



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:07 AM UTC

PDB ID : 6KET / pdb_00006ket
Title : Flavín-utilizing Monooxygenase (OX) Domain of Hybrid Polyketide/Non-Ribosomal Peptide Synthetase
Authors : Tian, Q.W.; Jiang, T.
Deposited on : 2019-07-05
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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
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

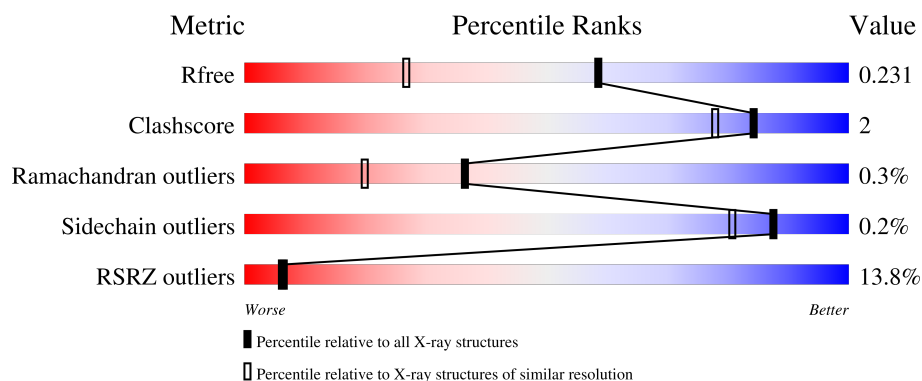
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	362	10% 91% 5% .
1	B	362	16% 85% 7% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5734 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 PuwE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2720	1732	464	515	9			
1	B	332	Total	C	N	O	S	0	0	0
			2587	1650	445	484	8			

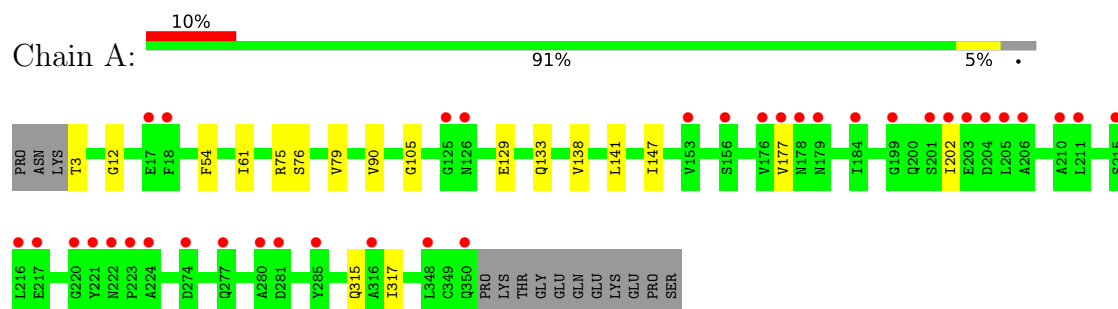
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	259	Total	O	0	0
			259	259		
2	B	168	Total	O	0	0
			168	168		

