



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 1IVS / pdb_00001ivs
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-
TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-
ADENYLATE ANALOGUE
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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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

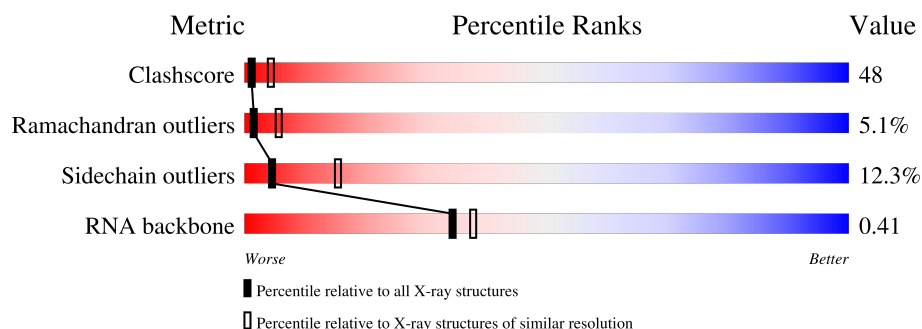
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	75	29% 40% 23% 8%
1	D	75	20% 53% 21% 5%
2	A	862	36% 51% 11% .
2	B	862	34% 52% 13% .

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.

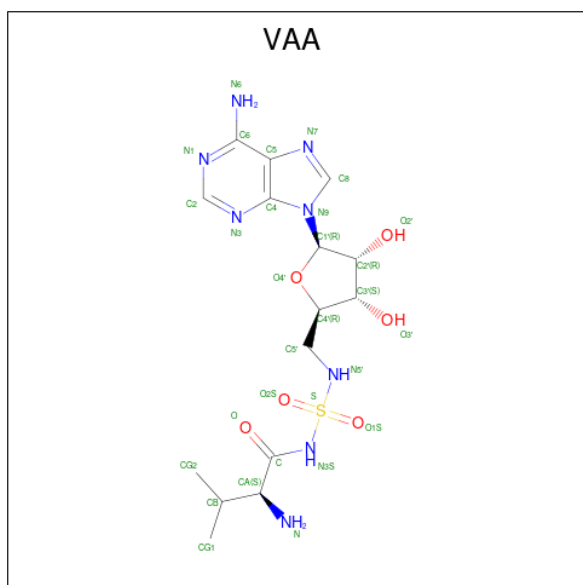
- Molecule 1 is a RNA chain called tRNA (Val).

