wwPDB X-ray Structure Validation Summary Report (i)

Nov 2, 2026 – 12:09 pm GMT

PDB ID	:	9T3N / pdb_00009t3n
Title	:	Type III polyketide synthase from Hypoxylon argillaceum CBS527.63
Authors	:	Zhang, L.; Groves, M.R.
Deposited on	:	2025-10-28
Resolution	:	2.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

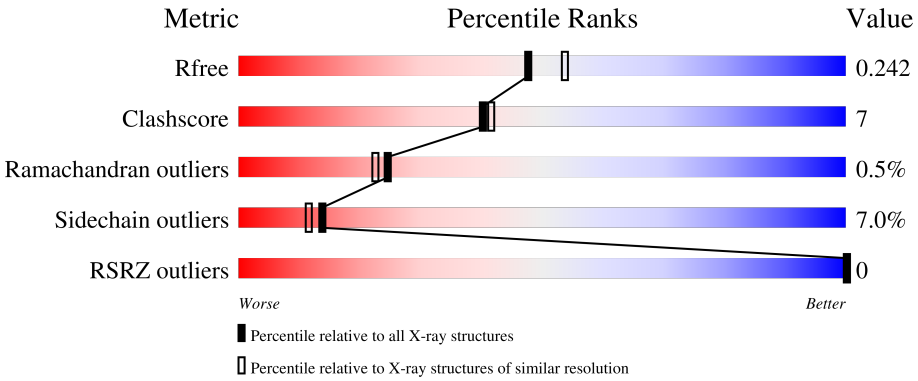
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 <=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	402	67% 21% • 8%
1	B	402	75% 13% • 8%
1	C	402	77% 13% • 8%
1	D	402	74% 15% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22268 atoms, of which 11158 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 Type III polyketide synthase from Hypoxylon argillaceum CBS527.63.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	H	N	O	S	80	1	0
			5532	1723	2788	491	512	18			
1	B	368	Total	C	H	N	O	S	79	2	0
			5541	1726	2793	492	513	17			
1	C	368	Total	C	H	N	O	S	80	2	0
			5536	1724	2789	492	514	17			
1	D	368	Total	C	H	N	O	S	80	1	0
			5532	1723	2788	491	513	17			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	38	Total	O	0	0
			38	38		
2	B	31	Total	O	0	0
			31	31		
2	C	27	Total	O	0	0
			27	27		
2	D	31	Total	O	0	0
			31	31		

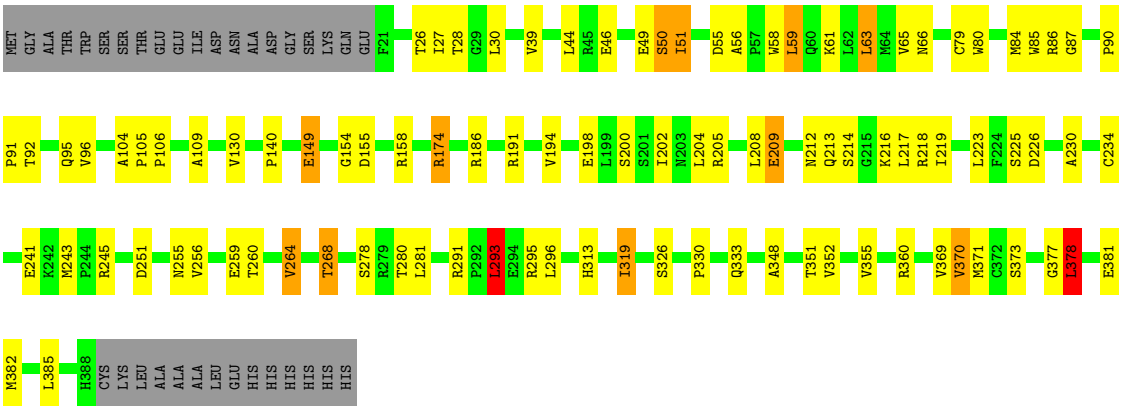
3 Residue-property plots (i)

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: Type III polyketide synthase from Hypoxylon argillaceum CBS527.63