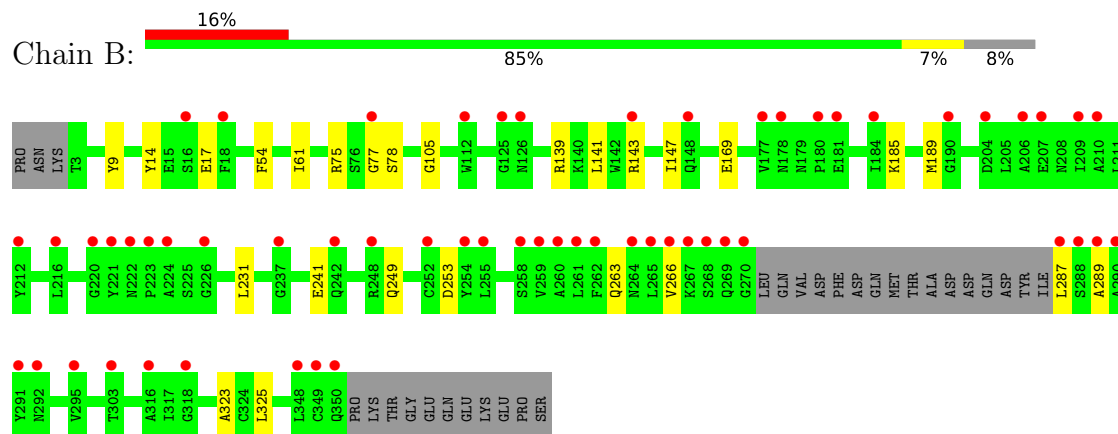
3 Residue-property plots

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: PuwE



• Molecule 1: PuwE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	95.61Å 103.55Å 77.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.29 – 1.60 23.29 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.29-1.60) 99.5 (23.29-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.13-2998	Depositor
R, R_{free}	0.220 , 0.239 0.211 , 0.231	Depositor DCC
R_{free} test set	2012 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5734	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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

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	0.37	2/2784 (0.1%)	0.53	0/3786
1	B	0.23	0/2648	0.49	0/3599
All	All	0.31	2/5432 (0.0%)	0.51	0/7385

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	SER	C-O	-7.80	1.14	1.24
1	A	79	VAL	C-O	-5.89	1.18	1.24

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	77	GLY	Mainchain,Peptide

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	2720	0	2648	9	0
1	B	2587	0	2533	15	0
2	A	259	0	0	0	0
2	B	168	0	0	1	0
All	All	5734	0	5181	24	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 2.

All (24) 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:B:139:ARG:O	1:B:143:ARG:HG3	1.97	0.64
1:A:3:THR:HA	1:A:315:GLN:HE22	1.71	0.56
1:B:263:GLN:HA	1:B:266:VAL:HG22	1.89	0.55
1:B:241:GLU:H	1:B:241:GLU:CD	2.18	0.52
1:B:287:LEU:HG	1:B:289:ALA:H	1.75	0.51
1:B:14:TYR:HE2	1:B:17:GLU:HA	1.75	0.50
1:B:249:GLN:NE2	1:B:253:ASP:OD2	2.33	0.47
1:A:61:ILE:H	1:A:61:ILE:HD12	1.79	0.47
1:A:141:LEU:HD21	1:A:147:ILE:HG12	1.97	0.47
1:B:75:ARG:HA	1:B:105:GLY:O	2.14	0.47
1:A:202:ILE:HG23	1:A:317:ILE:HD13	1.99	0.44
1:B:141:LEU:HD21	1:B:147:ILE:HG12	1.98	0.44
1:B:185:LYS:O	1:B:189:MET:HG3	2.17	0.44
1:A:3:THR:HA	1:A:315:GLN:NE2	2.32	0.43
1:A:75:ARG:HA	1:A:105:GLY:O	2.19	0.43
1:B:143:ARG:NE	1:B:169:GLU:OE2	2.48	0.43
1:B:9:TYR:CZ	1:B:231:LEU:HD12	2.53	0.43
1:B:143:ARG:NH2	2:B:405:HOH:O	2.52	0.42
1:B:231:LEU:HD21	1:B:325:LEU:HD12	2.03	0.41
1:A:129:GLU:HG3	1:A:133:GLN:NE2	2.35	0.41
1:A:90:VAL:HG22	1:A:138:VAL:HG13	2.03	0.41
1:A:12:GLY:HA2	1:A:54:PHE:CE2	2.56	0.40
1:B:9:TYR:HB2	1:B:323:ALA:HB1	2.03	0.40
1:B:61:ILE:HD12	1:B:61:ILE:H	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	346/362 (96%)	335 (97%)	10 (3%)	1 (0%)	36	20
1	B	328/362 (91%)	319 (97%)	8 (2%)	1 (0%)	36	20
All	All	674/724 (93%)	654 (97%)	18 (3%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	SER
1	A	177	VAL

