



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:35 PM GMT

PDB ID : 1GAX  
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-ADENYLATE ANALOGUE  
Authors : Fukai, S.; Nureki, O.; Sekine, S.; Shimada, A.; Tao, J.; Vassylyev, D.G.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
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 (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

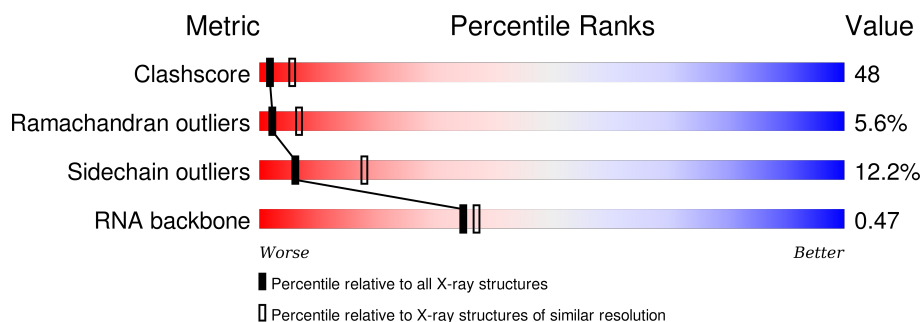
# 1 Overall quality at a glance

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  $\geq 3$ , 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% 39% 35%
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			

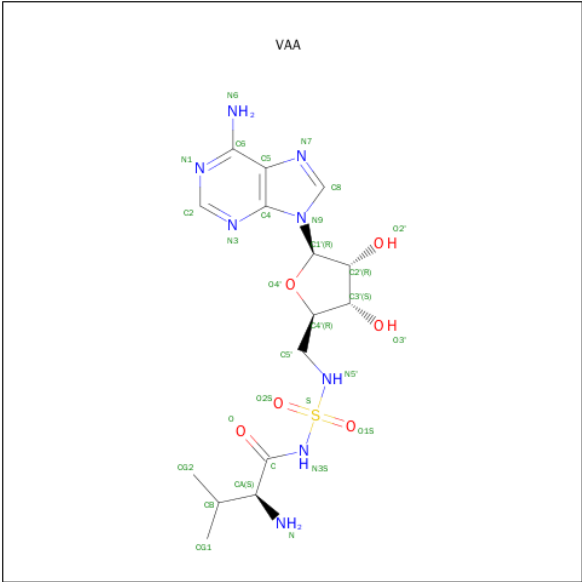
- Molecule 2 is a protein called VALYL-TRNA SYNTHETASE.

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.

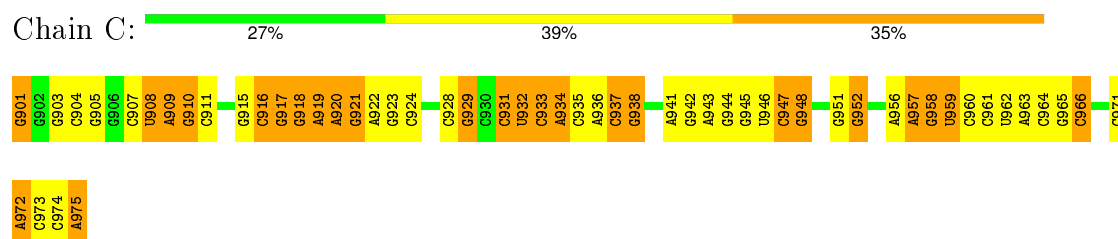
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	61	Total	O	0	0
			61	61		
5	C	19	Total	O	0	0
			19	19		
5	D	11	Total	O	0	0
			11	11		

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

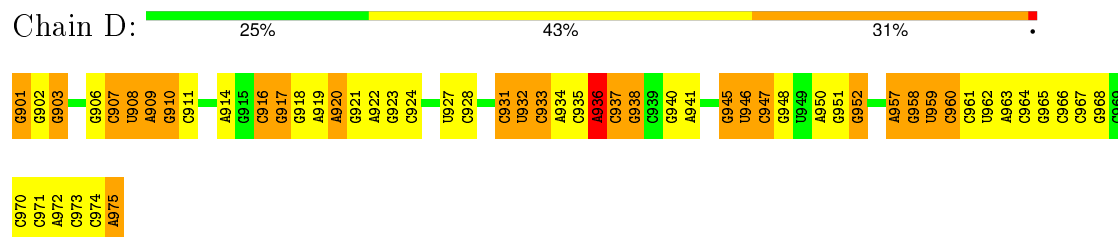
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