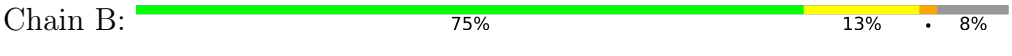
Chain A:

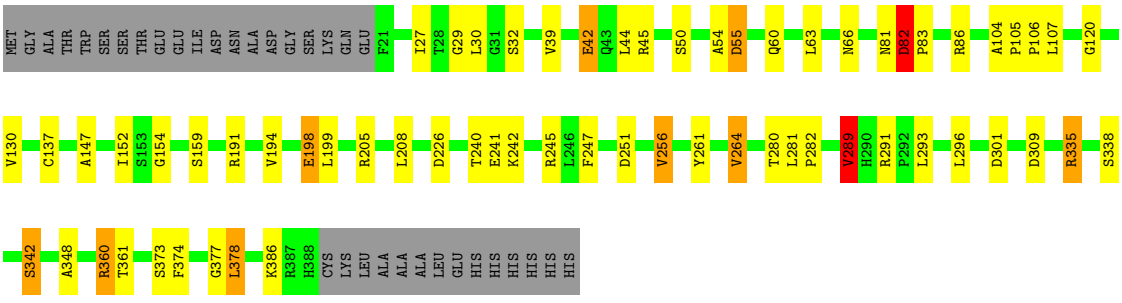




• Molecule 1: Type III polyketide synthase from Hypoxylon argillaceum CBS527.63

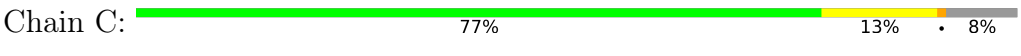
Chain B:

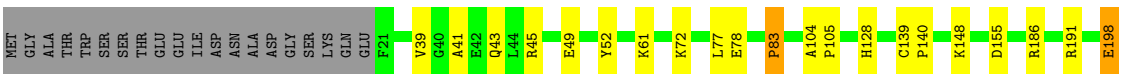


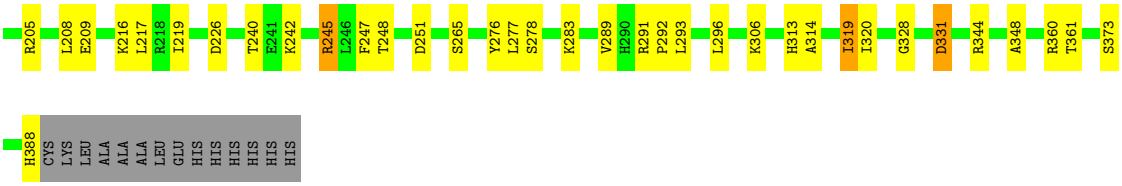


• Molecule 1: Type III polyketide synthase from Hypoxylon argillaceum CBS527.63

Chain C:

