Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 11:32 pm BST

PDB ID	:	2IU5
Title	:	Dihydroxyacetone kinase operon activator DhaS
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Deposited on	:	2006-05-27
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 (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 (1)) were used in the production of this report:

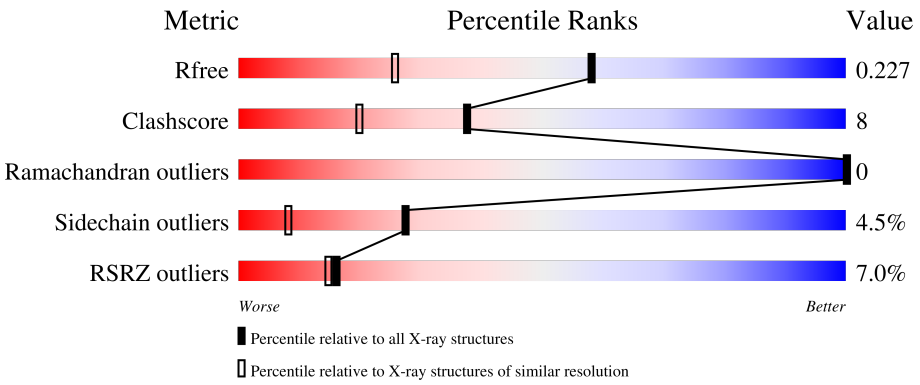
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	195	2%, 82%, 10%, •, 8%
1	B	195	11%, 74%, 15%, •, 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3328 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 HTH-TYPE DHAKLM OPERON TRANSCRIPTIONAL ACTIVATOR DHAS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	180	1527	992	248	282	5	0	0	1
1	B	178	1507	979	245	279	4	0	0	1

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	LEU	-	expression tag	UNP Q9CIV9
A	182	GLU	-	expression tag	UNP Q9CIV9
A	183	HIS	-	expression tag	UNP Q9CIV9
A	184	HIS	-	expression tag	UNP Q9CIV9
A	185	HIS	-	expression tag	UNP Q9CIV9
A	186	HIS	-	expression tag	UNP Q9CIV9
A	187	HIS	-	expression tag	UNP Q9CIV9
A	188	HIS	-	expression tag	UNP Q9CIV9
A	2	GLU	LYS	engineered mutation	UNP Q9CIV9
B	181	LEU	-	expression tag	UNP Q9CIV9
B	182	GLU	-	expression tag	UNP Q9CIV9
B	183	HIS	-	expression tag	UNP Q9CIV9
B	184	HIS	-	expression tag	UNP Q9CIV9
B	185	HIS	-	expression tag	UNP Q9CIV9
B	186	HIS	-	expression tag	UNP Q9CIV9
B	187	HIS	-	expression tag	UNP Q9CIV9
B	188	HIS	-	expression tag	UNP Q9CIV9
B	2	GLU	LYS	engineered mutation	UNP Q9CIV9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	181	181	181	0	0

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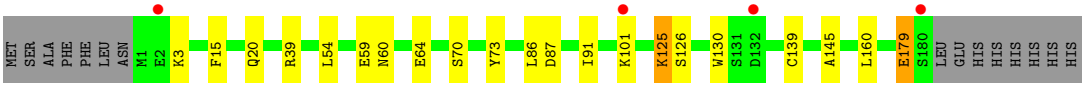
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	113	113	113	0	0

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.

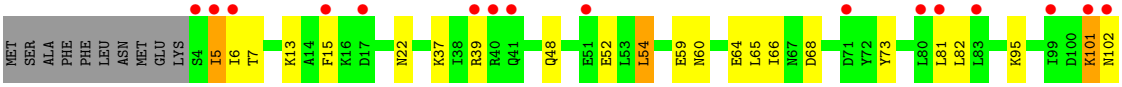
• Molecule 1: HTH-TYPE DHAKLM OPERON TRANSCRIPTIONAL ACTIVATOR DHAS

Chain A:



• Molecule 1: HTH-TYPE DHAKLM OPERON TRANSCRIPTIONAL ACTIVATOR DHAS

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.46Å 46.28Å 171.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.60 39.49 – 1.46	Depositor EDS
% Data completeness (in resolution range)	99.3 (40.00-1.60) 96.4 (39.49-1.46)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.46Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.230 0.199 , 0.227	Depositor DCC
R_{free} test set	2388 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å^2)	16.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3328	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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 (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	0.47	1/1560 (0.1%)	1.06	3/2104 (0.1%)
1	B	0.40	0/1540	0.64	0/2079
All	All	0.44	1/3100 (0.0%)	0.88	3/4183 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	GLU	C-N	-5.14	1.22	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	GLU	O-C-N	-28.19	77.59	122.70
1	A	179	GLU	CA-C-O	18.90	159.79	120.10
1	A	179	GLU	CA-C-N	-15.91	82.20	117.20

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	1527	0	1503	14	0
1	B	1507	0	1477	33	0
2	A	181	0	0	4	1
2	B	113	0	0	6	0
All	All	3328	0	2980	46	1

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 8.