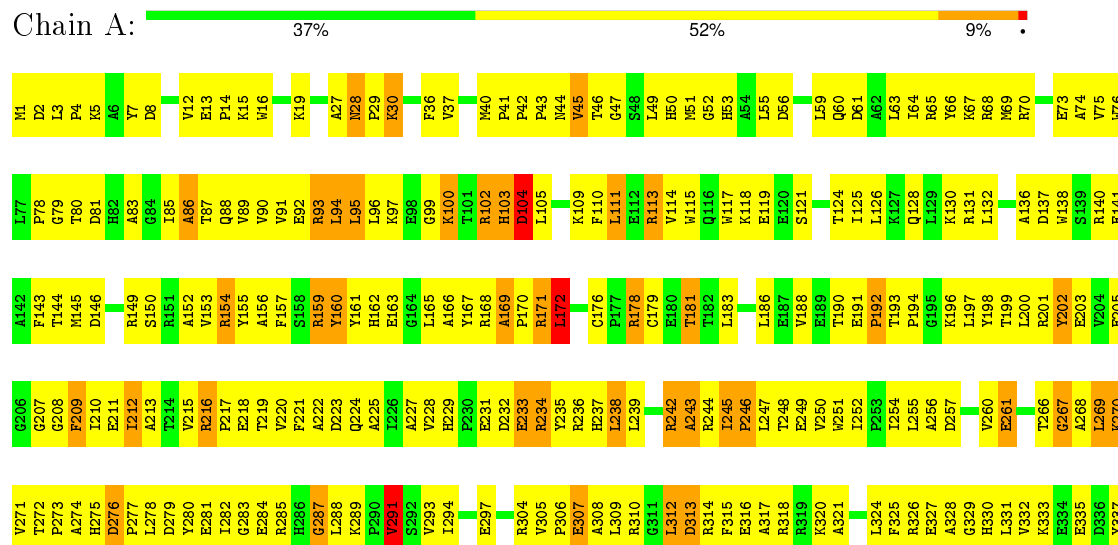
#### • Molecule 1: TRNA(VAL)

