



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 07:46 PM EDT

PDB ID : 3KG9  
Title : Dehydratase domain from CurK module of Curacin polyketide synthase  
Authors : Akey, D.L.; Smith, J.L.  
Deposited on : unknown  
Resolution : 1.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

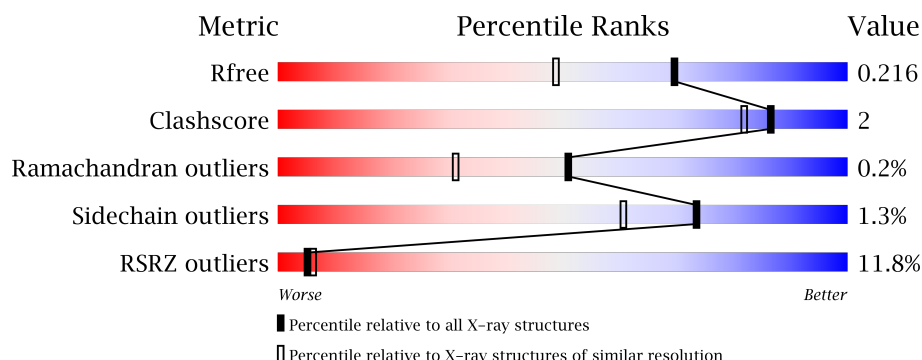
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	296	 11% 88% 7% 5%
1	B	296	 11% 89% 5% • 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4944 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 CurK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	5	0
			2232	1416	377	438	1			
1	B	279	Total	C	N	O	S	4	3	0
			2210	1406	375	428	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	955	SER	-	EXPRESSION TAG	UNP Q6DNE2
A	956	ASN	-	EXPRESSION TAG	UNP Q6DNE2
A	957	ALA	-	EXPRESSION TAG	UNP Q6DNE2
B	955	SER	-	EXPRESSION TAG	UNP Q6DNE2
B	956	ASN	-	EXPRESSION TAG	UNP Q6DNE2
B	957	ALA	-	EXPRESSION TAG	UNP Q6DNE2

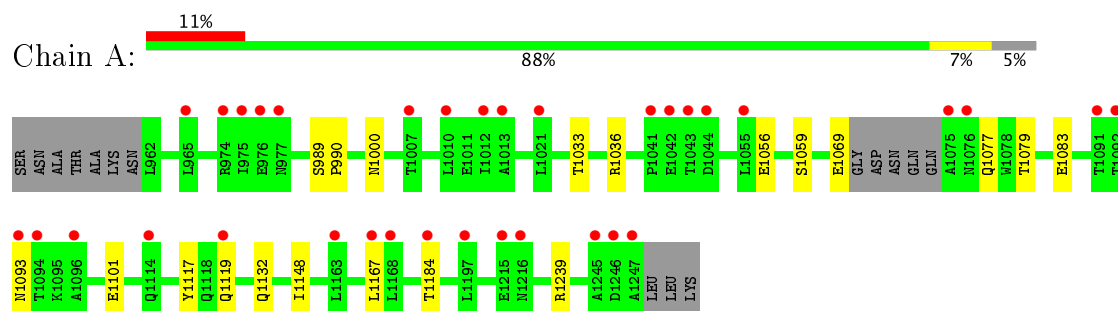
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	289	Total	O	0	0
			289	289		
2	B	213	Total	O	0	0
			213	213		

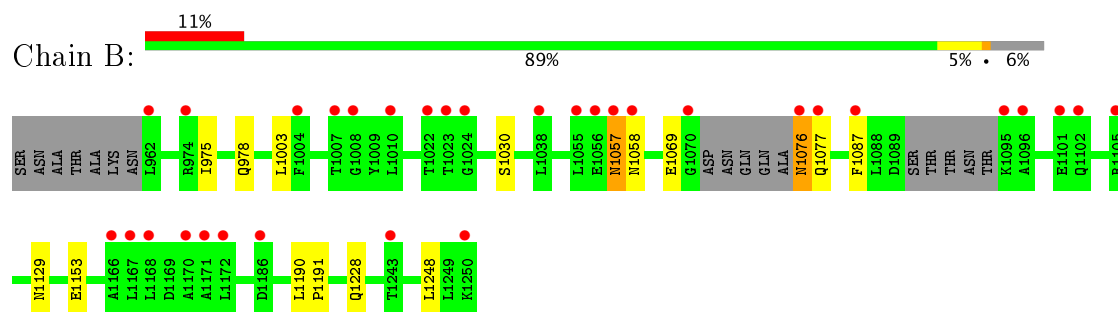
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: CurK



#### • Molecule 1: CurK



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.12Å 94.30Å 150.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.77 – 1.70 30.77 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.77-1.70) 97.9 (30.77-1.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.182 , 0.217 0.181 , 0.216	Depositor DCC
$R_{free}$ test set	3003 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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](#)

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	0.42	0/2269	0.57	0/3081
1	B	0.40	0/2246	0.56	0/3045
All	All	0.41	0/4515	0.56	0/6126

There are no bond length outliers.

There are no bond angle outliers.

