



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:07 PM UTC

PDB ID : 8QWB / pdb_00008qwb
Title : Crystal structure of citrate synthase from Methylophaga sulfidovorans
Authors : Mais, C.-N.; Bange, G.; Sendker, F.L.; Hochberg, G.
Deposited on : 2023-10-19
Resolution : 3.20 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
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

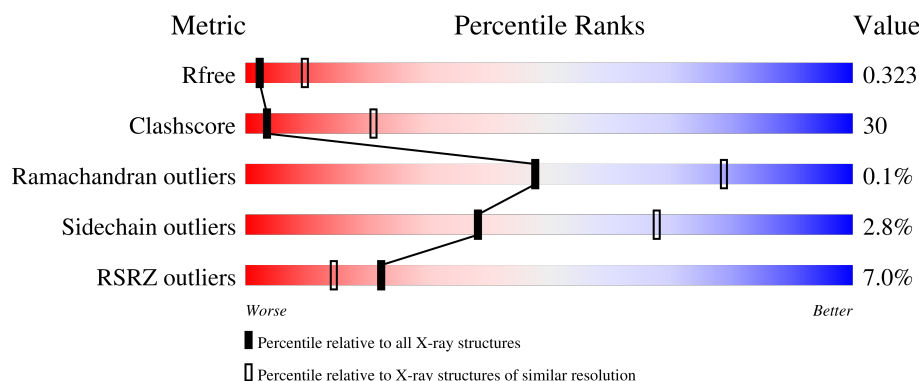
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	A	397	
1	B	397	
1	C	397	
1	D	397	
1	E	397	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	397	 6% 42% 37% 20%
1	G	397	 8% 36% 41% 21%
1	H	397	 6% 38% 40% 21%
1	I	397	 3% 41% 36% 22%
1	J	397	 6% 41% 40% 18%
1	K	397	 7% 39% 38% 22%
1	L	397	 3% 36% 42% 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30057 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	324	Total	C	N	O	S	0	0	0
			2555	1628	434	475	18			
1	B	327	Total	C	N	O	S	0	0	0
			2580	1642	437	482	19			
1	C	311	Total	C	N	O	S	0	0	0
			2441	1552	409	463	17			
1	D	324	Total	C	N	O	S	0	0	0
			2552	1623	434	477	18			
1	E	321	Total	C	N	O	S	0	0	0
			2533	1611	431	473	18			
1	F	318	Total	C	N	O	S	0	0	0
			2509	1597	427	468	17			
1	G	313	Total	C	N	O	S	0	0	0
			2457	1564	414	462	17			
1	H	315	Total	C	N	O	S	0	0	0
			2484	1581	421	465	17			
1	I	311	Total	C	N	O	S	0	0	0
			2446	1555	416	458	17			
1	J	326	Total	C	N	O	S	0	0	0
			2563	1632	433	480	18			
1	K	309	Total	C	N	O	S	0	0	0
			2433	1552	409	456	16			
1	L	317	Total	C	N	O	S	0	0	0
			2504	1594	423	469	18			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	LEU	-	expression tag	UNP A0A1I4B681
A	387	VAL	-	expression tag	UNP A0A1I4B681
A	388	PRO	-	expression tag	UNP A0A1I4B681
A	389	ARG	-	expression tag	UNP A0A1I4B681
A	390	LEU	-	expression tag	UNP A0A1I4B681

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	GLU	-	expression tag	UNP A0A1I4B681
A	392	HIS	-	expression tag	UNP A0A1I4B681
A	393	HIS	-	expression tag	UNP A0A1I4B681
A	394	HIS	-	expression tag	UNP A0A1I4B681
A	395	HIS	-	expression tag	UNP A0A1I4B681
A	396	HIS	-	expression tag	UNP A0A1I4B681
A	397	HIS	-	expression tag	UNP A0A1I4B681
B	386	LEU	-	expression tag	UNP A0A1I4B681
B	387	VAL	-	expression tag	UNP A0A1I4B681
B	388	PRO	-	expression tag	UNP A0A1I4B681
B	389	ARG	-	expression tag	UNP A0A1I4B681
B	390	LEU	-	expression tag	UNP A0A1I4B681
B	391	GLU	-	expression tag	UNP A0A1I4B681
B	392	HIS	-	expression tag	UNP A0A1I4B681
B	393	HIS	-	expression tag	UNP A0A1I4B681
B	394	HIS	-	expression tag	UNP A0A1I4B681
B	395	HIS	-	expression tag	UNP A0A1I4B681
B	396	HIS	-	expression tag	UNP A0A1I4B681
B	397	HIS	-	expression tag	UNP A0A1I4B681
C	386	LEU	-	expression tag	UNP A0A1I4B681
C	387	VAL	-	expression tag	UNP A0A1I4B681
C	388	PRO	-	expression tag	UNP A0A1I4B681
C	389	ARG	-	expression tag	UNP A0A1I4B681
C	390	LEU	-	expression tag	UNP A0A1I4B681
C	391	GLU	-	expression tag	UNP A0A1I4B681
C	392	HIS	-	expression tag	UNP A0A1I4B681
C	393	HIS	-	expression tag	UNP A0A1I4B681
C	394	HIS	-	expression tag	UNP A0A1I4B681
C	395	HIS	-	expression tag	UNP A0A1I4B681
C	396	HIS	-	expression tag	UNP A0A1I4B681
C	397	HIS	-	expression tag	UNP A0A1I4B681
D	386	LEU	-	expression tag	UNP A0A1I4B681
D	387	VAL	-	expression tag	UNP A0A1I4B681
D	388	PRO	-	expression tag	UNP A0A1I4B681
D	389	ARG	-	expression tag	UNP A0A1I4B681
D	390	LEU	-	expression tag	UNP A0A1I4B681
D	391	GLU	-	expression tag	UNP A0A1I4B681
D	392	HIS	-	expression tag	UNP A0A1I4B681
D	393	HIS	-	expression tag	UNP A0A1I4B681
D	394	HIS	-	expression tag	UNP A0A1I4B681
D	395	HIS	-	expression tag	UNP A0A1I4B681
D	396	HIS	-	expression tag	UNP A0A1I4B681

