



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:43 AM UTC

PDB ID : 2ZW9 / pdb_00002zw9
Title : Crystal structure of tRNA wybutosine synthesizing enzyme TYW4
Authors : Suzuki, Y.; Noma, A.; Suzuki, T.; Ishitani, R.; Nureki, O.
Deposited on : 2008-12-01
Resolution : 2.50 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)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

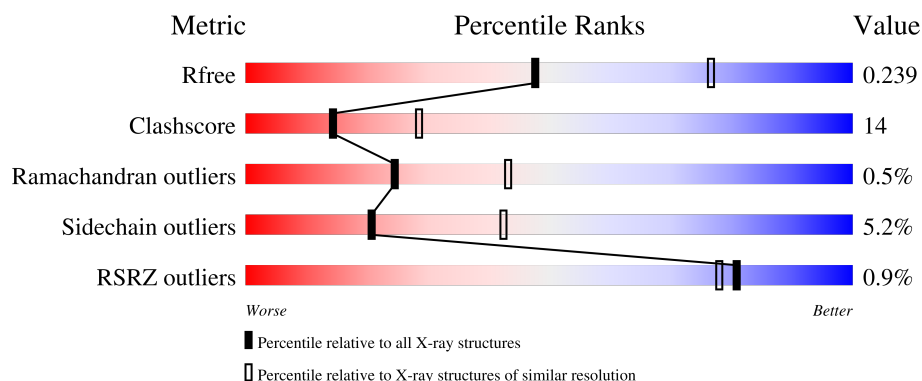
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

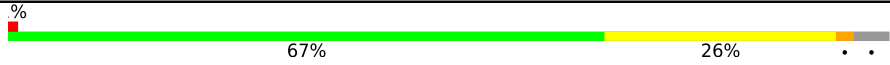
The reported resolution of this entry is 2.50 Å.

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	695	
1	B	695	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10810 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.

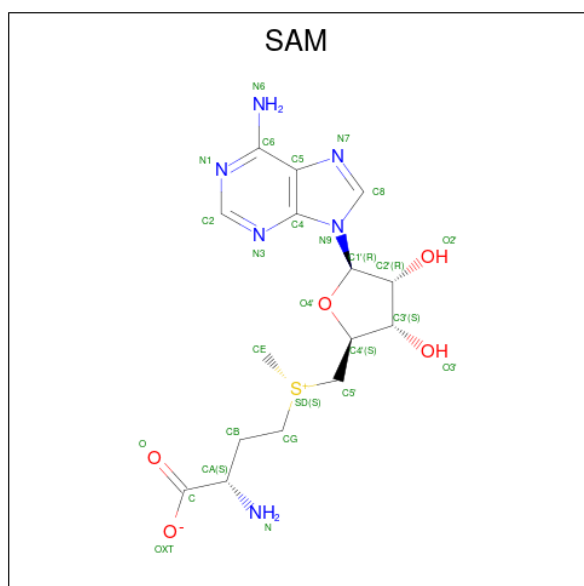
- Molecule 1 is a protein called Leucine carboxyl methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5329	3417	891	996	25			
1	B	664	Total	C	N	O	S	0	0	0
			5294	3396	880	992	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	LEU	MET	SEE REMARK 999	UNP Q08282
B	417	LEU	MET	SEE REMARK 999	UNP Q08282

