wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 08:51 pm BST

PDB ID	:	1IVS
Title	:	CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-ADENYLATE ANALOGUE
Authors	:	Fukai, S.; Nureki, O.; Sekine, S.-I.; Shimada, A.; Vassylyev, D.G.; Yokoyama, 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

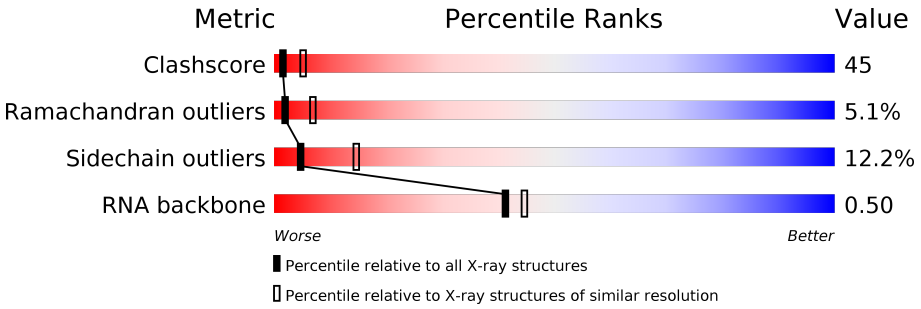
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	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 on 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	C	75	29% 43% 23% 5%
1	D	75	20% 53% 25% .
2	A	862	39% 51% 9% .
2	B	862	37% 51% 11% .

2 Entry composition

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.

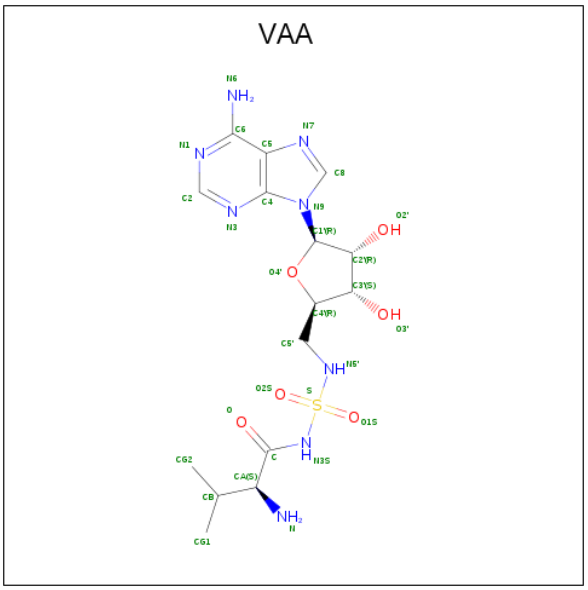
- Molecule 1 is a RNA chain called tRNA (Val).

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: $C_{15}H_{24}N_8O_6S$).



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	C	29	Total	O	0	0
			29	29		
4	D	13	Total	O	0	0
			13	13		
4	A	101	Total	O	0	0
			101	101		
4	B	75	Total	O	0	0
			75	75		

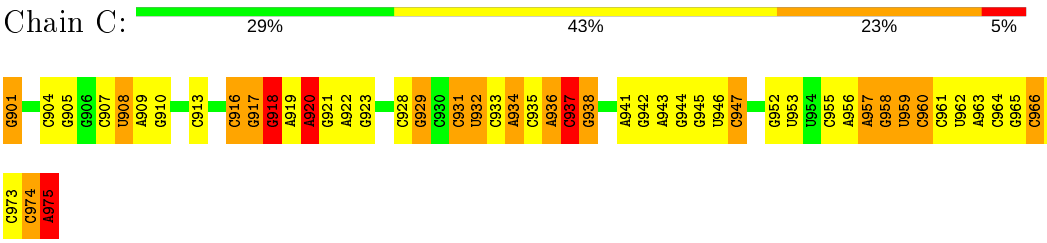
3 Residue-property plots (i)

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. 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.

