WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 12:39 PM EDT

|		
PDB ID	:	4YBO
Title	:	Structure of Citrate Synthase from the Thermoacidophilic Euryarchaeon Thermolasma acidophilum
Authors	:	Murphy, J.R.; Donini, S.; Kappock, T.J.
Deposited on	:	2015-02-19
Resolution	:	2.18 Å(reported)

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
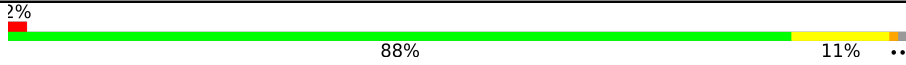*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.18 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.
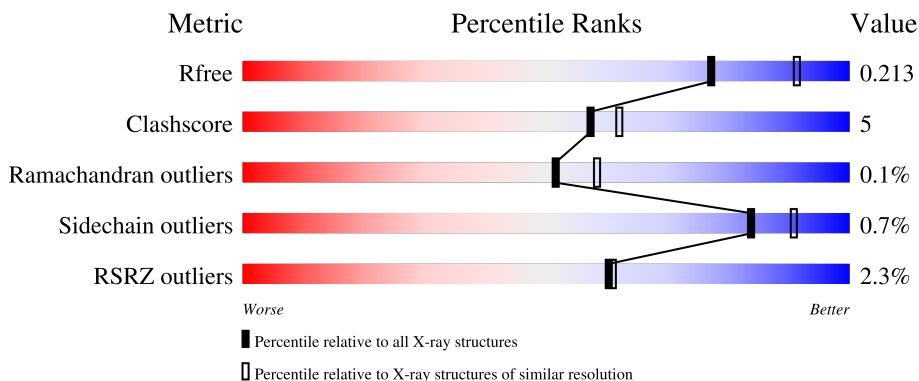
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	399	2% / 88% / 11% / ••
1	B	399	.% / 85% / 10% / 5%
1	C	399	3% / 87% / 8% / 5%
1	D	399	3% / 86% / 13% / •

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	BCT	B	400	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 13127 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3119	1993	536	578	12			
1	B	381	Total	C	N	O	S	0	0	0
			3003	1921	509	561	12			
1	C	380	Total	C	N	O	S	0	0	0
			2994	1915	507	560	12			
1	D	397	Total	C	N	O	S	0	0	0
			3135	2002	538	583	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	385	VAL	-	expression tag	UNP P21553
A	386	ASP	-	expression tag	UNP P21553
A	387	LYS	-	expression tag	UNP P21553
A	388	LEU	-	expression tag	UNP P21553
A	389	ALA	-	expression tag	UNP P21553
A	390	ALA	-	expression tag	UNP P21553
A	391	ALA	-	expression tag	UNP P21553
A	392	LEU	-	expression tag	UNP P21553
A	393	GLU	-	expression tag	UNP P21553
A	394	HIS	-	expression tag	UNP P21553
A	395	HIS	-	expression tag	UNP P21553
A	396	HIS	-	expression tag	UNP P21553
A	397	HIS	-	expression tag	UNP P21553
A	398	HIS	-	expression tag	UNP P21553
A	399	HIS	-	expression tag	UNP P21553
B	385	VAL	-	expression tag	UNP P21553
B	386	ASP	-	expression tag	UNP P21553
B	387	LYS	-	expression tag	UNP P21553
B	388	LEU	-	expression tag	UNP P21553
B	389	ALA	-	expression tag	UNP P21553
B	390	ALA	-	expression tag	UNP P21553

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	391	ALA	-	expression tag	UNP P21553
B	392	LEU	-	expression tag	UNP P21553
B	393	GLU	-	expression tag	UNP P21553
B	394	HIS	-	expression tag	UNP P21553
B	395	HIS	-	expression tag	UNP P21553
B	396	HIS	-	expression tag	UNP P21553
B	397	HIS	-	expression tag	UNP P21553
B	398	HIS	-	expression tag	UNP P21553
B	399	HIS	-	expression tag	UNP P21553
C	385	VAL	-	expression tag	UNP P21553
C	386	ASP	-	expression tag	UNP P21553
C	387	LYS	-	expression tag	UNP P21553
C	388	LEU	-	expression tag	UNP P21553
C	389	ALA	-	expression tag	UNP P21553
C	390	ALA	-	expression tag	UNP P21553
C	391	ALA	-	expression tag	UNP P21553
C	392	LEU	-	expression tag	UNP P21553
C	393	GLU	-	expression tag	UNP P21553
C	394	HIS	-	expression tag	UNP P21553
C	395	HIS	-	expression tag	UNP P21553
C	396	HIS	-	expression tag	UNP P21553
C	397	HIS	-	expression tag	UNP P21553
C	398	HIS	-	expression tag	UNP P21553
C	399	HIS	-	expression tag	UNP P21553
D	385	VAL	-	expression tag	UNP P21553
D	386	ASP	-	expression tag	UNP P21553
D	387	LYS	-	expression tag	UNP P21553
D	388	LEU	-	expression tag	UNP P21553
D	389	ALA	-	expression tag	UNP P21553
D	390	ALA	-	expression tag	UNP P21553
D	391	ALA	-	expression tag	UNP P21553
D	392	LEU	-	expression tag	UNP P21553
D	393	GLU	-	expression tag	UNP P21553
D	394	HIS	-	expression tag	UNP P21553
D	395	HIS	-	expression tag	UNP P21553
D	396	HIS	-	expression tag	UNP P21553
D	397	HIS	-	expression tag	UNP P21553
D	398	HIS	-	expression tag	UNP P21553
D	399	HIS	-	expression tag	UNP P21553