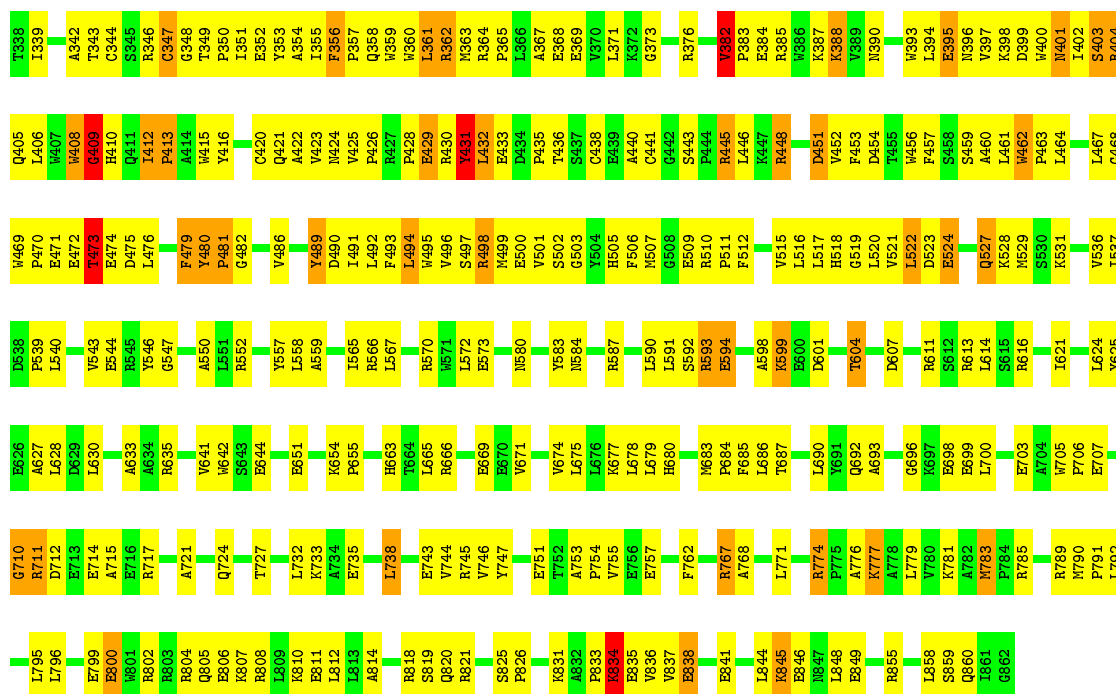


#### • Molecule 1: TRNA(VAL)



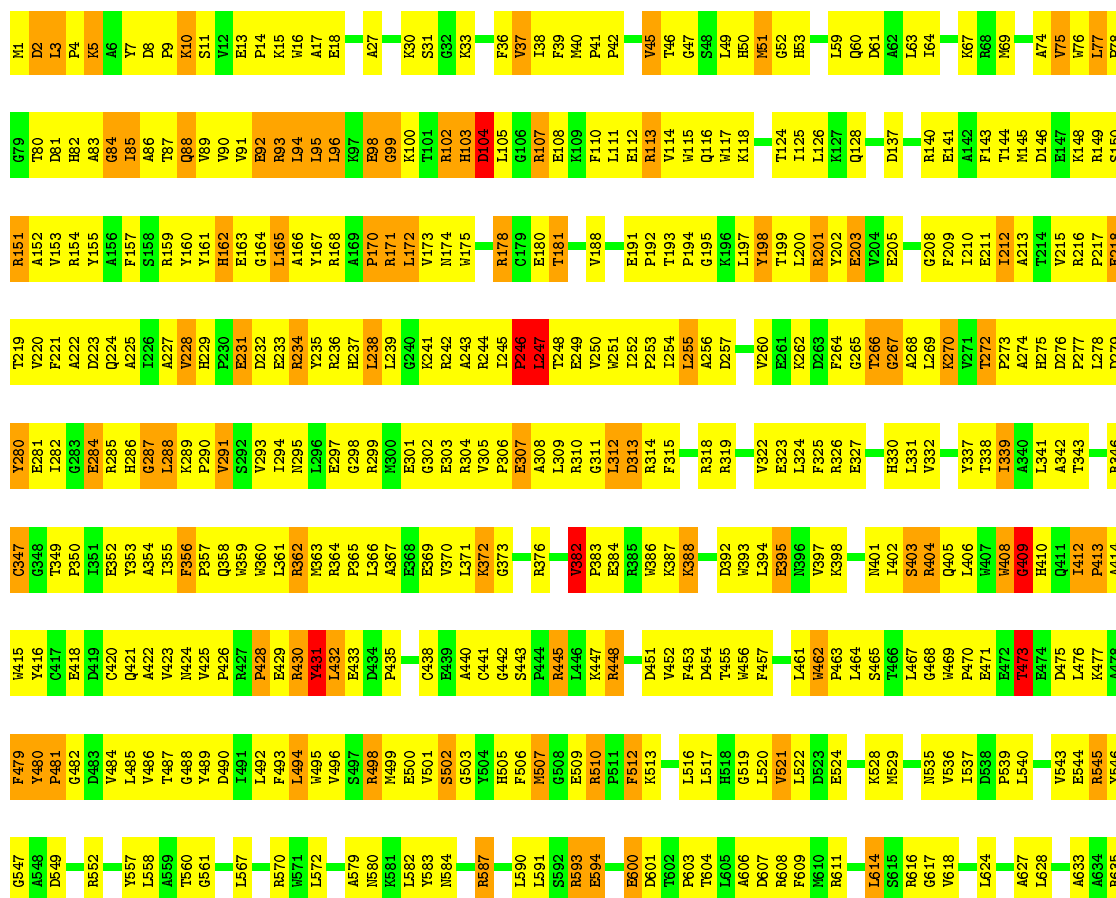
#### • Molecule 2: VALYL-TRNA SYNTHETASE