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			

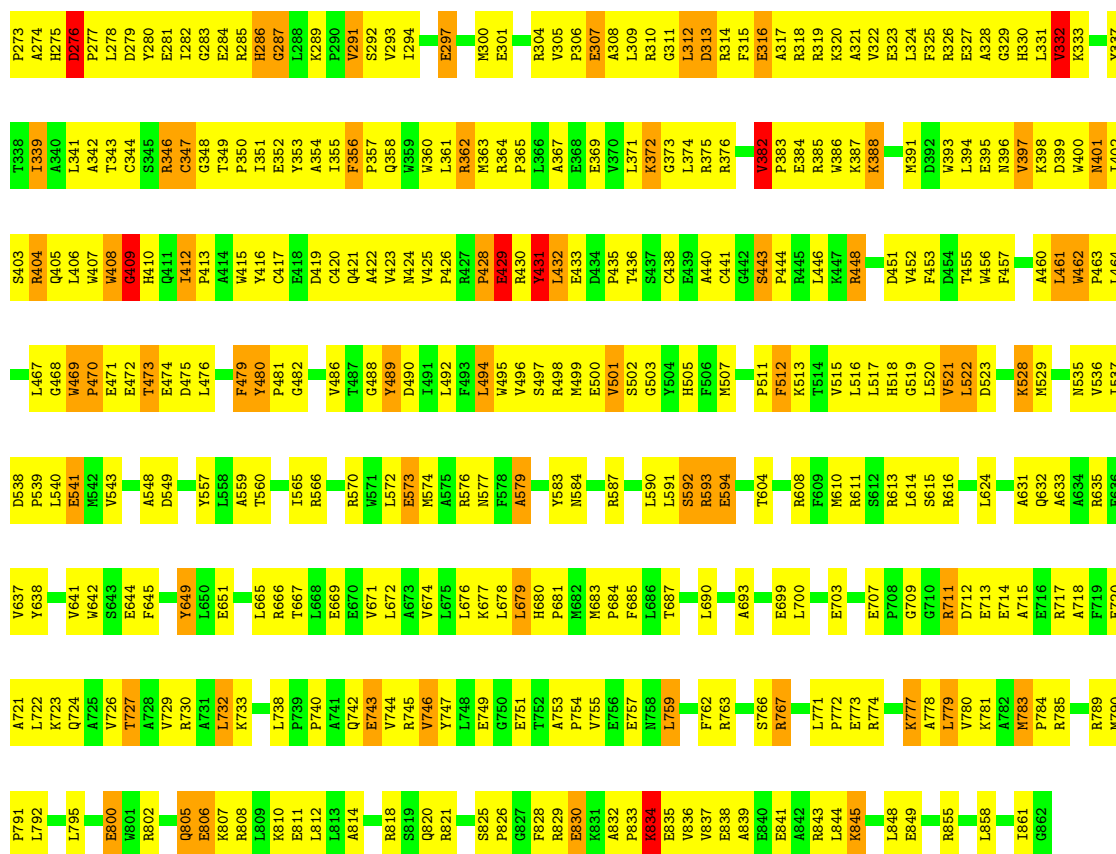
- Molecule 3 is N-[VALINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (CCD ID: VAA) (formula: $C_{15}H_{24}N_8O_6S$).



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		

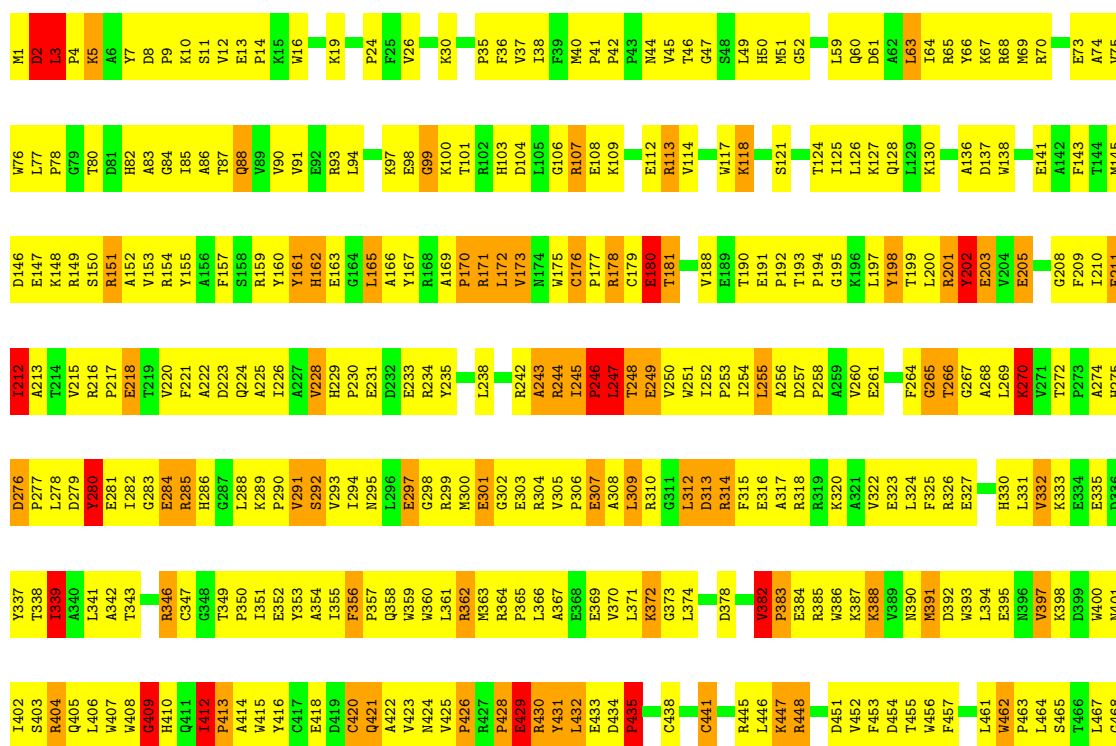
- Molecule 4 is water.