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	2232	0	2235	11	0
1	B	2210	0	2221	11	0
2	A	289	0	0	3	0
2	B	213	0	0	1	0
All	All	4944	0	4456	22	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 (22) 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:1057:ASN:HD22	1:B:1058:ASN:H	1.30	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1036:ARG:HD2	1:A:1079:THR:CG2	2.26	0.64
1:B:1057:ASN:HD22	1:B:1058:ASN:N	2.01	0.57
1:A:1056:GLU:HG2	1:A:1059:SER:HB3	1.86	0.57
1:A:1000:ASN:ND2	2:A:450:HOH:O	2.38	0.56
1:B:1129[B]:ASN:ND2	1:B:1153:GLU:OE2	2.27	0.56
1:B:1069:GLU:HA	1:B:1076:ASN:HD21	1.76	0.50
1:B:975:ILE:HG22	1:B:978:GLN:HB2	1.93	0.50
1:B:1003:LEU:HD21	1:B:1248:LEU:HB3	1.93	0.49
1:B:975:ILE:CG2	1:B:978:GLN:HB2	2.43	0.49
1:A:1148:ILE:HG22	1:A:1167[B]:LEU:CD1	2.42	0.49
1:A:1033[B]:THR:HG22	1:A:1239:ARG:HH22	1.77	0.49
1:B:1076:ASN:HB2	1:B:1077:GLN:H	1.62	0.46
1:A:1148:ILE:HG22	1:A:1167[B]:LEU:HD11	1.98	0.46
1:A:989:SER:HA	1:A:990:PRO:C	2.36	0.45
1:A:1036:ARG:HD2	1:A:1079:THR:HG23	1.97	0.45
1:A:1083:GLU:HB2	2:A:258:HOH:O	2.17	0.44
1:B:1190:LEU:HA	1:B:1191:PRO:HD3	1.95	0.42
1:A:1077:GLN:O	2:A:376:HOH:O	2.21	0.42
1:B:1228:GLN:NE2	2:B:413:HOH:O	2.54	0.41
1:B:1030:SER:HG	1:B:1087:PHE:HD2	1.69	0.41
1:A:1117:TYR:CZ	1:A:1132:GLN:HA	2.56	0.41

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	282/296 (95%)	274 (97%)	7 (2%)	1 (0%)	38	20
1	B	276/296 (93%)	270 (98%)	6 (2%)	0	100	100
All	All	558/592 (94%)	544 (98%)	13 (2%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN

### 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	243/250 (97%)	239 (98%)	4 (2%)	68	53
1	B	239/250 (96%)	237 (99%)	2 (1%)	85	78
All	All	482/500 (96%)	476 (99%)	6 (1%)	73	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1069	GLU
1	A	1101	GLU
1	A	1119	GLN
1	A	1184	THR
1	B	1057	ASN
1	B	1076	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1000	ASN
1	A	1093	ASN
1	B	1057	ASN
1	B	1115	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 carbohydrates 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<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	281/296 (94%)	0.71	34 (12%) 5 6	15, 22, 39, 58	2 (0%)
1	B	279/296 (94%)	0.78	32 (11%) 5 7	18, 25, 39, 48	6 (2%)
All	All	560/592 (94%)	0.74	66 (11%) 5 6	15, 24, 39, 58	8 (1%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1092	THR	11.2
1	A	1093	ASN	6.5
1	A	1094	THR	6.3
1	B	1070	GLY	6.3
1	B	1095	LYS	5.7
1	A	1043	THR	5.2
1	B	1076	ASN	5.1
1	A	1021	LEU	5.1
1	B	1096	ALA	5.0
1	A	1055	LEU	4.9
1	B	1024	GLY	4.8
1	A	974	ARG	4.5
1	A	1247	ALA	4.4
1	B	1058	ASN	4.3
1	B	962	LEU	4.3
1	B	1057	ASN	4.1
1	A	1215	GLU	4.1
1	B	1023	THR	4.0
1	A	1246	ASP	3.9
1	A	1216	ASN	3.7
1	B	1186	ASP	3.6
1	A	1075	ALA	3.6
1	A	1096	ALA	3.5
1	B	1250	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	1042	GLU	3.4
1	B	1087	PHE	3.4
1	B	1077	GLN	3.3
1	A	1076	ASN	3.2
1	A	1163	LEU	3.1
1	B	1056	GLU	3.0
1	B	1055	LEU	3.0
1	B	1022	THR	2.9
1	A	1114	GLN	2.9
1	A	1091	THR	2.8
1	B	1007	THR	2.7
1	A	976	GLU	2.7
1	A	1119	GLN	2.7
1	A	1044	ASP	2.7
1	A	975	ILE	2.7
1	A	1010	LEU	2.6
1	A	1184	THR	2.6
1	B	1105	ARG	2.6
1	A	1041	PRO	2.6
1	B	1008	GLY	2.6
1	A	1245	ALA	2.6
1	B	1168	LEU	2.6
1	B	1101	GLU	2.5
1	B	1170	ALA	2.5
1	A	1012	ILE	2.5
1	B	1010	LEU	2.5
1	B	974	ARG	2.4
1	A	1167[A]	LEU	2.4
1	B	1167	LEU	2.4
1	A	977	ASN	2.4
1	B	1166	ALA	2.4
1	A	1197	LEU	2.3
1	B	1004	PHE	2.3
1	B	1172	LEU	2.3
1	B	1243	THR	2.3
1	A	1007	THR	2.2
1	A	1013	ALA	2.2
1	B	1102	GLN	2.2
1	B	1171	ALA	2.2
1	A	1168	LEU	2.2
1	B	1038	LEU	2.1
1	A	965	LEU	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 carbohydrates 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.