Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:03 AM GMT

PDB ID	:	2ZE3
Title	:	Crystal Structure of DFA0005 Complexed with alpha-Ketoglutarate: A Novel Member of the ICL/PEPM Superfamily from Alkali-tolerant Deinococcus ficus
Authors	:	Liao, C.J.; Chin, K.H.; Chou, S.H.
Deposited on	:	2007-12-05
Resolution	:	1.65 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

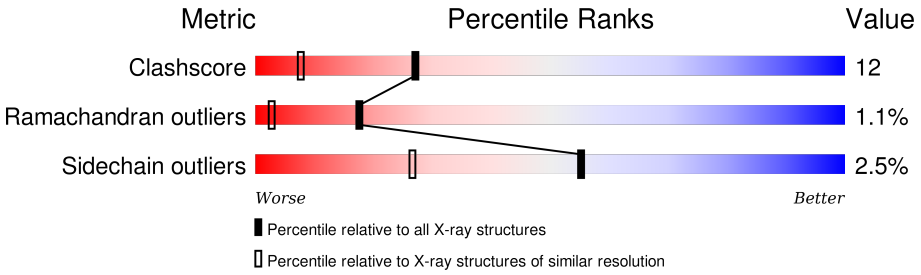
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.65 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))
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)

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 >=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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	275	80% 15%

2 Entry composition

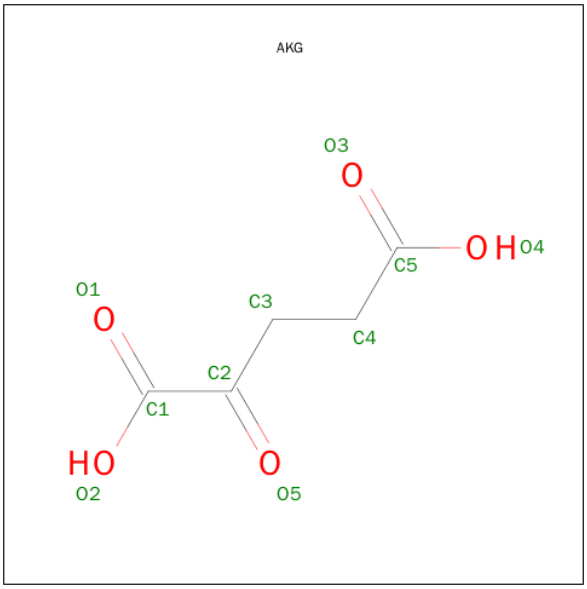
There are 3 unique types of molecules in this entry. The entry contains 2324 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DFA0005.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2061	1284	379	392	6			

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	253	Total	O	0	0
			253	253		

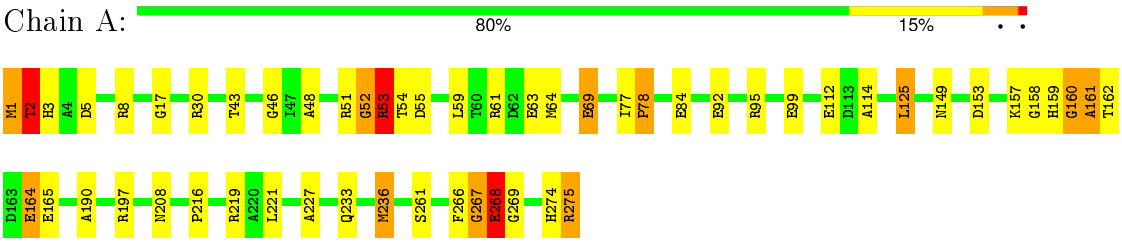
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: DFA0005

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	108.84Å 108.84Å 114.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.85 – 1.65	Depositor
% Data completeness (in resolution range)	99.7 (18.85-1.65)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2324	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG

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	1.24	25/2100 (1.2%)	1.25	35/2852 (1.2%)