● Molecule 2: VALYL-TRNA SYNTHETASE

Chain B: 36% 51% 12%



Q860	E639	R711	L795	R789	E644	E711	L796	R790	E649	E712	L797	R791	E650	E713	L798	R792	E651	E714	L799	E654	E715	L800	R801	E655	E716	L802	R803	E656	E717	L804	R805	E667	E718	L806	R807	E668	E719	L807	R808	E669	E720	L808	R809	E670	E721	L809	R810	E671	E722	L810	R811	E672	E723	L811	R812	E673	E724	L812	R813	E674	E725	L813	R814	E675	E726	L814	R815	E676	E727	L815	R816	E677	E728	L816	R817	E678	E729	L817	R818	E679	E730	L818	R819	E680	E731	L819	R820	E681	E732	L820	R821	E682	E733	L821	R822	E683	E734	L822	R823	E684	E735	L823	R824	E685	E736	L824	R825	E686	E737	L825	R826	E687	E738	L826	R827	E688	E739	L827	R828	E689	E740	L828	R829	E690	E741	L829	R830	E691	E742	L830	R831	E692	E743	L831	R832	E693	E744	L832	R833	E694	E745	L833	R834	E695	E746	L834	R835	E696	E747	L835	R836	E697	E748	L836	R837	E698	E749	L837	R838	E699	E750	L838	R839	E700	E751	L839	R840	E701	E752	L840	R841	E702	E753	L841	R842	E703	E754	L842	R843	E704	E755	L843	R844	E705	E756	L844	R845	E706	E757	L845	R846	E707	E758	L846	R847	E708	E759	L847	R848	E709	E760	L848	R849	E710	E761	L849	R850	E711	E762	L850	R851	E712	E763	L851	R852	E713	E764	L852	R853	E714	E765	L853	R854	E715	E766	L854	R855	E716	E767	L855	R856	E717	E768	L856	R857	E718	E769	L857	R858	E719	E770	L858	R859	E720	E771	L859	R860	E721	E772	L860	R861	E722	E773	L861	R862	E723	E774	L862	R863	E724	E775	L863	R864	E725	E776	L864	R865	E726	E777	L865	R866	E727	E778	L866	R867	E728	E779	L867	R868	E729	E780	L868	R869	E730	E781	L869	R870	E731	E782	L870	R871	E732	E783	L871	R872	E733	E784	L872	R873	E734	E785	L873	R874	E735	E786	L874	R875	E736	E787	L875	R876	E737	E788	L876	R877	E738	E789	L877	R878	E739	E790	L878	R879	E740	E791	L879	R880	E741	E792	L880	R881	E742	E793	L881	R882	E743	E794	L882	R883	E744	E795	L883	R884	E745	E796	L884	R885	E746	E797	L885	R886	E747	E798	L886	R887	E748	E799	L887	R888	E749	E800	L888	R889	E750	E801	L889	R890	E751	E802	L890	R891	E752	E803	L891	R892	E753	E804	L892	R893	E754	E805	L893	R894	E755	E806	L894	R895	E756	E807	L895	R896	E757	E808	L896	R897	E758	E809	L897	R898	E759	E810	L898	R899	E760	E811	L899	R900	E761	E812	L900	R901	E762	E813	L901	R902	E763	E814	L902	R903	E764	E815	L903	R904	E765	E816	L904	R905	E766	E817	L905	R906	E767	E818	L906	R907	E768	E819	L907	R908	E769	E820	L908	R909	E770	E821	L909	R910	E771	E822	L910	R911	E772	E823	L911	R912	E773	E824	L912	R913	E774	E825	L913	R914	E775	E826	L914	R915	E776	E827	L915	R916	E777	E828	L916	R917	E778	E829	L917	R918	E779	E830	L918	R919	E780	E831	L919	R920	E781	E832	L920	R921	E782	E833	L921	R922	E783	E834	L922	R923	E784	E835	L923	R924	E785	E836	L924	R925	E786	E837	L925	R926	E787	E838	L926	R927	E788	E839	L927	R928	E789	E840	L928	R929	E790	E841	L929	R930	E791	E842	L930	R931	E792	E843	L931	R932	E793	E844	L932	R933	E794	E845	L933	R934	E795	E846	L934	R935	E796	E847	L935	R936	E797	E848	L936	R937	E798	E849	L937	R938	E799	E850	L938	R939	E800	E851	L939	R940	E801	E852	L940	R941	E802	E853	L941	R942	E803	E854	L942	R943	E804	E855	L943	R944	E805	E856	L944	R945	E806	E857	L945	R946	E807	E858	L946	R947	E808	E859	L947	R948	E809	E860	L948	R949	E810	E861	L949	R950	E811	E862	L950	R951	E812	E863	L951	R952	E813	E864	L952	R953	E814	E865	L953	R954	E815	E866	L954	R955	E816	E867	L955	R956	E817	E868	L956	R957	E818	E869	L957	R958	E819	E870	L958	R959	E820	E871	L959	R960	E821	E872	L960	R961	E822	E873	L961	R962	E823	E874	L962	R963	E824	E875	L963	R964	E825	E876	L964	R965	E826	E877	L965	R966	E827	E878	L966	R967	E828	E879	L967	R968	E829	E880	L968	R969	E830	E881	L969	R970	E831	E882	L970	R971	E832	E883	L971	R972	E833	E884	L972	R973	E834	E885	L973	R974	E835	E886	L974	R975	E836	E887	L975	R976	E837	E888	L976	R977	E838	E889	L977	R978	E839	E890	L978	R979	E840	E891	L979	R980	E841	E892	L980	R981	E842	E893	L981	R982	E843	E894	L982	R983	E844	E895	L983	R984	E845	E896	L984	R985	E846	E897	L985	R986	E847	E898	L986	R987	E848	E899	L987	R988	E849	E900	L988	R989	E850	E901	L989	R990	E851	E902	L990	R991	E852	E903	L991	R992	E853	E904	L992	R993	E854	E905	L993	R994	E855	E906	L994	R995	E856	E907	L995	R996	E857	E908	L996	R997	E858	E909	L997	R998	E859	E910	L998	R999	E860	E911	L999	R1000	E861	E912	L1000	R1001	E862	E913	L1001	R1002	E863	E914	L1002	R1003	E864	E915	L1003	R1004	E865	E916	L1004	R1005	E866	E917	L1005	R1006	E867	E918	L1006	R1007	E868	E919	L1007	R1008	E869	E920	L1008	R1009	E870	E921	L1009	R1010	E871	E922	L1010	R1011	E872	E923	L1011	R1012	E873	E924	L1012	R1013	E874	E925	L1013	R1014	E875	E926	L1014	R1015	E876	E927	L1015	R1016	E877	E928	L1016	R1017	E878	E929	L1017	R1018	E879	E930	L1018	R1019	E880	E931	L1019	R1020	E881	E932	L1020	R1021	E882	E933	L1021	R1022	E883	E934	L1022	R1023	E884	E935	L1023	R1024	E885	E936	L1024	R1025	E886	E937	L1025	R1026	E887	E938	L1026	R1027	E888	E939	L1027	R1028	E889	E940	L1028	R1029	E890	E941	L1029	R1030	E891	E942	L1030	R1031	E892	E943	L1031	R1032	E893	E944	L1032	R1033	E894	E945	L1033	R1034	E895	E946	L1034	R1035	E896	E947	L1035	R1036	E897	E948	L1036	R1037	E898	E949	L1037	R1038	E899	E950	L1038	R1039	E900	E951	L1039	R1040	E901	E952	L1040	R1041	E902	E953	L1041	R1042	E903	E954	L1042	R1043	E904	E955	L10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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, $\alpha$ , $\beta$ , $\gamma$	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	6
All	All	1720/1724 (100%)	1328 (77%)	295 (17%)	97 (6%)	2	7