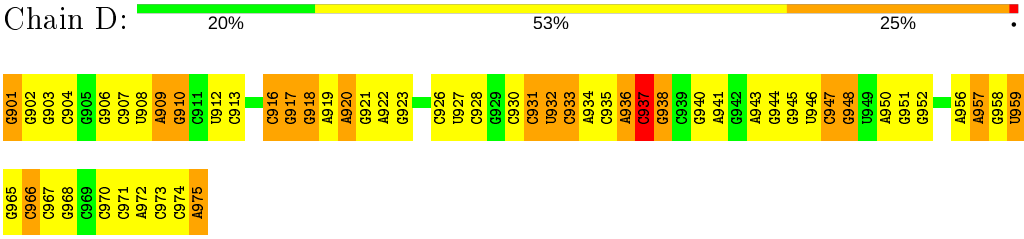
- Molecule 1: tRNA (Val)

Chain C:



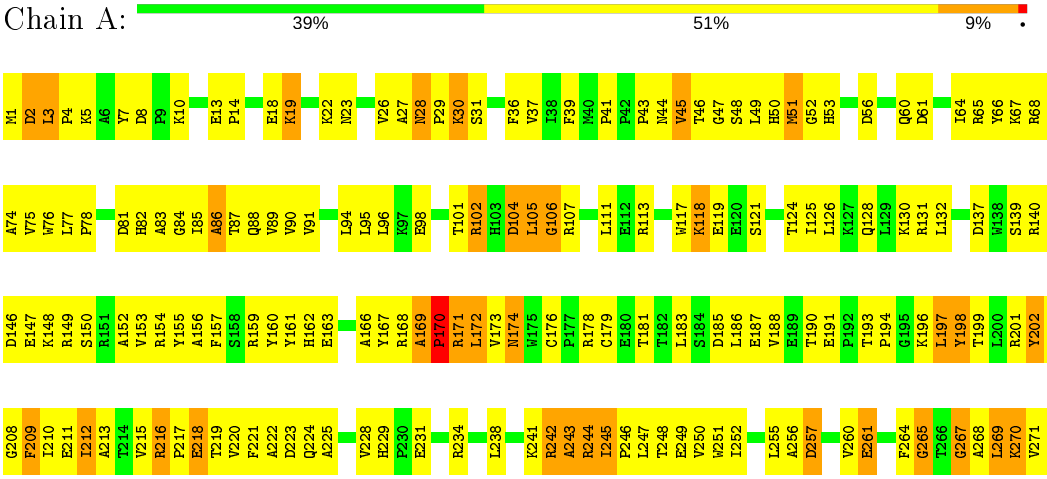
- Molecule 1: tRNA (Val)

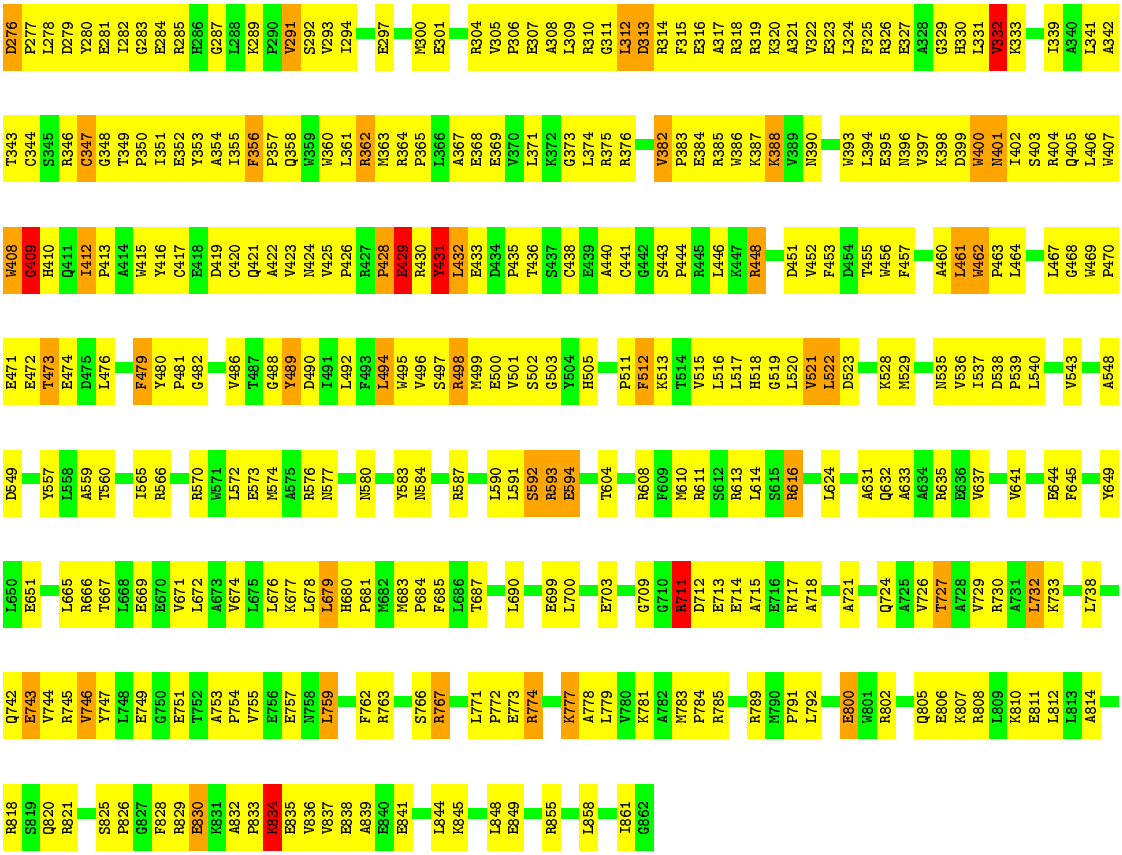
Chain D:



- Molecule 2: Valyl-tRNA synthetase

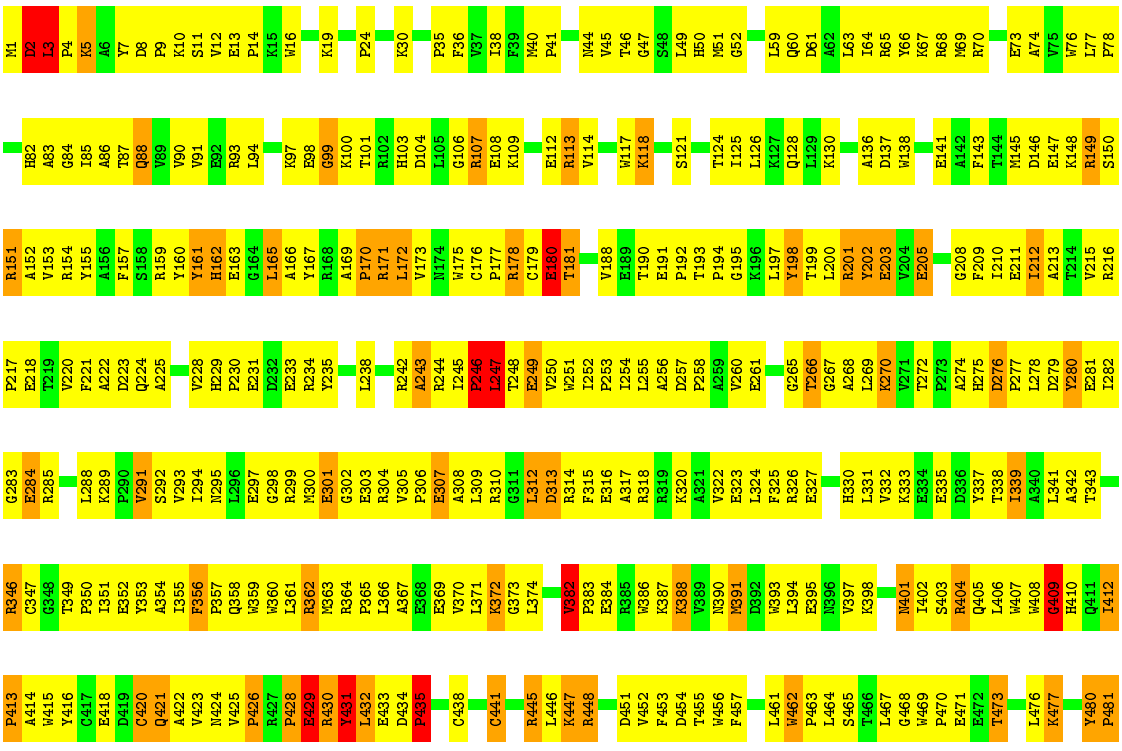
Chain A:

