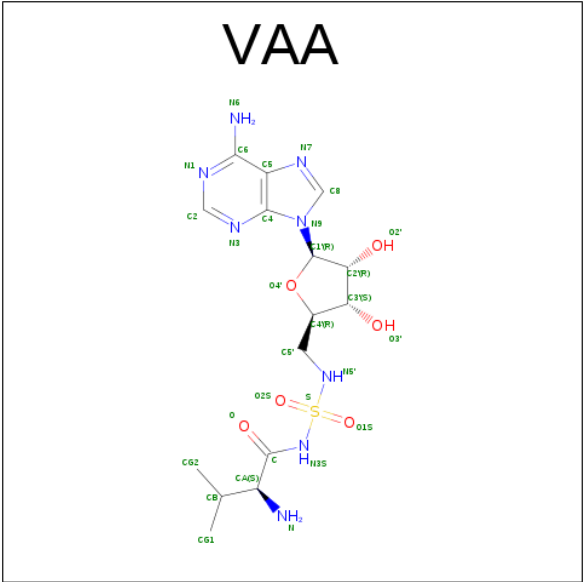
- Molecule 2 is a protein called VALYL-TRNA SYNTHETASE.

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 ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is N-[VALINYLYL]-N'-[ADENOSYL]-DIAMINOSUFONE (three-letter code: VAA) (formula: C<sub>15</sub>H<sub>24</sub>N<sub>8</sub>O<sub>6</sub>S).



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

- Molecule 5 is water.

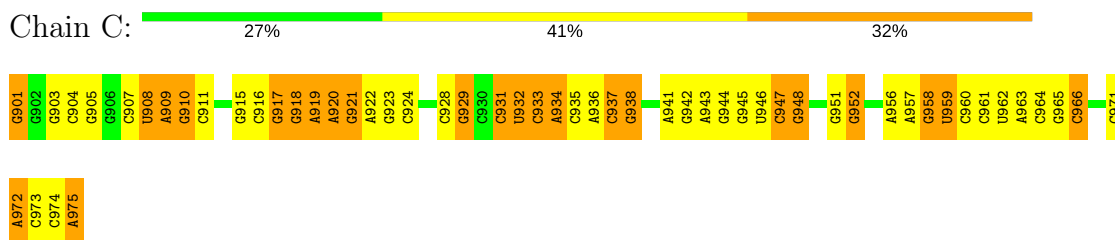
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	61	Total	O	0	0
			61	61		
5	C	19	Total	O	0	0
			19	19		
5	D	11	Total	O	0	0
			11	11		

### 3 Residue-property plots [i](#)

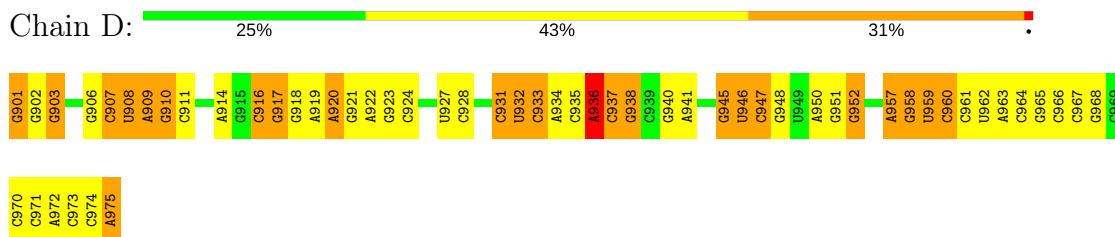
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

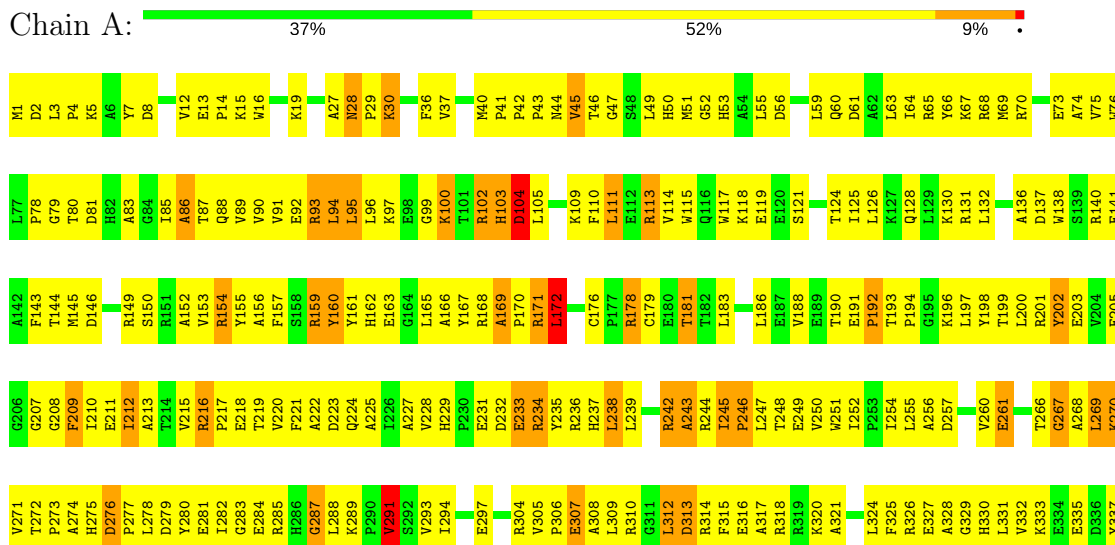
#### • Molecule 1: TRNA(VAL)