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	3	2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ARG	CD-NE	-19.51	1.13	1.46
1	A	219	ARG	CD-NE	-19.46	1.13	1.46
1	A	52	GLY	N-CA	-13.80	1.25	1.46
1	A	267	GLY	CA-C	-13.26	1.30	1.51
1	A	53	ARG	CB-CG	-12.99	1.17	1.52
1	A	53	ARG	N-CA	11.63	1.69	1.46
1	A	274	HIS	C-N	11.40	1.60	1.34
1	A	2	THR	N-CA	-11.16	1.24	1.46
1	A	161	ALA	N-CA	10.59	1.67	1.46
1	A	69	GLU	CB-CG	10.07	1.71	1.52
1	A	267	GLY	N-CA	-9.27	1.32	1.46
1	A	159	HIS	N-CA	9.15	1.64	1.46
1	A	30	ARG	CD-NE	-9.09	1.31	1.46
1	A	158	GLY	C-N	9.08	1.54	1.34
1	A	53	ARG	CG-CD	-8.99	1.29	1.51
1	A	1	MET	CA-C	-8.62	1.30	1.52
1	A	2	THR	CA-CB	7.98	1.74	1.53
1	A	125	LEU	CB-CG	6.98	1.72	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	GLY	CA-C	-6.77	1.41	1.51
1	A	160	GLY	CA-C	-6.37	1.41	1.51
1	A	160	GLY	C-N	6.16	1.48	1.34
1	A	153	ASP	C-N	5.54	1.46	1.34
1	A	78	PRO	CG-CD	-5.47	1.32	1.50
1	A	53	ARG	CA-CB	-5.39	1.42	1.53
1	A	274	HIS	CA-C	-5.13	1.39	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	53	ARG	N-CA-CB	17.38	141.88	110.60
1	A	53	ARG	CA-CB-CG	15.70	147.93	113.40
1	A	53	ARG	CB-CG-CD	15.42	151.68	111.60
1	A	158	GLY	N-CA-C	14.68	149.81	113.10
1	A	275	ARG	CA-C-O	-13.10	92.59	120.10
1	A	53	ARG	CD-NE-CZ	11.13	139.18	123.60
1	A	52	GLY	CA-C-O	10.88	140.19	120.60
1	A	219	ARG	CG-CD-NE	10.77	134.42	111.80
1	A	52	GLY	CA-C-N	-10.46	94.18	117.20
1	A	1	MET	CB-CA-C	10.43	131.26	110.40
1	A	275	ARG	N-CA-CB	10.14	128.85	110.60
1	A	236	MET	CG-SD-CE	-9.66	84.74	100.20
1	A	69	GLU	CB-CG-CD	9.54	139.97	114.20
1	A	159	HIS	N-CA-CB	-9.54	93.42	110.60
1	A	219	ARG	CD-NE-CZ	9.29	136.60	123.60
1	A	53	ARG	CG-CD-NE	9.07	130.85	111.80
1	A	53	ARG	CB-CA-C	8.21	126.82	110.40
1	A	53	ARG	N-CA-C	-8.15	89.00	111.00
1	A	274	HIS	CA-C-O	7.98	136.87	120.10
1	A	52	GLY	C-N-CA	-7.11	103.93	121.70
1	A	43	THR	CA-CB-CG2	7.09	122.32	112.40
1	A	159	HIS	N-CA-C	7.02	129.94	111.00
1	A	268	GLU	N-CA-CB	7.00	123.20	110.60
1	A	158	GLY	CA-C-N	-6.82	102.19	117.20
1	A	125	LEU	CB-CG-CD2	-6.72	99.57	111.00
1	A	1	MET	CA-C-N	-6.69	102.48	117.20
1	A	274	HIS	O-C-N	-5.79	113.43	122.70
1	A	2	THR	CA-CB-CG2	-5.70	104.43	112.40
1	A	160	GLY	C-N-CA	-5.55	107.83	121.70
1	A	2	THR	N-CA-CB	5.42	120.59	110.30
1	A	267	GLY	CA-C-N	-5.39	105.34	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	HIS	CB-CA-C	5.36	121.12	110.40
1	A	267	GLY	O-C-N	5.33	131.23	122.70
1	A	190	ALA	N-CA-C	-5.06	97.34	111.00
1	A	2	THR	CB-CA-C	5.05	125.24	111.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1	MET	CA
1	A	2	THR	CA
1	A	275	ARG	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	GLY	Peptide
1	A	53	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	2061	0	2017	49	0
2	A	10	0	2	0	0
3	A	253	0	0	6	4
All	All	2324	0	2019	49	4

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 12.