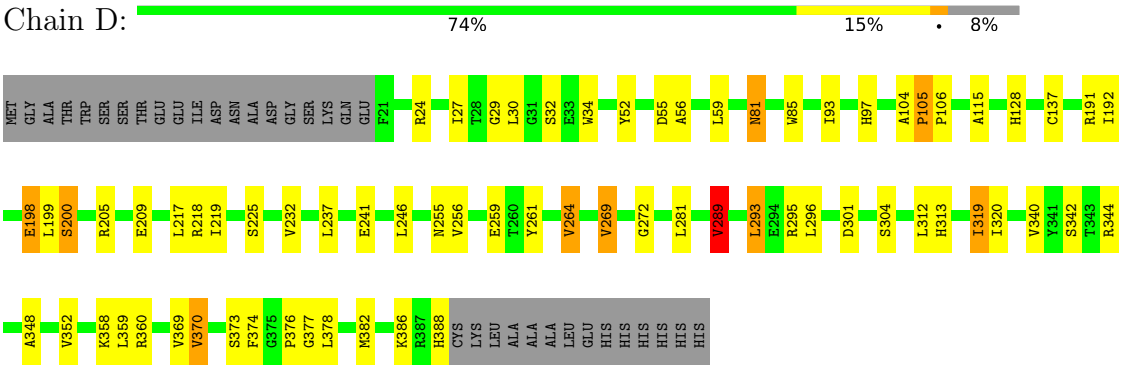






• Molecule 1: Type III polyketide synthase from Hypoxylon argillaceum CBS527.63

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.33Å 68.41Å 94.23Å 78.17° 78.91° 66.68°	Depositor
Resolution (Å)	43.15 – 2.10 43.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.8 (43.15-2.10) 91.8 (43.15-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.186 , 0.243 0.186 , 0.242	Depositor DCC
R_{free} test set	4044 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 30.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.168 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22268	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.71	0/2799	1.27	11/3806 (0.3%)
1	B	0.71	0/2805	1.26	9/3815 (0.2%)
1	C	0.70	0/2807	1.26	12/3817 (0.3%)
1	D	0.70	0/2799	1.27	7/3806 (0.2%)
All	All	0.70	0/11210	1.26	39/15244 (0.3%)

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	A	0	5
1	B	0	5
1	C	0	3
1	D	0	4
All	All	0	17

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	269	VAL	N-CA-CB	-8.57	100.52	112.52
1	A	155	ASP	CA-CB-CG	7.97	120.57	112.60
1	B	335	ARG	CD-NE-CZ	7.58	135.02	124.40
1	C	331	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	174	ARG	CD-NE-CZ	7.18	134.45	124.40

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Sidechain
1	A	191	ARG	Sidechain
1	A	291	ARG	Sidechain
1	A	377	GLY	Peptide,Mainchain
1	B	191	ARG	Sidechain

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	2744	2788	2779	67	0
1	B	2748	2793	2778	37	0
1	C	2747	2789	2768	19	0
1	D	2744	2788	2779	36	0
2	A	38	0	0	0	0
2	B	31	0	0	3	0
2	C	27	0	0	0	0
2	D	31	0	0	0	0
All	All	11110	11158	11104	146	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 7.

The worst 5 of 146 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:D:198:GLU:HG2	1:D:348:ALA:HB3	1.58	0.86
1:D:255:ASN:HD21	1:D:295:ARG:HH11	1.20	0.85
1:D:289:VAL:HG13	1:D:374:PHE:HZ	1.40	0.85
1:D:81:ASN:C	1:D:81:ASN:HD22	1.90	0.80
1:A:28:THR:HG21	1:A:243:MET:CE	2.13	0.79

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	367/402 (91%)	351 (96%)	15 (4%)	1 (0%)	36	36
1	B	368/402 (92%)	355 (96%)	11 (3%)	2 (0%)	24	22
1	C	368/402 (92%)	356 (97%)	10 (3%)	2 (0%)	24	22
1	D	367/402 (91%)	350 (95%)	15 (4%)	2 (0%)	24	22
All	All	1470/1608 (91%)	1412 (96%)	51 (4%)	7 (0%)	24	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	LEU
1	B	378	LEU
1	D	217	LEU
1	D	378	LEU
1	B	82	ASP

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	287/313 (92%)	267 (93%)	20 (7%)	14	11
1	B	287/313 (92%)	265 (92%)	22 (8%)	12	9
1	C	288/313 (92%)	273 (95%)	15 (5%)	21	20
1	D	287/313 (92%)	263 (92%)	24 (8%)	10	7
All	All	1149/1252 (92%)	1068 (93%)	81 (7%)	14	11

5 of 81 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	24	ARG
1	D	293	LEU
1	D	59	LEU
1	D	237	LEU
1	D	319	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	212	ASN
1	D	43	GLN
1	D	255	ASN
1	C	324	GLN
1	D	60	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)

There are no ligands in this entry.

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

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^{th} 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	368/402 (91%)	-1.25	0	100	100	16, 40, 79, 115	1 (0%)
1	B	368/402 (91%)	-1.25	0	100	100	16, 41, 79, 99	1 (0%)
1	C	368/402 (91%)	-1.22	0	100	100	14, 42, 84, 112	1 (0%)
1	D	368/402 (91%)	-1.19	0	100	100	15, 44, 84, 102	1 (0%)
All	All	1472/1608 (91%)	-1.23	0	100	100	14, 42, 82, 115	4 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.