



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:43 PM UTC

PDB ID : 2AET / pdb\_00002aet  
Title : R304K trichodiene synthase: Complex with Mg, pyrophosphate, and (4S)-7-azabisabolene  
Authors : Vedula, L.S.; Cane, D.E.; Christianson, D.W.  
Deposited on : 2005-07-23  
Resolution : 2.75 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

<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>.

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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  
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

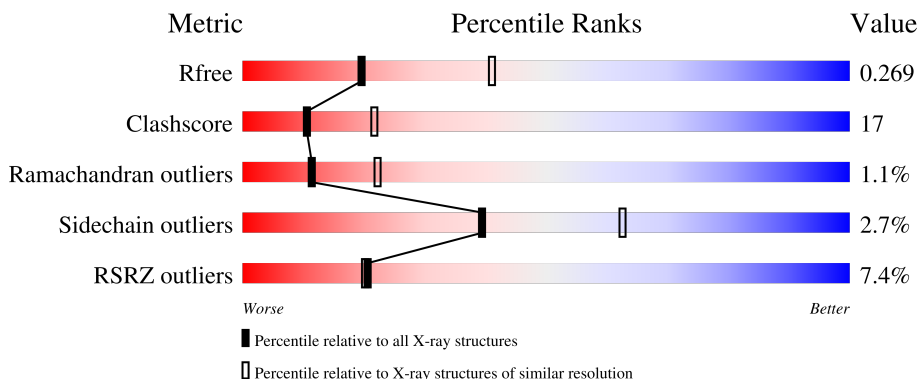
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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  $\geq 3$ , 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	374	 2% 61% 32% 6%
1	B	374	 11% 63% 28% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	751	-	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5956 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.

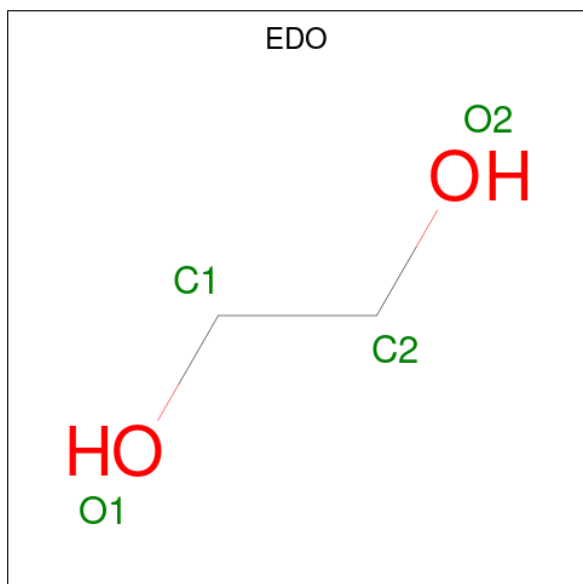
- Molecule 1 is a protein called Trichodiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	352	2921	1872	489	543	17	89	0	0
1	B	353	2926	1874	489	546	17	197	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	304	LYS	ARG	engineered mutation	UNP P13513
B	304	LYS	ARG	engineered mutation	UNP P13513

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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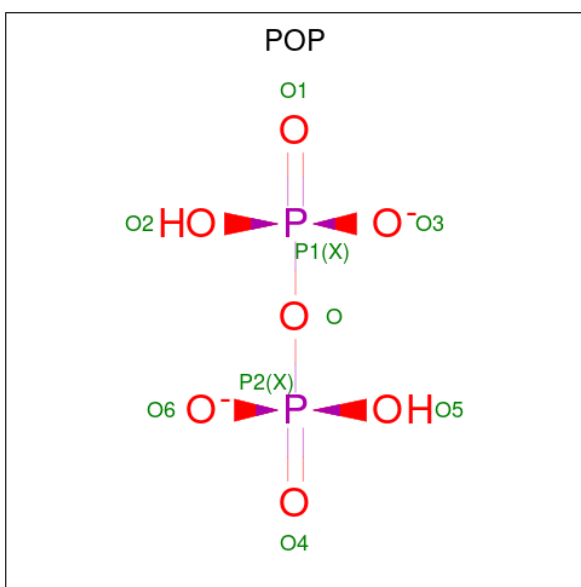
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	41	Total	O	0	0
			41	41		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.38Å 122.38Å 151.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.00 – 2.75 60.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	88.8 (60.00-2.75) 88.7 (60.00-2.75)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.73Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.256 0.235 , 0.269	Depositor DCC
$R_{free}$ test set	1523 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.8	Xtrriage
Anisotropy	0.265	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POP, EDO, MG