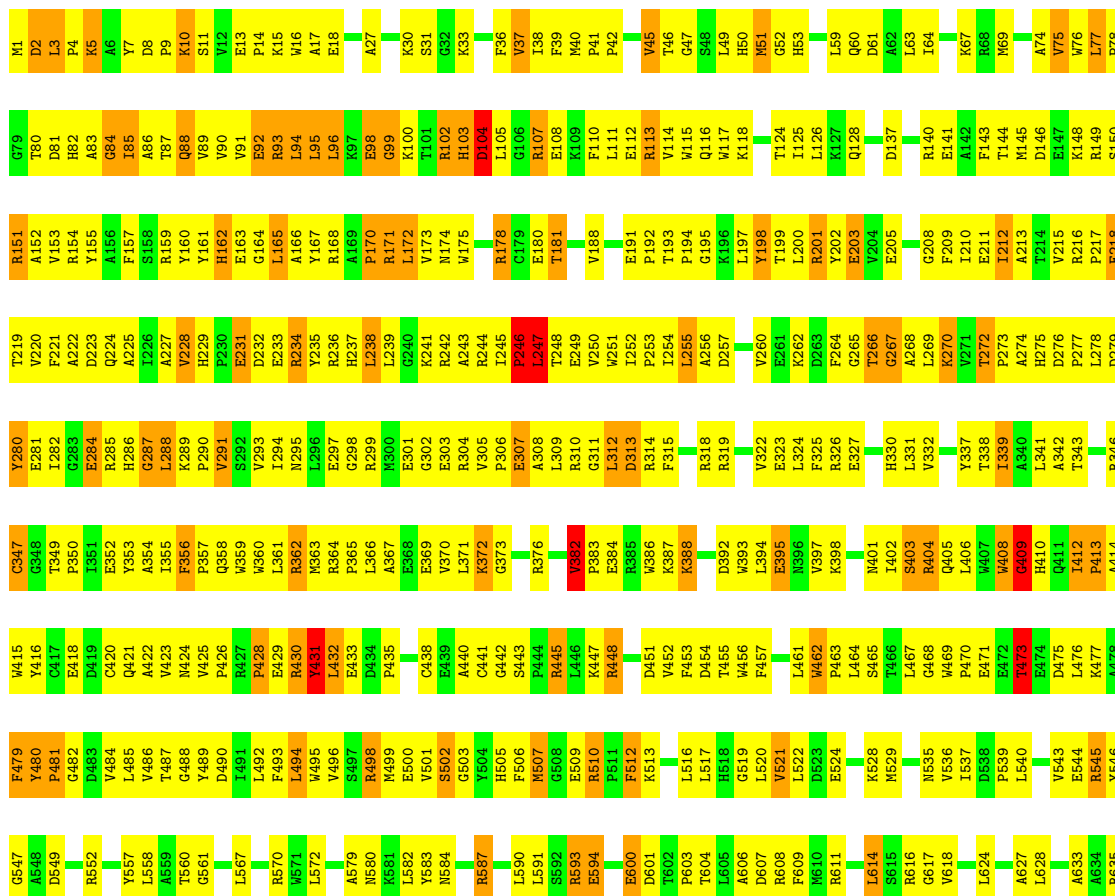


#### • Molecule 1: TRNA(VAL)



#### • Molecule 2: VALYL-TRNA SYNTHETASE





Q860	W790	E639	R789	W790	D711	E644	L795	E716	R717	Y649	W797	E798	E799	L722	L650	E651	E654	A725	W726	T727	Q805	E806	E807	A808	L809	K810	A734	E811	E735	A736	G737	L738	P739	E669	E670	W671	E675	L676	K677	L678	L679	H680	P681	H682	H683	P684	F685	L686	T687	S688	D689	E690	H691	Q692	A693	G696	K697	E698	V699	K700	P706	E707	P708	G709	G710																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
L861	L792	E641	L796	E715	E714	F645	L796	E716	R717	Y649	W797	E798	E799	L722	L650	E651	E654	A725	W726	T727	Q805	E806	E807	A808	L809	K810	A734	E811	E735	A736	G737	L738	P739	E669	E670	W671	E675	L676	K677	L678	L679	H680	P681	H682	H683	P684	F685	L686	T687	S688	D689	E690	H691	Q692	A693	G696	K697	E698	V699	K700	P706	E707	P708	G709	G710																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	411.81Å 411.81Å 81.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (30.00-2.90)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.245 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17368	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	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: ZN, 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	0.47	1/1791 (0.1%)	0.78	0/2789
1	D	0.46	1/1791 (0.1%)	0.78	1/2789 (0.0%)
2	A	0.44	0/7143	0.69	3/9678 (0.0%)
2	B	0.43	0/7143	0.68	2/9678 (0.0%)
All	All	0.44	2/17868 (0.0%)	0.71	6/24934 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	901	G	OP3-P	-7.02	1.52	1.61
1	D	901	G	OP3-P	-6.91	1.52	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	172	LEU	CA-CB-CG	7.55	132.66	115.30
1	D	936	A	N9-C1'-C2'	6.97	123.06	114.00
2	B	382	VAL	C-N-CD	5.74	140.45	128.40
2	B	409	GLY	N-CA-C	5.50	126.84	113.10
2	A	409	GLY	N-CA-C	5.13	125.93	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	67	0
1	D	1603	0	816	66	0
2	A	6970	0	6943	728	0
2	B	6970	0	6942	751	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	30	0	24	3	0
4	B	30	0	24	4	0
5	A	67	0	0	13	0
5	B	61	0	0	17	0
5	C	19	0	0	0	0
5	D	11	0	0	1	0
All	All	17368	0	15565	1571	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 48.

The worst 5 of 1571 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:777:LYS:H	2:B:777:LYS:HE3	1.06	1.18
2:B:201:ARG:HE	2:B:211:GLU:HB3	1.02	1.17
