



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 08:04 PM UTC

PDB ID : 6Y01 / pdb_00006y01
Title : The structure of the molybdenum cofactor binding protein from the phototrophic bacterium *Rippkaea orientalis*
Authors : Krausze, J.
Deposited on : 2020-02-05
Resolution : 1.23 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
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

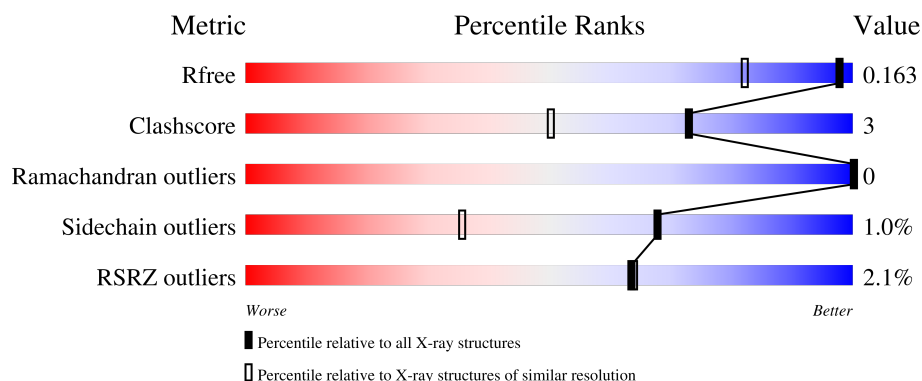
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.23 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	1630 (1.26-1.22)
Clashscore	190562	1668 (1.26-1.22)
Ramachandran outliers	187476	1635 (1.26-1.22)
Sidechain outliers	187428	1633 (1.26-1.22)
RSRZ outliers	180081	1630 (1.26-1.22)

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	AAA	178	3% 88% • 8%
1	BBB	178	% 88% • 7%
1	CCC	178	2% 86% 5% • 8%
1	DDD	178	2% 86% 7% • 7%

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	IMD	BBB	201	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5248 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 p450 cytochrome, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	164	Total	C	N	O	S	0	1	0
			1202	760	207	230	5			
1	BBB	165	Total	C	N	O	S	0	2	0
			1217	764	211	238	4			
1	CCC	163	Total	C	N	O	S	0	2	0
			1206	758	206	237	5			
1	DDD	166	Total	C	N	O	S	0	2	0
			1210	763	207	235	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-11	MET	-	initiating methionine	UNP B7K4Z0
AAA	-10	ARG	-	expression tag	UNP B7K4Z0
AAA	-9	GLY	-	expression tag	UNP B7K4Z0
AAA	-8	SER	-	expression tag	UNP B7K4Z0
AAA	-7	HIS	-	expression tag	UNP B7K4Z0
AAA	-6	HIS	-	expression tag	UNP B7K4Z0
AAA	-5	HIS	-	expression tag	UNP B7K4Z0
AAA	-4	HIS	-	expression tag	UNP B7K4Z0
AAA	-3	HIS	-	expression tag	UNP B7K4Z0
AAA	-2	HIS	-	expression tag	UNP B7K4Z0
AAA	-1	GLY	-	expression tag	UNP B7K4Z0
AAA	0	SER	-	expression tag	UNP B7K4Z0
AAA	164	LYS	-	expression tag	UNP B7K4Z0
AAA	165	LEU	-	expression tag	UNP B7K4Z0
AAA	166	ASN	-	expression tag	UNP B7K4Z0
BBB	-11	MET	-	initiating methionine	UNP B7K4Z0
BBB	-10	ARG	-	expression tag	UNP B7K4Z0
BBB	-9	GLY	-	expression tag	UNP B7K4Z0
BBB	-8	SER	-	expression tag	UNP B7K4Z0
BBB	-7	HIS	-	expression tag	UNP B7K4Z0
BBB	-6	HIS	-	expression tag	UNP B7K4Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-5	HIS	-	expression tag	UNP B7K4Z0
BBB	-4	HIS	-	expression tag	UNP B7K4Z0
BBB	-3	HIS	-	expression tag	UNP B7K4Z0
BBB	-2	HIS	-	expression tag	UNP B7K4Z0
BBB	-1	GLY	-	expression tag	UNP B7K4Z0
BBB	0	SER	-	expression tag	UNP B7K4Z0
BBB	164	LYS	-	expression tag	UNP B7K4Z0
BBB	165	LEU	-	expression tag	UNP B7K4Z0
BBB	166	ASN	-	expression tag	UNP B7K4Z0
CCC	-11	MET	-	initiating methionine	UNP B7K4Z0
CCC	-10	ARG	-	expression tag	UNP B7K4Z0
CCC	-9	GLY	-	expression tag	UNP B7K4Z0
CCC	-8	SER	-	expression tag	UNP B7K4Z0
CCC	-7	HIS	-	expression tag	UNP B7K4Z0
CCC	-6	HIS	-	expression tag	UNP B7K4Z0
CCC	-5	HIS	-	expression tag	UNP B7K4Z0
CCC	-4	HIS	-	expression tag	UNP B7K4Z0
CCC	-3	HIS	-	expression tag	UNP B7K4Z0
CCC	-2	HIS	-	expression tag	UNP B7K4Z0
CCC	-1	GLY	-	expression tag	UNP B7K4Z0
CCC	0	SER	-	expression tag	UNP B7K4Z0
CCC	164	LYS	-	expression tag	UNP B7K4Z0
CCC	165	LEU	-	expression tag	UNP B7K4Z0
CCC	166	ASN	-	expression tag	UNP B7K4Z0
DDD	-11	MET	-	initiating methionine	UNP B7K4Z0
DDD	-10	ARG	-	expression tag	UNP B7K4Z0
DDD	-9	GLY	-	expression tag	UNP B7K4Z0
DDD	-8	SER	-	expression tag	UNP B7K4Z0
DDD	-7	HIS	-	expression tag	UNP B7K4Z0
DDD	-6	HIS	-	expression tag	UNP B7K4Z0
DDD	-5	HIS	-	expression tag	UNP B7K4Z0
DDD	-4	HIS	-	expression tag	UNP B7K4Z0
DDD	-3	HIS	-	expression tag	UNP B7K4Z0
DDD	-2	HIS	-	expression tag	UNP B7K4Z0
DDD	-1	GLY	-	expression tag	UNP B7K4Z0
DDD	0	SER	-	expression tag	UNP B7K4Z0
DDD	164	LYS	-	expression tag	UNP B7K4Z0
DDD	165	LEU	-	expression tag	UNP B7K4Z0
DDD	166	ASN	-	expression tag	UNP B7K4Z0