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

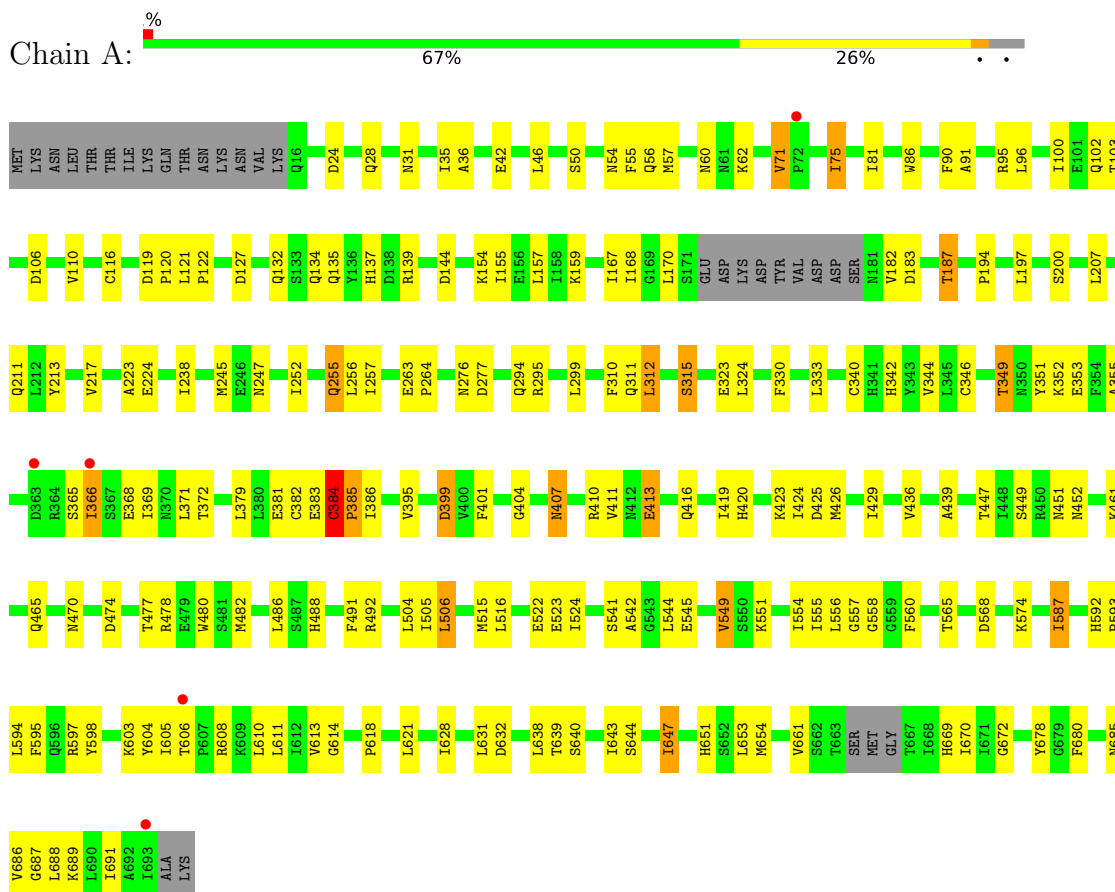
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	75	Total	O	0	0
			75	75		

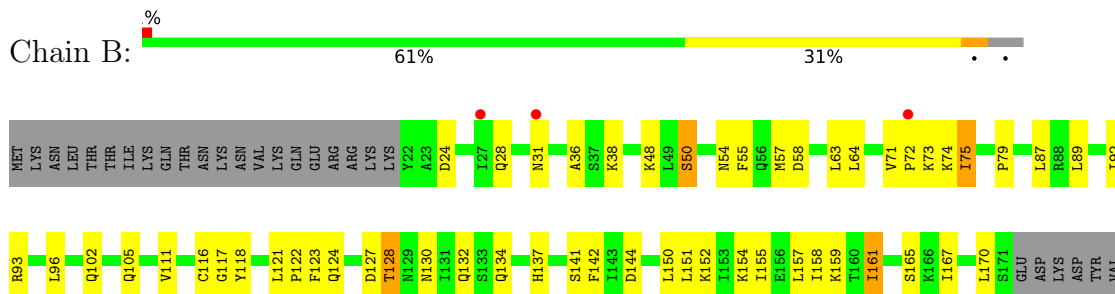
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