All (46) 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:5:ILE:H	1:B:5:ILE:CD1	1.27	1.38
1:B:5:ILE:N	1:B:5:ILE:HD12	1.44	1.13
1:A:139:CYS:HB3	2:A:2152:HOH:O	0.80	0.96
1:B:176:LYS:HD3	2:B:2108:HOH:O	1.68	0.93
1:B:105:HIS:H	1:B:105:HIS:CD2	1.78	0.91
1:B:105:HIS:H	1:B:105:HIS:HD2	1.19	0.89
1:B:5:ILE:H	1:B:5:ILE:HD12	0.73	0.88
1:B:13:LYS:HD2	2:B:2003:HOH:O	1.75	0.85
1:B:5:ILE:CD1	1:B:5:ILE:N	2.10	0.85
1:B:48:GLN:HG3	1:B:52:GLU:OE2	1.77	0.83
1:B:105:HIS:CD2	1:B:105:HIS:N	2.50	0.80
1:B:73:TYR:OH	1:B:81:LEU:HD22	1.91	0.70
1:B:101:LYS:HE3	2:B:2060:HOH:O	2.00	0.61
1:B:130:TRP:CD1	1:B:135:LYS:HE2	2.38	0.59
1:B:102:ASN:HA	1:B:105:HIS:NE2	2.17	0.59
1:B:73:TYR:OH	1:B:81:LEU:CD2	2.52	0.58
1:A:39:ARG:HG3	1:A:39:ARG:NH1	2.18	0.57
1:B:105:HIS:HD2	1:B:105:HIS:N	1.93	0.57
1:A:39:ARG:HG3	1:A:39:ARG:HH11	1.70	0.56
1:B:59:GLU:HG3	2:B:2039:HOH:O	2.05	0.56
1:B:6:ILE:HG23	1:B:7:THR:N	2.21	0.55
1:A:20:GLN:NE2	1:A:91:ILE:HD12	2.22	0.54
1:A:86:LEU:HB2	1:A:160:LEU:HD22	1.88	0.54
1:B:64:GLU:OE2	1:B:64:GLU:HA	2.07	0.53
1:A:73:TYR:CD1	1:A:125:LYS:HE2	2.45	0.52
1:B:138:ILE:HD11	1:B:178:PHE:CE1	2.45	0.52
1:B:5:ILE:H	1:B:5:ILE:HD13	1.53	0.50
1:A:87:ASP:OD1	1:A:160:LEU:HD13	2.14	0.48
1:A:160:LEU:CD1	2:A:2163:HOH:O	2.62	0.47
1:B:22:ASN:O	1:B:95:LYS:NZ	2.48	0.47
1:A:39:ARG:HH11	1:A:39:ARG:CG	2.27	0.47
1:A:15:PHE:HE2	1:A:54:LEU:CD2	2.28	0.46
1:B:15:PHE:HE2	1:B:54:LEU:HD13	1.81	0.45
1:A:60:ASN:O	1:A:64:GLU:HG3	2.17	0.45
1:B:127:ASP:HA	2:B:2080:HOH:O	2.15	0.45
1:B:162:LYS:HG3	2:B:2097:HOH:O	2.16	0.44
1:A:179:GLU:C	2:A:2179:HOH:O	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:HB2	1:B:37:LYS:HE2	1.85	0.43
1:B:64:GLU:OE2	1:B:68:ASP:HB2	2.20	0.42
1:A:59:GLU:OE2	2:A:2084:HOH:O	2.21	0.42
1:B:65:LEU:HD13	1:B:82:LEU:HD23	2.02	0.42
1:A:145:ALA:HB2	1:B:145:ALA:HB2	2.01	0.41
1:B:73:TYR:CZ	1:B:81:LEU:HD22	2.56	0.41
1:B:60:ASN:O	1:B:64:GLU:HG2	2.20	0.41
1:B:15:PHE:CE2	1:B:54:LEU:HD13	2.57	0.40
1:B:73:TYR:CE2	1:B:81:LEU:HD22	2.56	0.40

All (1) 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)
2:A:2014:HOH:O	2:A:2142:HOH:O[3_645]	1.97	0.23

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	178/195 (91%)	175 (98%)	3 (2%)	0	100	100
1	B	176/195 (90%)	176 (100%)	0	0	100	100
All	All	354/390 (91%)	351 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	167/182 (92%)	161 (96%)	6 (4%)	35 12
1	B	165/182 (91%)	156 (94%)	9 (6%)	21 5
All	All	332/364 (91%)	317 (96%)	15 (4%)	27 8

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	70	SER
1	A	101	LYS
1	A	125	LYS
1	A	126	SER
1	A	130	TRP
1	B	5	ILE
1	B	39	ARG
1	B	54	LEU
1	B	66	ILE
1	B	101	LYS
1	B	105	HIS
1	B	124	LYS
1	B	126	SER
1	B	130	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	169	ASN
1	B	76	GLN
1	B	105	HIS
1	B	113	ASN
1	B	158	ASN
1	B	166	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 monosaccharides 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 (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	A	180/195 (92%)	0.38	4 (2%) 62 60	17, 22, 30, 37	0
1	B	178/195 (91%)	1.09	21 (11%) 4 3	12, 21, 31, 37	0
All	All	358/390 (91%)	0.73	25 (6%) 16 15	12, 22, 31, 37	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ILE	7.9
1	B	101	LYS	7.0
1	B	4	SER	6.3
1	B	6	ILE	4.7
1	A	101	LYS	4.6
1	B	39	ARG	4.4
1	B	41	GLN	4.3
1	B	99	ILE	3.2
1	B	40	ARG	3.1
1	B	81	LEU	3.1
1	A	2	GLU	2.5
1	B	127	ASP	2.5
1	B	83	LEU	2.5
1	B	17	ASP	2.4
1	B	80	LEU	2.3
1	B	102	ASN	2.3
1	A	132	ASP	2.3
1	B	105	HIS	2.2
1	B	118	VAL	2.2
1	B	15	PHE	2.1
1	A	180	SER	2.1
1	B	51	GLU	2.1
1	B	180	SER	2.1
1	B	133	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	71	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 monosaccharides 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.