2:A:102:ARG:HH21	2:A:104:ASP:HA	1.04	1.16
2:A:382:VAL:HG11	2:A:516:LEU:HD12	1.19	1.16
2:A:28:ASN:HD21	2:A:30:LYS:HG2	1.05	1.13

There are no symmetry-related clashes.

## 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%)	676 (79%)	139 (16%)	45 (5%)	2	8
2	B	860/862 (100%)	652 (76%)	156 (18%)	52 (6%)	2	5
All	All	1720/1724 (100%)	1328 (77%)	295 (17%)	97 (6%)	2	6

5 of 97 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	94	LEU
2	A	103	HIS
2	A	104	ASP
2	A	234	ARG
2	A	312	LEU

### 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	724/724 (100%)	641 (88%)	83 (12%)	6	20
2	B	724/724 (100%)	630 (87%)	94 (13%)	5	15
All	All	1448/1448 (100%)	1271 (88%)	177 (12%)	6	17

5 of 177 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	834	LYS
2	B	178	ARG
2	B	733	LYS
2	A	845	LYS
2	B	75	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	758	ASN

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Mol	Chain	Res	Type
2	B	116	GLN
2	B	692	GLN
2	A	860	GLN
2	B	50	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	26 (35%)	0
1	D	74/75 (98%)	27 (36%)	0
All	All	148/150 (98%)	53 (35%)	0

5 of 53 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	903	G
1	C	907	C
1	C	908	U
1	C	909	A
1	C	910	G

There are no RNA pucker outliers to report.

## 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 ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	VAA	A	990	-	25,32,32	3.19	10 (40%)	24,48,48	2.02	3 (12%)
4	VAA	B	1990	-	25,32,32	3.04	9 (36%)	24,48,48	1.87	6 (25%)

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	VAA	A	990	-	-	0/19/39/39	0/3/3/3
4	VAA	B	1990	-	-	0/19/39/39	0/3/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	990	VAA	C5'-N5'	-8.66	1.31	1.47
4	B	1990	VAA	C5'-N5'	-7.81	1.33	1.47
4	A	990	VAA	C5'-C4'	-4.58	1.41	1.52
4	B	1990	VAA	C5'-C4'	-3.91	1.42	1.52
4	A	990	VAA	C8-N7	-3.62	1.27	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	990	VAA	O2S-S-O1S	-6.45	111.01	120.19
4	B	1990	VAA	O2S-S-O1S	-5.59	112.23	120.19
4	A	990	VAA	C-N3S-S	-3.64	117.87	124.09
4	B	1990	VAA	C-N3S-S	-2.87	119.18	124.09
4	B	1990	VAA	O1S-S-N5'	-2.84	101.73	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	990	VAA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1990	VAA	4	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 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.