• Molecule 1: Leucine carboxyl methyltransferase 2



• Molecule 1: Leucine carboxyl methyltransferase 2



I691	K603	M482	S392	R275	ASP
A694	Y604	I483	V393	K285	ASP
LYS	I605	L486	D394	K286	SER
	T606	S487	V395	T288	N181
	P607	H488	A396	T289	V182
	R608		G397	E290	T186
	K609	N502	N398	S291	K189
	L610	L506	D399	Q292	Y190
	L611		F401	Y303	L191
	I612	V509	N407	D308	P194
	V613			K309	C195
	G614	M515	N412	F310	D196
	G615	L516	E413	Q311	L197
	T616	L517	I414	L312	N198
	S617	N518	L415	W313	D199
	P618	N519	Q416	K321	N202
	R624	D527	L417	K322	T205
		V528	S418	E323	L206
	T628	T529	I419	L324	L207
	I629	P530	H420	L325	N208
		K531	Y421	E328	E209
	L634	D532	D422	E332	Q210
	S635	E533	K423	L333	Q211
	E636	F534	I424	H337	L212
	E637		D425	V344	Y213
	T637	L539	M426	C346	D214
	L638		K427		V217
	I641		N428		V218
	P642	T554	I429	T349	K219
	I643	T555		N350	E224
	S644	L556	S433	Y351	L227
	R645	G557	L345	K352	P232
	R646		A439	A355	E233
	I647	F560	F445	I366	L238
	W648	M561		T369	M245
	E649		I448	N370	E246
		S652	S449	L371	N247
	L653	L571		L379	L252
	V661	E578	N452	L380	Q255
	S662	N579	Q453	E383	L256
	T663	A580	L454	C384	I257
	S664		L455	P385	P258
	G665	T585	R460	I386	F262
	G666	V586	K461	K387	E263
	T667	I587	A462	R388	P264
	I668	K588	P463		
	H669	K589	N470		
	L670	L590	W471		
	I671	H592	D474		
	G672	P593			
		L594	T477		
	V686	F595	W480		
	G687	Q596	S481		
	L688	K597			
	K689	Y598			
	L690				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.44Å 88.63Å 256.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.50 46.32 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.0 (46.32-2.50) 90.8 (46.32-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.245 0.188 , 0.239	Depositor DCC
R_{free} test set	2600 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10810	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	A	0.29	0/5443	0.79	8/7359 (0.1%)
1	B	0.29	0/5409	0.77	8/7318 (0.1%)
All	All	0.29	0/10852	0.78	16/14677 (0.1%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ILE	CA-C-N	7.96	127.62	119.82
1	A	257	ILE	C-N-CA	7.96	127.62	119.82
1	A	384	CYS	CA-C-N	6.97	128.55	119.84
1	A	384	CYS	C-N-CA	6.97	128.55	119.84
1	A	71	VAL	CA-C-N	6.63	126.13	119.24

There are no chirality outliers.

There are no planarity outliers.

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	A	5329	0	5346	151	0
1	B	5294	0	5303	157	0
2	A	27	0	22	2	0
2	B	27	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	58	0	0	0	0
3	B	75	0	0	1	0
All	All	10810	0	10693	302	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 14.

The worst 5 of 302 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)
1:A:384:CYS:SG	1:A:424:ILE:HB	1.85	1.16
1:A:461:LYS:HD3	1:B:482:MET:HE1	1.37	1.04
1:B:102:GLN:HE22	1:B:355:ALA:H	1.11	0.96
1:A:71:VAL:HG11	1:A:75:ILE:HD11	1.48	0.96
1:B:606:THR:HG22	1:B:608:ARG:H	1.30	0.95

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	
1	A	660/695 (95%)	618 (94%)	40 (6%)	2 (0%)	36	55
1	B	660/695 (95%)	612 (93%)	44 (7%)	4 (1%)	21	38
All	All	1320/1390 (95%)	1230 (93%)	84 (6%)	6 (0%)	24	43

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	ASN
1	A	385	PRO

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Mol	Chain	Res	Type
1	B	195	CYS
1	B	383	GLU
1	B	483	ILE

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	
1	A	603/630 (96%)	578 (96%)	25 (4%)	27	53
1	B	599/630 (95%)	561 (94%)	38 (6%)	16	34
All	All	1202/1260 (95%)	1139 (95%)	63 (5%)	21	42

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	105	GLN
1	B	605	ILE
1	B	275	ARG
1	B	597	ARG
1	B	634	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	102	GLN
1	B	592	HIS
1	B	132	GLN
1	B	416	GLN
1	B	124	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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$
2	SAM	A	801	-	27,29,29	1.10	4 (14%)	34,42,42	2.06	9 (26%)
2	SAM	B	801	-	27,29,29	1.08	4 (14%)	34,42,42	1.99	9 (26%)