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		



• Molecule 2: Valyl-tRNA synthetase

Chain B: 34% 52% 13%





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, 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	0.40	0/1791	0.88	9/2789 (0.3%)
1	D	0.40	0/1791	0.87	4/2789 (0.1%)
2	A	0.54	0/7143	1.05	45/9678 (0.5%)
2	B	0.54	0/7143	1.09	53/9678 (0.5%)
All	All	0.51	0/17868	1.03	111/24934 (0.4%)

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

There are no bond length outliers.

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	975	A	C4'-C3'-O3'	11.97	127.36	109.40
2	B	382	VAL	CA-C-N	-11.00	106.09	119.84
2	B	382	VAL	C-N-CA	-11.00	106.09	119.84
2	A	244	ARG	N-CA-C	-9.27	96.79	110.23
1	D	937	C	C2'-C3'-O3'	9.10	123.14	109.50

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	65	0
1	D	1603	0	816	58	0
2	A	6970	0	6949	719	1
2	B	6970	0	6949	765	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	1	0
4	D	13	0	0	1	0
All	All	17424	0	15578	1570	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 48.

The worst 5 of 1570 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%)	2	9
2	B	860/862 (100%)	670 (78%)	139 (16%)	51 (6%)	1	4
All	All	1720/1724 (100%)	1353 (79%)	280 (16%)	87 (5%)	1	6

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%)	641 (88%)	83 (12%)	5	18
2	B	724/724 (100%)	629 (87%)	95 (13%)	4	13
All	All	1448/1448 (100%)	1270 (88%)	178 (12%)	4	15

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	266	THR

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Mol	Chain	Res	Type
2	B	510	ARG
2	B	291	VAL
2	B	420	CYS
2	B	580	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	505	HIS
2	B	724	GLN
2	B	518	HIS
2	B	584	ASN
2	B	820	GLN

5.3.3 RNA ⓘ

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	D	937	C
1	D	959	U
1	D	957	A
1	C	959	U
1	D	936	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 oligosaccharides 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	B	991	-	31,32,32	3.23	9 (29%)	42,48,48	1.86	7 (16%)
3	VAA	A	990	-	31,32,32	3.21	10 (32%)	42,48,48	1.66	8 (19%)

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	B	991	-	-	5/23/39/39	0/3/3/3
3	VAA	A	990	-	-	1/23/39/39	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)
3	A	990	VAA	C5'-N5'	-9.41	1.32	1.47
3	B	991	VAA	S-N5'	9.24	1.72	1.61
3	B	991	VAA	C5'-N5'	-9.14	1.33	1.47
3	B	991	VAA	O1S-S	7.33	1.53	1.43
3	A	990	VAA	O1S-S	7.15	1.53	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	991	VAA	O2S-S-O1S	-7.19	109.75	120.34
3	A	990	VAA	O2S-S-O1S	-6.11	111.34	120.34
3	B	991	VAA	O4'-C1'-N9	4.47	116.67	108.09
3	B	991	VAA	C1'-N9-C8	3.97	135.90	127.09
3	A	990	VAA	C1'-N9-C8	3.27	134.36	127.09

There are no chirality outliers.