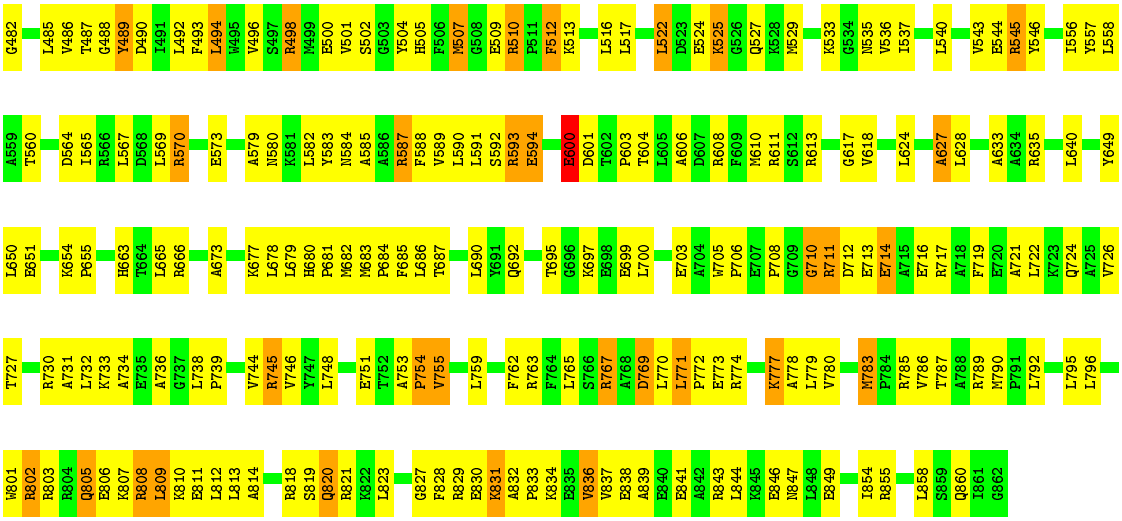




- Molecule 2: Valyl-tRNA synthetase

Chain B:




G482 L485 V486 T487 G488 Y489 D490 I491 L492 F493 L494 W495 V496 S497 R498 M499 E500 V501 S502 G503 Y504 H505 F506 M507 G508 E509 R510 P511 F512 K513 L516 L517 L522 D523 E524 K525 G526 Q527 K528 M529 K533 G534 N535 V536 I537 L540 V543 E544 R545 Y546 I556 Y557 L558
A559 T560 D564 I565 R566 L567 D568 L569 R570 E573 A579 N580 K581 L582 Y583 N584 A585 A586 R587 F588 V589 L590 L591 S592 R593 E594 E600 D601 T602 P603 T604 L605 A606 D607 R608 F609 M610 R611 S612 R613 G617 V618 L624 A627 L628 A633 A634 R635 L640 Y649
L650 E651 K654 P655 H663 T664 L665 R666 A673 K677 L678 L679 H680 P681 M682 M683 P684 F685 L686 T687 L690 Y691 Q692 T695 G696 K697 E698 E699 L700 E703 A704 W705 P706 E707 P708 G709 G710 R711 D712 E713 E714 A715 E716 R717 A718 F719 E720 A721 L722 K723 Q724 A725 V726
T727 R730 A731 L732 K733 A734 E735 A736 G737 L738 P739 V744 R745 V746 Y747 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
W801 R802 R803 R804 Q805 E806 K807 R808 L809 K810 E811 L812 L813 A814 R818 S819 Q820 R821 K822 L823 G827 F828 R829 E830 K831 A832 P833 K834 E835 V836 V837 E838 A839 E840 E841 A842 R843 L844 K845 E846 N847 L848 E849 I854 R855 L858 S859 Q860 I861 G862

4 Data and refinement statistics (i)

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, 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

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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:A:777:LYS:H	2:A:777:LYS:HD3	0.98	1.12
2:B:382:VAL:HG23	2:B:383:PRO:HD3	1.29	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 10
2	B	860/862 (100%)	670 (78%)	139 (16%)	51 (6%)	1 5
All	All	1720/1724 (100%)	1353 (79%)	280 (16%)	87 (5%)	2 7

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%)	5 16
2	B	724/724 (100%)	632 (87%)	92 (13%)	4 13
All	All	1448/1448 (100%)	1272 (88%)	176 (12%)	5 15

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 (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)

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	-	27,32,32	3.17	10 (37%)	30,48,48	1.80	7 (23%)
3	VAA	B	991	-	27,32,32	3.22	8 (29%)	30,48,48	1.90	5 (16%)