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
2	SAM	A	801	-	-	1/17/33/33	0/3/3/3
2	SAM	B	801	-	-	2/17/33/33	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SAM	C2-N1	2.68	1.38	1.33
2	B	801	SAM	C2-N1	2.62	1.38	1.33
2	A	801	SAM	C2-N3	2.58	1.38	1.33
2	B	801	SAM	C2-N3	2.45	1.38	1.33
2	A	801	SAM	OXT-C	-2.14	1.23	1.30

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	SAM	N3-C2-N1	-5.76	119.87	128.58
2	B	801	SAM	N3-C2-N1	-5.60	120.10	128.58
2	A	801	SAM	C5-C4-N3	-4.51	120.51	126.72
2	B	801	SAM	C5-C4-N3	-4.13	121.03	126.72
2	A	801	SAM	N9-C8-N7	-3.94	108.35	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

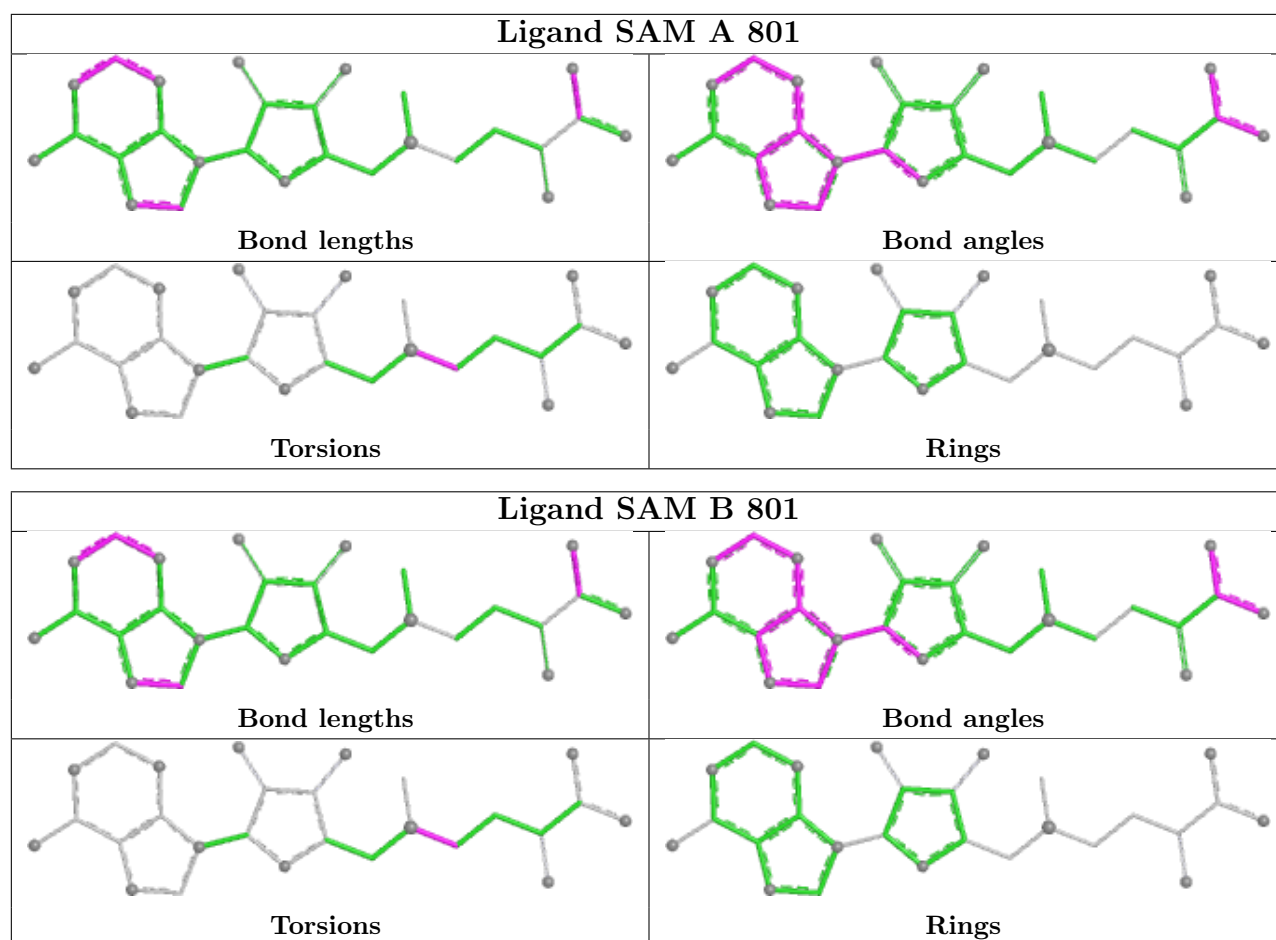
Mol	Chain	Res	Type	Atoms
2	B	801	SAM	CB-CG-SD-C5'
2	B	801	SAM	CB-CG-SD-CE
2	A	801	SAM	CB-CG-SD-C5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SAM	2	0
2	B	801	SAM	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 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.