All (49) 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:53:ARG:CA	1:A:53:ARG:N	1.69	1.55
1:A:161:ALA:N	1:A:161:ALA:CA	1.67	1.51
1:A:275:ARG:CG	1:A:275:ARG:O	1.97	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:H	1:A:54:THR:H	1.03	0.98
1:A:275:ARG:HG2	1:A:275:ARG:O	1.60	0.96
1:A:53:ARG:N	1:A:54:THR:N	2.18	0.92
1:A:53:ARG:H	1:A:54:THR:N	1.70	0.90
1:A:53:ARG:C	1:A:53:ARG:N	2.24	0.89
1:A:52:GLY:C	1:A:53:ARG:CA	2.41	0.88
1:A:216:PRO:HG2	1:A:221:LEU:HD21	1.58	0.85
1:A:53:ARG:N	1:A:54:THR:H	1.75	0.83
1:A:149:ASN:HD21	1:A:208:ASN:HD22	1.24	0.83
1:A:2:THR:HG22	3:A:491:HOH:O	1.80	0.82
1:A:164:GLU:CD	1:A:164:GLU:H	1.90	0.75
1:A:160:GLY:C	1:A:161:ALA:CA	2.55	0.74
1:A:162:THR:HB	1:A:164:GLU:OE1	1.91	0.70
1:A:160:GLY:O	1:A:161:ALA:HB3	1.97	0.64
1:A:54:THR:HG22	1:A:54:THR:O	2.01	0.61
1:A:233:GLN:HG2	3:A:464:HOH:O	2.02	0.59
1:A:51:ARG:HH11	1:A:51:ARG:HG3	1.66	0.59
1:A:268:GLU:N	1:A:268:GLU:OE1	2.36	0.58
1:A:1:MET:HG2	1:A:3:HIS:H	1.68	0.58
1:A:59:LEU:HD12	1:A:64:MET:CE	2.34	0.58
1:A:54:THR:HG21	1:A:63:GLU:OE2	2.04	0.57
1:A:114:ALA:HB1	1:A:157:LYS:HE3	1.91	0.52
1:A:51:ARG:O	1:A:52:GLY:C	2.45	0.52
1:A:52:GLY:O	1:A:53:ARG:CA	2.57	0.52
1:A:275:ARG:HG3	1:A:275:ARG:O	2.04	0.50
1:A:51:ARG:NH1	1:A:51:ARG:HG3	2.27	0.49
1:A:149:ASN:ND2	1:A:208:ASN:HD22	2.03	0.47
1:A:161:ALA:N	1:A:161:ALA:CB	2.67	0.46
1:A:160:GLY:O	1:A:165:GLU:OE2	2.33	0.45
1:A:46:GLY:O	1:A:236:MET:HE1	2.15	0.45
1:A:268:GLU:CD	1:A:268:GLU:H	2.19	0.45
1:A:266:PHE:CD1	1:A:269:GLY:HA3	2.52	0.45
1:A:197:ARG:NH2	3:A:478:HOH:O	2.50	0.45
1:A:59:LEU:HD12	1:A:64:MET:HE1	1.98	0.45
1:A:261:SER:OG	3:A:526:HOH:O	1.99	0.45
1:A:5:ASP:OD1	1:A:8:ARG:NH2	2.49	0.45
1:A:48:ALA:HB1	1:A:53:ARG:HB3	1.99	0.44
1:A:125:LEU:HD12	1:A:125:LEU:O	2.19	0.43
1:A:77:ILE:HB	1:A:78:PRO:HD2	2.01	0.43
1:A:92:GLU:HG2	3:A:303:HOH:O	2.19	0.42
1:A:1:MET:HG2	1:A:3:HIS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ARG:HD3	3:A:294:HOH:O	2.20	0.42
1:A:84:GLU:O	1:A:112:GLU:HG2	2.21	0.41
1:A:95:ARG:O	1:A:99:GLU:HG3	2.21	0.41
1:A:162:THR:OG1	1:A:164:GLU:HG2	2.21	0.40
1:A:17:GLY:HA2	1:A:227:ALA:O	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:482:HOH:O	3:A:482:HOH:O[12_555]	1.12	1.08
3:A:372:HOH:O	3:A:372:HOH:O[2_655]	1.16	1.04
3:A:481:HOH:O	3:A:481:HOH:O[2_655]	1.37	0.83
3:A:354:HOH:O	3:A:354:HOH:O[12_555]	2.07	0.13

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	273/275 (99%)	261 (96%)	9 (3%)	3 (1%)	17 3

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	55	ASP
1	A	268	GLU

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	202/202 (100%)	197 (98%)	5 (2%)	55 26

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

Mol	Chain	Res	Type
1	A	2	THR
1	A	53	ARG
1	A	69	GLU
1	A	164	GLU
1	A	268	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	100	HIS
1	A	149	ASN
1	A	233	GLN
1	A	274	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	AKG	A	276	-	3,9,9	12.46	2 (66%)	4,11,11	7.09	4 (100%)

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	AKG	A	276	-	-	0/3/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	276	AKG	C3-C2	-20.43	1.18	1.51
2	A	276	AKG	O5-C2	-6.89	1.10	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	276	AKG	C3-C2-C1	-4.80	110.00	121.51
2	A	276	AKG	C3-C4-C5	5.16	122.21	112.75
2	A	276	AKG	C4-C3-C2	8.60	134.73	112.98
2	A	276	AKG	O5-C2-C3	8.81	136.92	120.28

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.