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	N	0	0
			5	3	2		
2	BBB	1	Total	C	N	0	0
			5	3	2		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	3	Total	Cl	0	0
			3	3		
3	BBB	3	Total	Cl	0	0
			3	3		
3	CCC	3	Total	Cl	0	0
			3	3		
3	DDD	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	100	Total	O	0	0
			100	100		
4	BBB	96	Total	O	0	0
			96	96		
4	CCC	105	Total	O	0	0
			105	105		

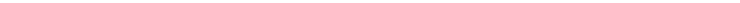
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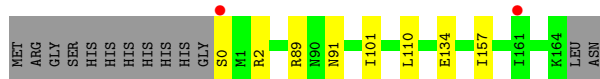
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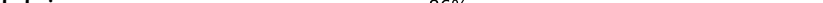
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	DDD	92	Total	O	0	0
			92	92		

- Molecule 1: p450 cytochrome, putative

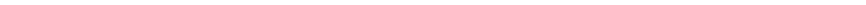


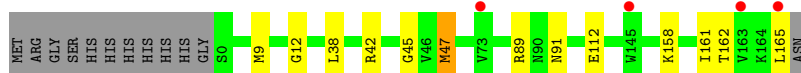
- Chain BBB:  88% 7%



- Chain CCC:  86% 2% 5% 8%



- Chain DDD:  2% 86% 7% • 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.58Å 72.04Å 70.26Å 90.00° 113.33° 90.00°	Depositor
Resolution (Å)	64.52 – 1.23 64.52 – 1.23	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.52-1.23) 100.0 (64.52-1.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.23Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.142 , 0.163 0.143 , 0.163	Depositor DCC
R_{free} test set	8868 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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: IMD, CL

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	AAA	1.13	2/1217 (0.2%)	1.13	0/1658
1	BBB	1.07	1/1230 (0.1%)	1.08	0/1676
1	CCC	1.12	1/1219 (0.1%)	1.04	0/1658
1	DDD	1.04	0/1223	1.05	1/1667 (0.1%)
All	All	1.09	4/4889 (0.1%)	1.08	1/6659 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	CCC	71	HIS	CE1-NE2	5.92	1.38	1.32
1	AAA	18	THR	C-O	5.81	1.30	1.24
1	AAA	49	HIS	CE1-NE2	5.46	1.38	1.32
1	BBB	134	GLU	CD-OE1	-5.11	1.15	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	47	MET	CG-SD-CE	5.63	113.29	100.90

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	AAA	1202	0	1231	3	0
1	BBB	1217	0	1237	6	0
1	CCC	1206	0	1237	6	0
1	DDD	1210	0	1234	17	0
2	AAA	5	0	5	0	0
2	BBB	5	0	5	0	0
3	AAA	3	0	0	0	0
3	BBB	3	0	0	0	0
3	CCC	3	0	0	0	0
3	DDD	1	0	0	0	0
4	AAA	100	0	0	0	0
4	BBB	96	0	0	1	0
4	CCC	105	0	0	2	0
4	DDD	92	0	0	1	0
All	All	5248	0	4949	31	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 3.