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	292/305 (96%)	292 (100%)	0	100	100
1	B	277/305 (91%)	276 (100%)	1 (0%)	84	75
All	All	569/610 (93%)	568 (100%)	1 (0%)	87	81

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	54	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	101	GLN
1	A	148	GLN
1	A	150	GLN
1	A	160	GLN
1	A	315	GLN
1	B	5	GLN
1	B	148	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, 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	348/362 (96%)	0.52	36 (10%)	12 12	11, 21, 39, 47	0
1	B	332/362 (91%)	0.99	58 (17%)	4 3	12, 27, 52, 60	0
All	All	680/724 (93%)	0.75	94 (13%)	6 6	11, 24, 46, 60	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	LEU	5.9
1	B	262	PHE	5.2
1	B	270	GLY	5.0
1	B	223	PRO	4.9
1	B	259	VAL	4.8
1	B	265	LEU	4.1
1	A	224	ALA	3.8
1	B	237	GLY	3.8
1	A	223	PRO	3.8
1	A	153	VAL	3.7
1	A	222	ASN	3.5
1	B	289	ALA	3.3
1	B	224	ALA	3.2
1	B	291	TYR	3.2
1	B	221	TYR	3.2
1	B	350	GLN	3.2
1	B	77	GLY	3.2
1	B	210	ALA	3.2
1	A	126	ASN	3.1
1	B	222	ASN	3.1
1	A	202	ILE	3.1
1	B	18	PHE	3.0
1	B	268	SER	2.9
1	A	221	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	292	ASN	2.9
1	B	266	VAL	2.8
1	B	216	LEU	2.8
1	A	199	GLY	2.8
1	B	295	VAL	2.8
1	A	201	SER	2.7
1	A	17	GLU	2.6
1	B	220	GLY	2.6
1	B	349	CYS	2.6
1	B	267	LYS	2.6
1	B	206	ALA	2.6
1	A	220	GLY	2.5
1	A	280	ALA	2.5
1	B	242	GLN	2.5
1	B	269	GLN	2.5
1	B	177	VAL	2.5
1	A	178	ASN	2.4
1	A	211	LEU	2.4
1	A	206	ALA	2.4
1	A	277	GLN	2.4
1	A	204	ASP	2.4
1	A	203	GLU	2.4
1	B	16	SER	2.4
1	B	316	ALA	2.4
1	B	126	ASN	2.4
1	A	285	TYR	2.4
1	B	348	LEU	2.4
1	B	226	GLY	2.3
1	B	181	GLU	2.3
1	A	205	LEU	2.3
1	B	290	ALA	2.3
1	B	190	GLY	2.3
1	B	252	CYS	2.3
1	B	254	TYR	2.3
1	B	178	ASN	2.3
1	B	125	GLY	2.3
1	A	216	LEU	2.3
1	B	255	LEU	2.3
1	B	143	ARG	2.3
1	A	184	ILE	2.3
1	A	177	VAL	2.3
1	A	350	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	210	ALA	2.2
1	B	260	ALA	2.2
1	A	156	SER	2.2
1	A	18	PHE	2.2
1	B	212	TYR	2.2
1	B	184	ILE	2.2
1	B	303	THR	2.2
1	A	179	ASN	2.2
1	B	258	SER	2.2
1	B	261	LEU	2.2
1	A	217	GLU	2.2
1	B	318	GLY	2.2
1	A	125	GLY	2.1
1	A	348	LEU	2.1
1	B	288	SER	2.1
1	B	180	PRO	2.1
1	B	207	GLU	2.1
1	A	274	ASP	2.1
1	B	148	GLN	2.1
1	B	248	ARG	2.1
1	A	176	VAL	2.1
1	B	264	ASN	2.1
1	A	215	SER	2.1
1	A	316	ALA	2.0
1	B	204	ASP	2.0
1	B	112	TRP	2.0
1	B	209	ILE	2.0
1	A	281	ASP	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.