5 of 6 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	O4'-C4'-C5'-N5'
3	B	991	VAA	C5'-N5'-S-O2S
3	A	990	VAA	C5'-N5'-S-O1S

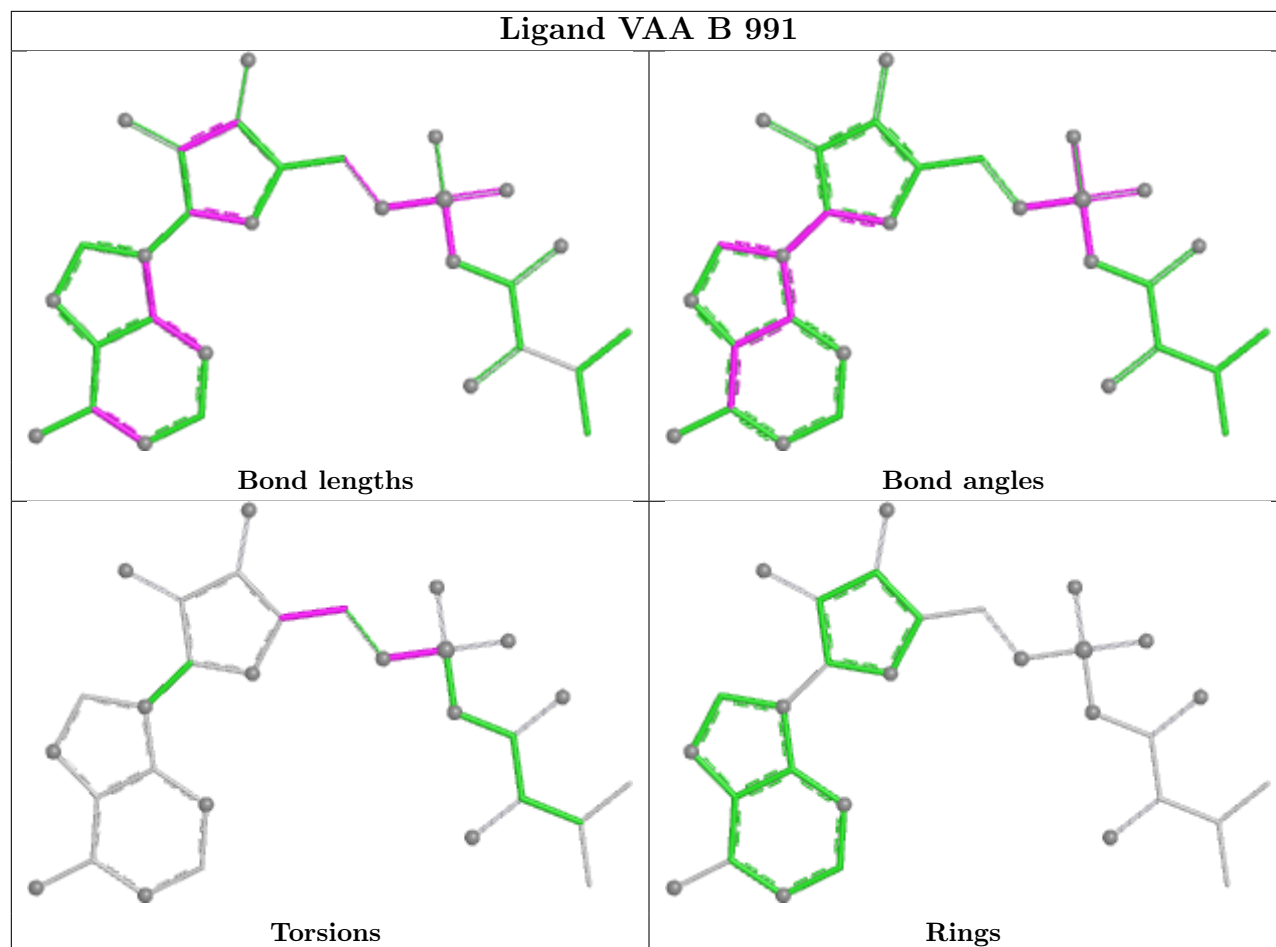
There are no ring outliers.