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	0.46	0/3006	0.91	6/4081 (0.1%)
1	B	0.44	0/3011	0.92	11/4089 (0.3%)
All	All	0.45	0/6017	0.92	17/8170 (0.2%)

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	264	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	B	28	THR	N-CA-C	-7.92	97.04	109.72
1	A	103	LYS	N-CA-C	-7.87	103.80	113.41
1	B	276	VAL	N-CA-C	7.17	117.96	110.72

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	A	2921	0	2775	99	0
1	B	2926	0	2770	96	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
4	B	9	0	0	0	0
5	A	48	0	0	1	0
5	B	41	0	0	1	0
All	All	5956	0	5557	182	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 17.

The worst 5 of 182 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:27:TYR:HB3	1:A:32:ARG:HH12	1.40	0.85
1:B:240:GLN:NE2	1:B:245:LYS:HE2	1.94	0.82
1:A:12:THR:HG21	1:A:263:THR:HG22	1.61	0.80
1:A:69:THR:HG23	1:A:298:TRP:HZ2	1.48	0.78
1:A:107:TYR:HB3	1:A:108:PRO:HD3	1.66	0.78

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	350/374 (94%)	329 (94%)	19 (5%)	2 (1%)	21	38
1	B	351/374 (94%)	320 (91%)	25 (7%)	6 (2%)	7	14
All	All	701/748 (94%)	649 (93%)	44 (6%)	8 (1%)	11	22

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	304	LYS
1	B	306	ARG
1	B	102	SER
1	A	198	LYS
1	A	275	ALA

### 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	
1	A	318/340 (94%)	310 (98%)	8 (2%)	42	64
1	B	318/340 (94%)	309 (97%)	9 (3%)	38	61
All	All	636/680 (94%)	619 (97%)	17 (3%)	39	62

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	209	GLU
1	B	259	LEU
1	A	335	VAL
1	B	29	ARG
1	B	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	ASN
1	B	216	GLN
1	B	175	HIS
1	B	225	ASN
1	A	272	GLN

### 5.3.3 RNA [i](#)

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](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
2	EDO	A	750	-	3,3,3	2.34	2 (66%)	2,2,2	0.53	0
4	POP	B	700	3	6,8,8	1.57	1 (16%)	12,13,13	1.60	1 (8%)
2	EDO	B	751	-	3,3,3	2.35	2 (66%)	2,2,2	0.48	0

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	EDO	A	750	-	-	0/1/1/1	-
4	POP	B	700	3	-	0/6/6/6	-
2	EDO	B	751	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	751	EDO	O2-C2	2.94	1.57	1.42
2	A	750	EDO	O2-C2	2.92	1.57	1.42
2	A	750	EDO	O1-C1	2.69	1.55	1.42
2	B	751	EDO	O1-C1	2.65	1.55	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	POP	P2-O6	-2.50	1.45	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	POP	O2-P1-O	4.68	120.34	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	751	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	342/374 (91%)	0.08	8 (2%) 61 59	33, 51, 77, 100	0
1	B	333/374 (89%)	0.58	42 (12%) 8 6	4, 56, 100, 125	1 (0%)
All	All	675/748 (90%)	0.33	50 (7%) 20 20	4, 53, 92, 125	1 (0%)

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	GLU	7.5
1	B	54	GLN	7.4
1	B	314	VAL	7.1
1	B	316	GLU	7.0
1	B	22	TYR	6.5

### 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, 95<sup>th</sup> 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
3	MG	B	703	1/1	0.74	0.29	91,91,91,91	0
3	MG	B	702	1/1	0.83	0.15	68,68,68,68	0
4	POP	B	700	9/9	0.83	0.13	116,117,119,119	0
2	EDO	B	751	4/4	0.90	0.13	44,46,49,50	0
2	EDO	A	750	4/4	0.90	0.15	49,52,52,53	0
3	MG	B	701	1/1	0.96	0.10	71,71,71,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.