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

BCT

O1

O

C

OH O3

O⁻

O2
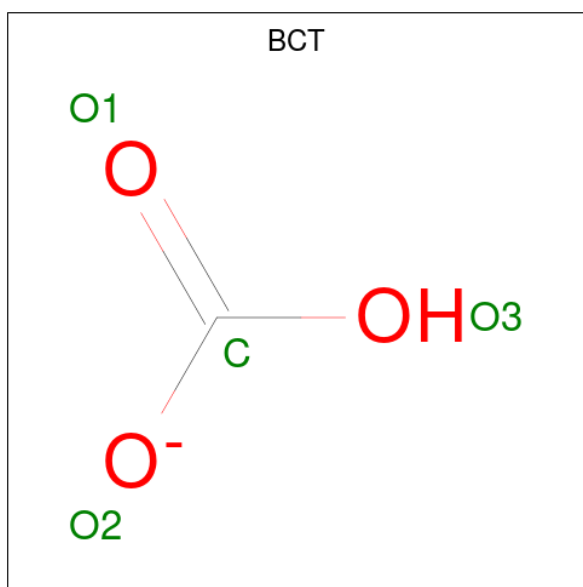
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 4	C 1	O 3	0	0
2	C	1	Total 4	C 1	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total 234	O 234	0	0
3	B	239	Total 239	O 239	0	0
3	C	198	Total 198	O 198	0	0
3	D	197	Total 197	O 197	0	0

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.
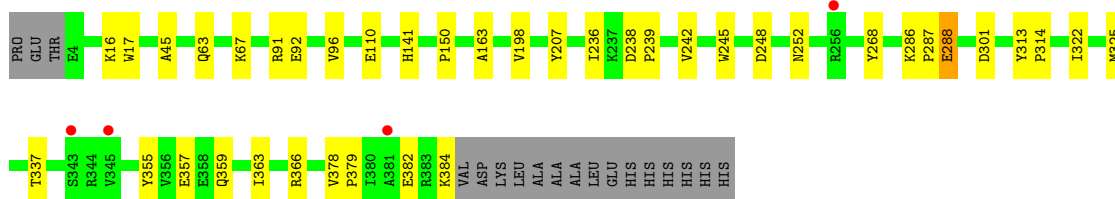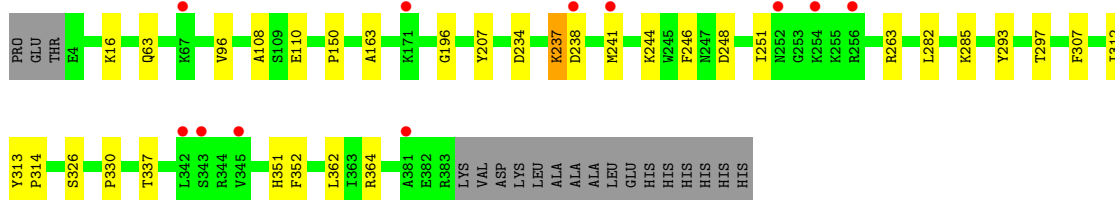
• Molecule 1: Citrate synthase

Chain A:
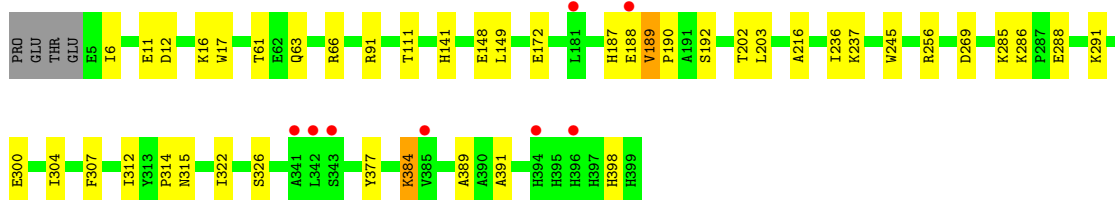
• Molecule 1: Citrate synthase

Chain B:

• Molecule 1: Citrate synthase
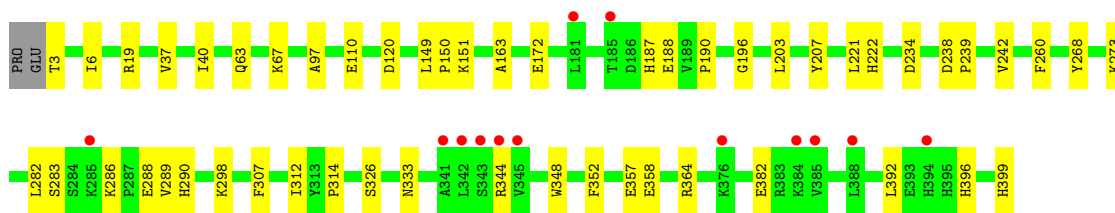
Chain C:

• Molecule 1: Citrate synthase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.51Å 113.41Å 120.07Å 90.00° 95.08° 90.00°	Depositor
Resolution (Å)	29.15 – 2.18 29.90 – 2.18	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.15-2.18) 89.8 (29.90-2.18)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.23	Depositor
$<I/\sigma(I)>$ [1]	1.88 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.164 , 0.212 0.166 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (2.63%)	wwPDB-VP
Wilson B-factor (Å^2)	24.9	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 37.5	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13127	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.59	0/3189	0.59	0/4309
1	B	0.62	0/3067	0.60	0/4144
1	C	0.55	0/3058	0.59	0/4133
1	D	0.53	0/3205	0.57	0/4331
All	All	0.58	0/12519	0.59	0/16917

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 ⓘ

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	3119	0	3114	35	0
1	B	3003	0	3009	32	0
1	C	2994	0	2996	23	0
1	D	3135	0	3127	38	0
2	B	4	0	0	3	0
2	C	4	0	0	0	0
3	A	234	0	0	4	0
3	B	239	0	0	6	0
3	C	198	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	197	0	0	5	0
All	All	13127	0	12246	119	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 5.

The worst 5 of 119 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:188:GLU:HG2	1:A:189:VAL:H	1.14	1.11
1:D:188:GLU:OE2	3:D:401:HOH:O	1.70	1.07
1:A:63:GLN:OE1	1:A:66:ARG:NH1	1.94	1.00
1:B:301:ASP:OD1	3:B:501:HOH:O	1.84	0.95
1:A:288:GLU:N	1:A:288:GLU:OE1	2.01	0.92

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	393/399 (98%)	385 (98%)	8 (2%)	0	100	100
1	B	379/399 (95%)	372 (98%)	7 (2%)	0	100	100
1	C	378/399 (95%)	370 (98%)	7 (2%)	1 (0%)	41	43
1	D	395/399 (99%)	386 (98%)	9 (2%)	0	100	100
All	All	1545/1596 (97%)	1513 (98%)	31 (2%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	237	LYS

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	322/326 (99%)	318 (99%)	4 (1%)	71	81
1	B	311/326 (95%)	308 (99%)	3 (1%)	76	85
1	C	310/326 (95%)	310 (100%)	0	100	100
1	D	324/326 (99%)	322 (99%)	2 (1%)	86	92
All	All	1267/1304 (97%)	1258 (99%)	9 (1%)	84	91

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	222	HIS
1	D	382	GLU
1	A	384	LYS
1	B	288	GLU
1	B	366	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	BCT	B	400	-	2,3,3	0.50	0	2,3,3	0.44	0
2	BCT	C	400	-	2,3,3	0.76	0	2,3,3	0.23	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	BCT	3	0

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 ⓘ

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	395/399 (98%)	-0.06	8 (2%)	65	66	19, 30, 57, 75	0
1	B	381/399 (95%)	-0.16	4 (1%)	82	82	17, 26, 46, 79	0
1	C	380/399 (95%)	-0.00	11 (2%)	51	52	19, 30, 60, 93	0
1	D	397/399 (99%)	0.06	13 (3%)	46	47	21, 34, 61, 83	0
All	All	1553/1596 (97%)	-0.04	36 (2%)	60	61	17, 30, 57, 93	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	VAL	5.5
1	D	385	VAL	4.1
1	D	345	VAL	4.1
1	A	188	GLU	4.1
1	C	381	ALA	3.8

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($Å^2$)	Q<0.9
2	BCT	B	400	4/4	0.91	0.17	53,53,53,54	0
2	BCT	C	400	4/4	0.96	0.09	35,36,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.