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	-	-	1/19/39/39	0/3/3/3
3	VAA	B	991	-	-	3/19/39/39	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	991	VAA	S-N5'	9.06	1.72	1.61
3	A	990	VAA	C5'-N5'	-8.69	1.32	1.47
3	B	991	VAA	C5'-N5'	-8.44	1.33	1.47
3	B	991	VAA	O1S-S	6.82	1.53	1.43
3	A	990	VAA	O1S-S	6.66	1.53	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	991	VAA	O2S-S-O1S	-7.12	109.75	120.40
3	A	990	VAA	O2S-S-O1S	-6.06	111.34	120.40
3	B	991	VAA	C1'-N9-C4	-3.58	120.36	126.64
3	A	990	VAA	C-N3S-S	-3.02	119.22	124.23
3	B	991	VAA	C-N3S-S	-2.88	119.45	124.23

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	991	VAA	C5'-N5'-S-O1S
3	B	991	VAA	C5'-N5'-S-N3S
3	B	991	VAA	C5'-N5'-S-O2S
3	A	990	VAA	C5'-N5'-S-O1S

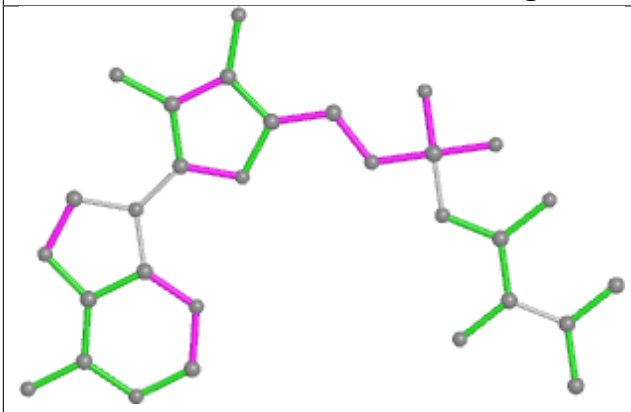
There are no ring outliers.

2 monomers are involved in 6 short contacts:

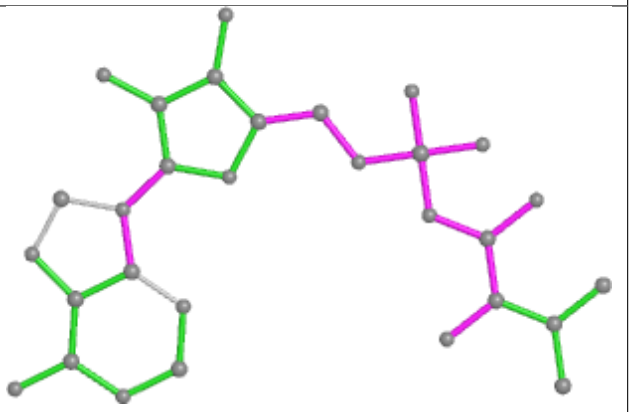
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	990	VAA	5	0
3	B	991	VAA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