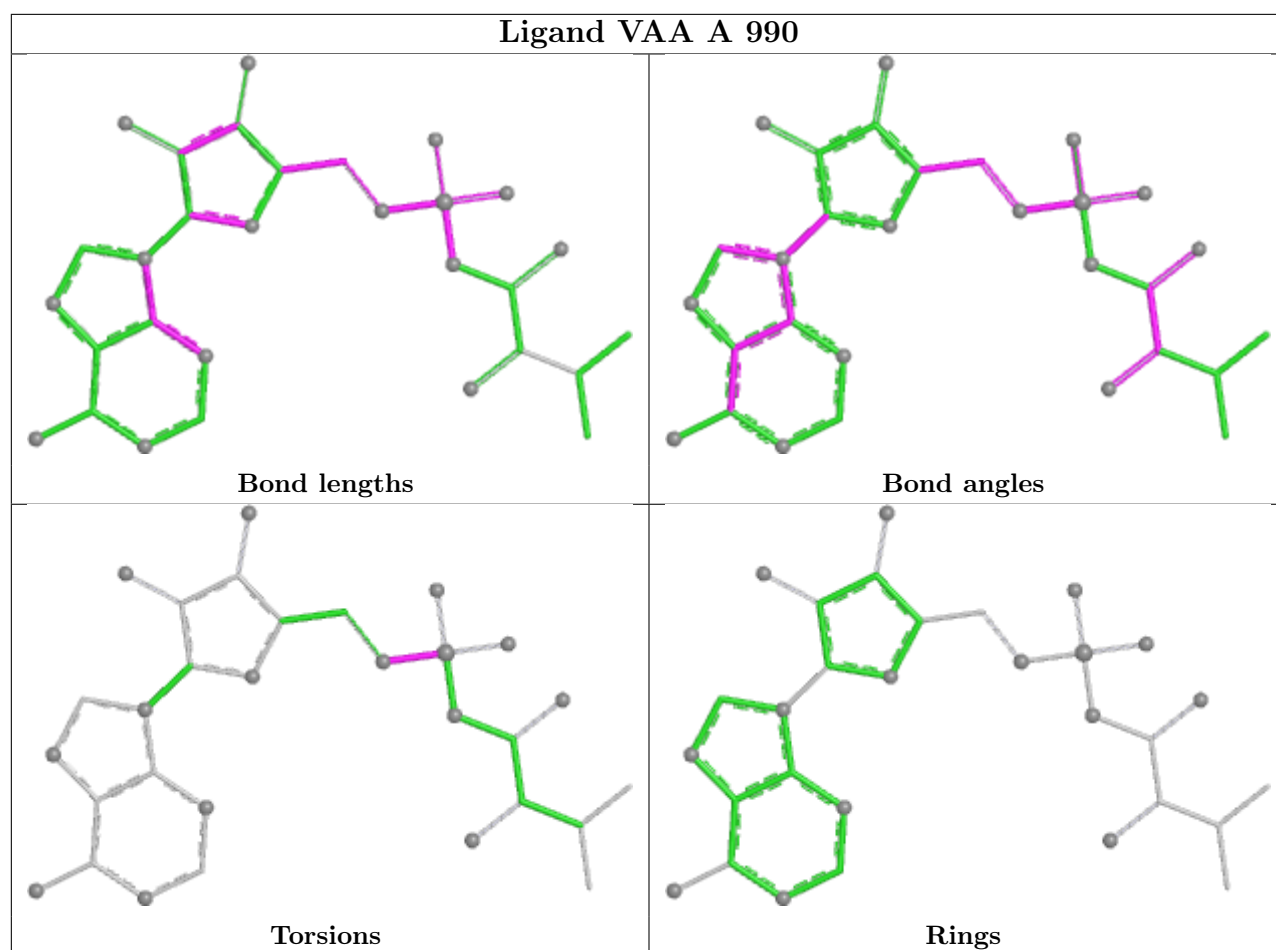
2 monomers are involved in 6 short contacts:

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