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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/695 (95%)	-0.04	5 (0%) 82 80	39, 61, 94, 127	0
1	B	664/695 (95%)	-0.03	7 (1%) 78 75	37, 61, 93, 131	0
All	All	1330/1390 (95%)	-0.03	12 (0%) 81 78	37, 61, 94, 131	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	366	ILE	3.8
1	B	72	PRO	3.4
1	B	31	ASN	3.4
1	B	27	ILE	3.3
1	B	384	CYS	2.8

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

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

6.3 Carbohydrates [i](#)

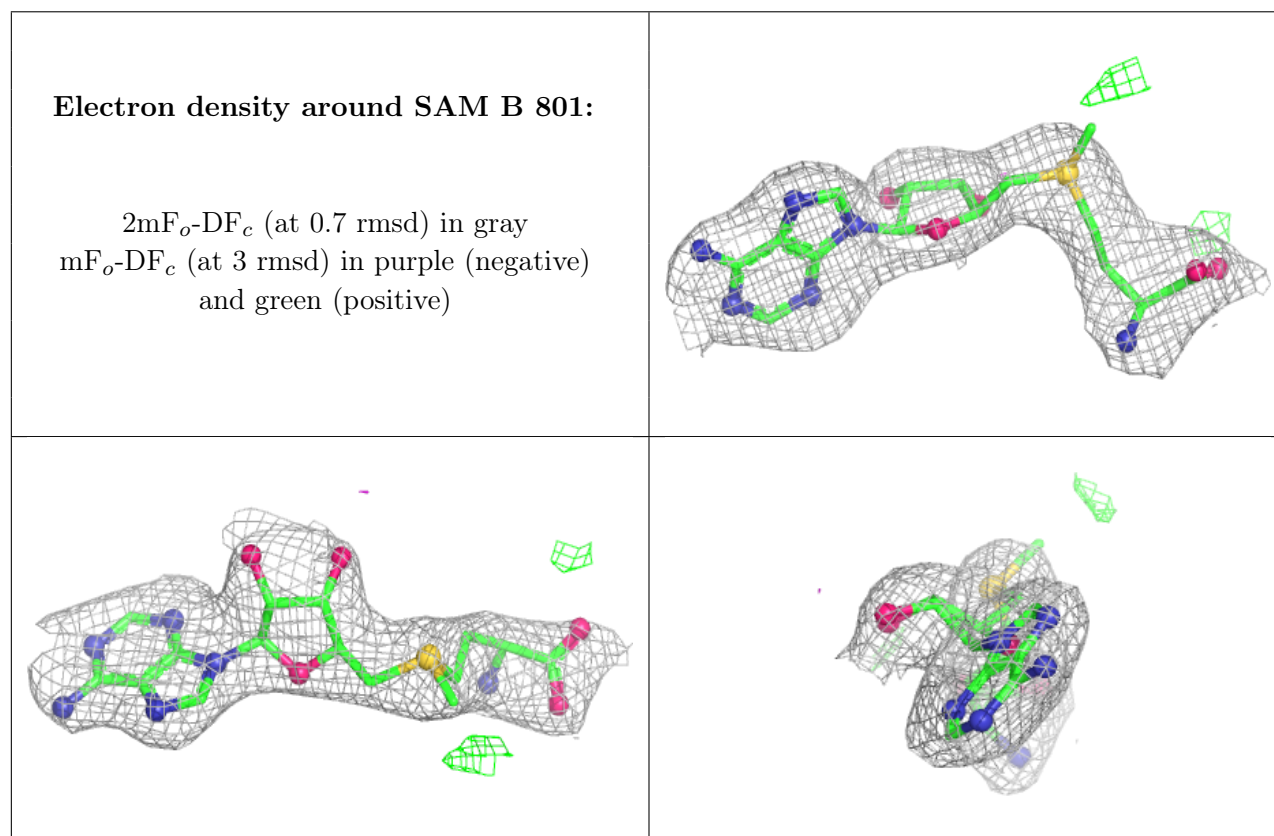
There are no oligosaccharides in this entry.