The worst 5 of 31 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:DDD:9:MET:SD	1:DDD:112:GLU:OE1	1.96	1.24
1:DDD:42:ARG:H	1:DDD:47:MET:CE	1.54	1.20
1:DDD:42:ARG:CB	1:DDD:47:MET:HE2	1.71	1.19
1:DDD:42:ARG:N	1:DDD:47:MET:HE3	1.57	1.18
1:DDD:42:ARG:HB2	1:DDD:47:MET:HE2	1.15	1.14

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	AAA	163/178 (92%)	161 (99%)	2 (1%)	0	100	100
1	BBB	165/178 (93%)	163 (99%)	2 (1%)	0	100	100
1	CCC	163/178 (92%)	161 (99%)	2 (1%)	0	100	100
1	DDD	166/178 (93%)	166 (100%)	0	0	100	100
All	All	657/712 (92%)	651 (99%)	6 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	AAA	129/146 (88%)	128 (99%)	1 (1%)	73	44
1	BBB	131/146 (90%)	130 (99%)	1 (1%)	73	44
1	CCC	132/146 (90%)	130 (98%)	2 (2%)	57	22
1	DDD	130/146 (89%)	129 (99%)	1 (1%)	73	44
All	All	522/584 (89%)	517 (99%)	5 (1%)	68	36

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	89	ARG
1	BBB	89	ARG
1	CCC	43	ASN
1	CCC	89	ARG
1	DDD	89	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 10 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	$\# Z > 2$
2	IMD	AAA	201	-	5,5,5	0.30	0	5,5,5	0.61	0
2	IMD	BBB	201	-	5,5,5	5.86	4 (80%)	5,5,5	3.15	1 (20%)

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	IMD	AAA	201	-	-	-	0/1/1/1
2	IMD	BBB	201	-	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	201	IMD	C5-C4	8.98	1.67	1.35
2	BBB	201	IMD	C4-N3	7.27	1.63	1.37
2	BBB	201	IMD	C2-N3	5.34	1.55	1.32
2	BBB	201	IMD	C5-N1	3.08	1.46	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	BBB	201	IMD	C5-C4-N3	-6.70	88.47	109.11

There are no chirality outliers.

There are no torsion outliers.

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, 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	AAA	164/178 (92%)	-0.06	5 (3%)	52	53	17, 25, 50, 79	1 (0%)
1	BBB	165/178 (92%)	0.01	2 (1%)	76	77	16, 28, 47, 70	2 (1%)
1	CCC	163/178 (91%)	-0.11	3 (1%)	67	68	12, 24, 42, 79	2 (1%)
1	DDD	166/178 (93%)	0.17	4 (2%)	59	61	12, 29, 50, 81	2 (1%)
All	All	658/712 (92%)	0.00	14 (2%)	63	64	12, 26, 50, 81	7 (1%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	163	VAL	4.3
1	CCC	162	THR	3.8
1	DDD	165	LEU	3.3
1	AAA	142	ASN	2.5
1	AAA	0	SER	2.3

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	IMD	AAA	201	5/5	0.76	0.18	61,63,70,75	0
2	IMD	BBB	201	5/5	0.83	0.28	85,100,110,111	0
3	CL	AAA	202	1/1	0.99	0.08	34,34,34,34	0
3	CL	AAA	203	1/1	0.99	0.06	28,28,28,28	0
3	CL	BBB	202	1/1	0.99	0.09	36,36,36,36	0
3	CL	BBB	204	1/1	0.99	0.07	37,37,37,37	0
3	CL	CCC	201	1/1	0.99	0.13	37,37,37,37	0
3	CL	AAA	204	1/1	1.00	0.07	35,35,35,35	0
3	CL	BBB	203	1/1	1.00	0.04	28,28,28,28	0
3	CL	CCC	202	1/1	1.00	0.04	28,28,28,28	0
3	CL	CCC	203	1/1	1.00	0.09	33,33,33,33	0
3	CL	DDD	201	1/1	1.00	0.06	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.