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%)	7	21
2	B	724/724 (100%)	630 (87%)	94 (13%)	5	15
All	All	1448/1448 (100%)	1271 (88%)	177 (12%)	6	18

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%)	10 (13%)
1	D	74/75 (98%)	27 (36%)	7 (9%)
All	All	148/150 (98%)	53 (35%)	17 (11%)

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

5 of 17 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	947	C
1	C	957	A
1	D	937	C
1	C	937	C
1	D	947	C

## 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	3.54	11 (44%)	27,48,48	1.93	5 (18%)
4	VAA	B	1990	-	25,32,32	3.37	9 (36%)	27,48,48	1.82	7 (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	-	-	0/17/39/39	0/3/3/3
4	VAA	B	1990	-	-	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)
4	A	990	VAA	C5'-N5'	-8.16	1.31	1.47
4	B	1990	VAA	C5'-N5'	-7.35	1.33	1.47
4	A	990	VAA	C5'-C4'	-4.31	1.41	1.51
4	B	1990	VAA	C5'-C4'	-3.67	1.42	1.51
4	A	990	VAA	C8-N7	-3.50	1.27	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	990	VAA	O2S-S-O1S	-5.53	111.01	120.04
4	B	1990	VAA	O2S-S-O1S	-4.79	112.23	120.04
4	A	990	VAA	C-N3S-S	-4.42	117.87	124.05
4	B	1990	VAA	C-N3S-S	-3.48	119.18	124.05
4	B	1990	VAA	C1'-N9-C4	-3.14	122.21	126.94

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
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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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