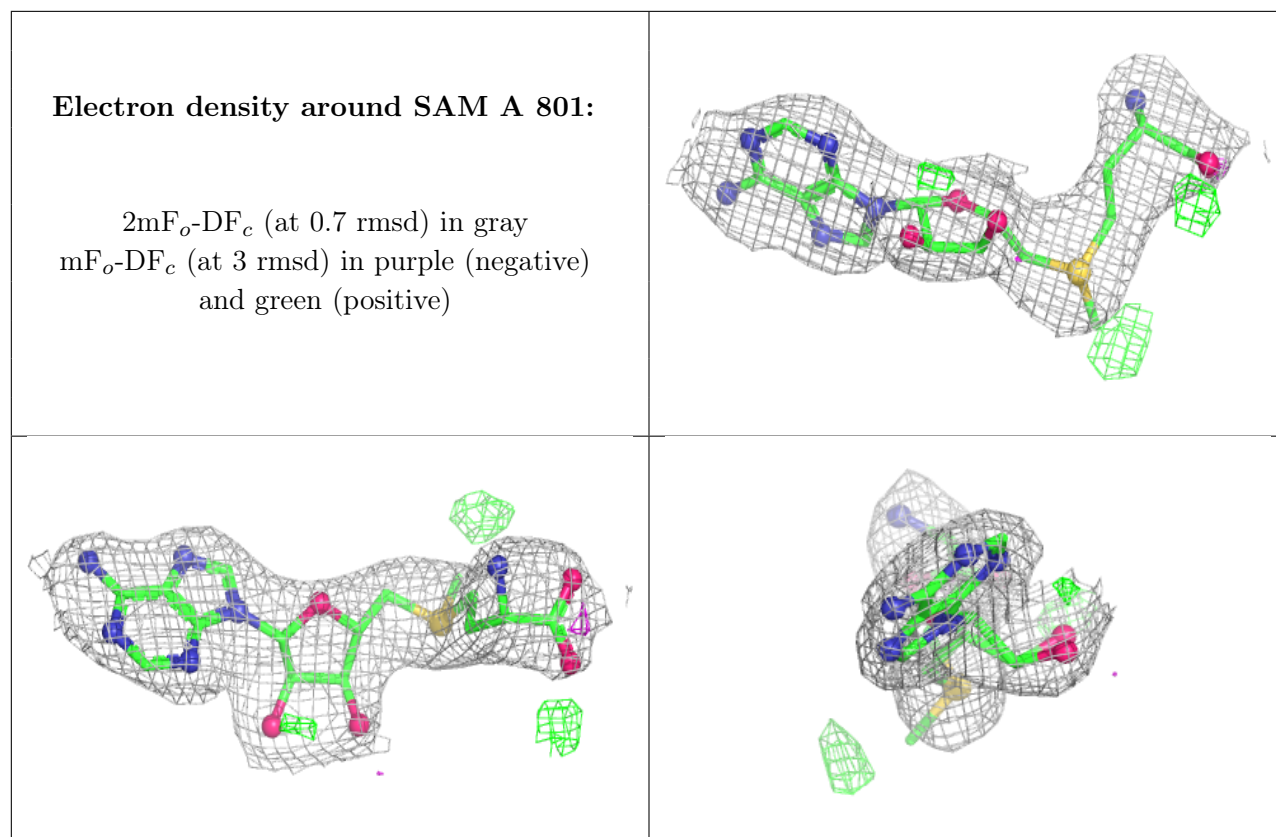
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAM	B	801	27/27	0.92	0.10	62,72,79,89	0
2	SAM	A	801	27/27	0.93	0.09	52,64,78,82	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.