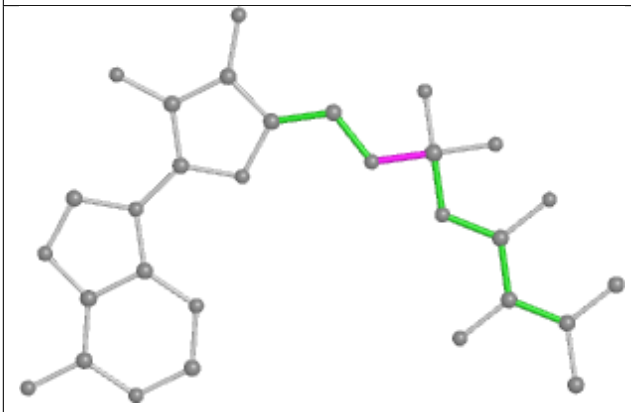
Ligand VAA A 990



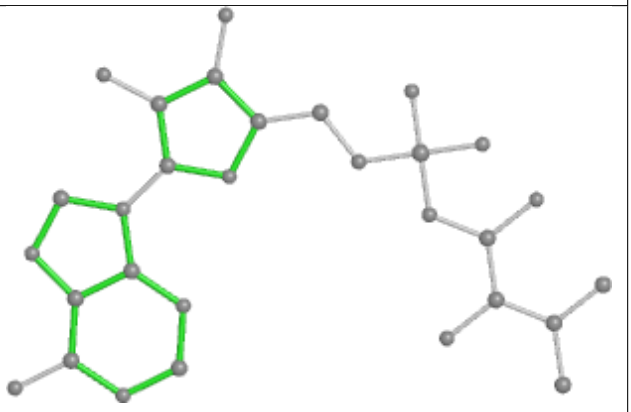
Bond lengths



Bond angles

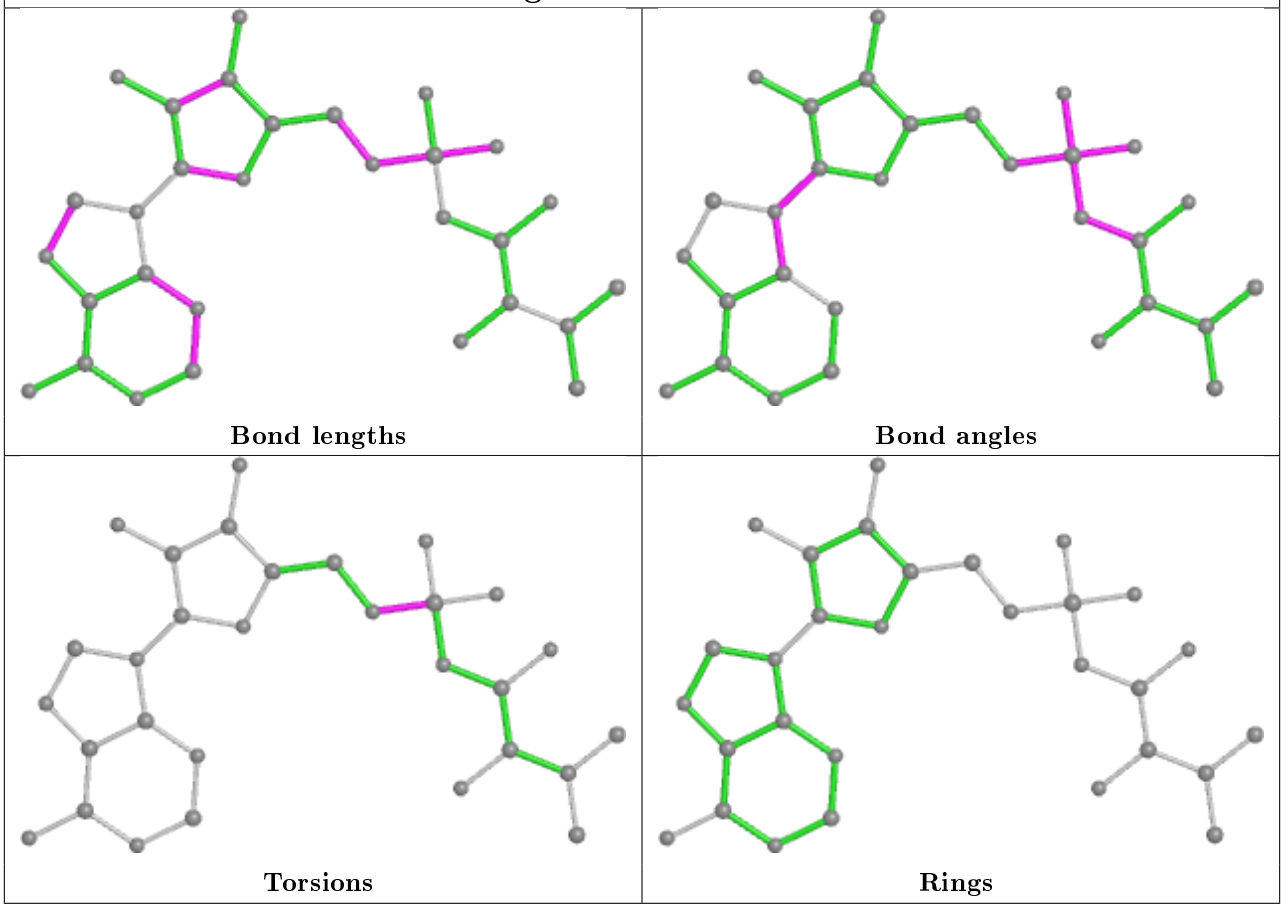


Torsions



Rings

Ligand VAA B 991



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.