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	397	HIS	-	expression tag	UNP A0A1I4B681
E	386	LEU	-	expression tag	UNP A0A1I4B681
E	387	VAL	-	expression tag	UNP A0A1I4B681
E	388	PRO	-	expression tag	UNP A0A1I4B681
E	389	ARG	-	expression tag	UNP A0A1I4B681
E	390	LEU	-	expression tag	UNP A0A1I4B681
E	391	GLU	-	expression tag	UNP A0A1I4B681
E	392	HIS	-	expression tag	UNP A0A1I4B681
E	393	HIS	-	expression tag	UNP A0A1I4B681
E	394	HIS	-	expression tag	UNP A0A1I4B681
E	395	HIS	-	expression tag	UNP A0A1I4B681
E	396	HIS	-	expression tag	UNP A0A1I4B681
E	397	HIS	-	expression tag	UNP A0A1I4B681
F	386	LEU	-	expression tag	UNP A0A1I4B681
F	387	VAL	-	expression tag	UNP A0A1I4B681
F	388	PRO	-	expression tag	UNP A0A1I4B681
F	389	ARG	-	expression tag	UNP A0A1I4B681
F	390	LEU	-	expression tag	UNP A0A1I4B681
F	391	GLU	-	expression tag	UNP A0A1I4B681
F	392	HIS	-	expression tag	UNP A0A1I4B681
F	393	HIS	-	expression tag	UNP A0A1I4B681
F	394	HIS	-	expression tag	UNP A0A1I4B681
F	395	HIS	-	expression tag	UNP A0A1I4B681
F	396	HIS	-	expression tag	UNP A0A1I4B681
F	397	HIS	-	expression tag	UNP A0A1I4B681
G	386	LEU	-	expression tag	UNP A0A1I4B681
G	387	VAL	-	expression tag	UNP A0A1I4B681
G	388	PRO	-	expression tag	UNP A0A1I4B681
G	389	ARG	-	expression tag	UNP A0A1I4B681
G	390	LEU	-	expression tag	UNP A0A1I4B681
G	391	GLU	-	expression tag	UNP A0A1I4B681
G	392	HIS	-	expression tag	UNP A0A1I4B681
G	393	HIS	-	expression tag	UNP A0A1I4B681
G	394	HIS	-	expression tag	UNP A0A1I4B681
G	395	HIS	-	expression tag	UNP A0A1I4B681
G	396	HIS	-	expression tag	UNP A0A1I4B681
G	397	HIS	-	expression tag	UNP A0A1I4B681
H	386	LEU	-	expression tag	UNP A0A1I4B681
H	387	VAL	-	expression tag	UNP A0A1I4B681
H	388	PRO	-	expression tag	UNP A0A1I4B681
H	389	ARG	-	expression tag	UNP A0A1I4B681
H	390	LEU	-	expression tag	UNP A0A1I4B681

Continued on next page...

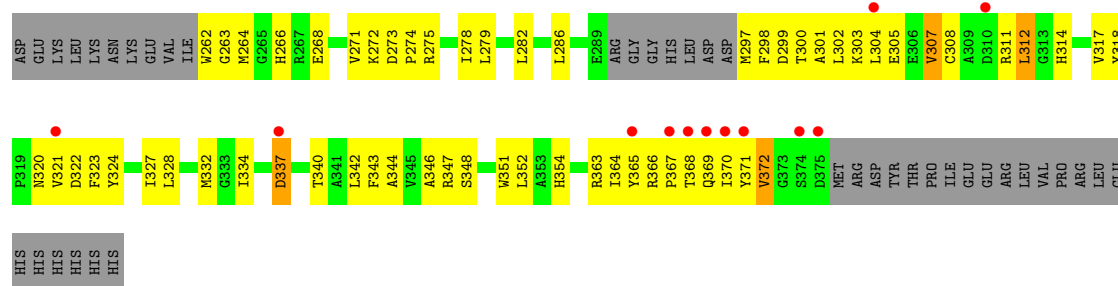
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	391	GLU	-	expression tag	UNP A0A1I4B681
H	392	HIS	-	expression tag	UNP A0A1I4B681
H	393	HIS	-	expression tag	UNP A0A1I4B681
H	394	HIS	-	expression tag	UNP A0A1I4B681
H	395	HIS	-	expression tag	UNP A0A1I4B681
H	396	HIS	-	expression tag	UNP A0A1I4B681
H	397	HIS	-	expression tag	UNP A0A1I4B681
I	386	LEU	-	expression tag	UNP A0A1I4B681
I	387	VAL	-	expression tag	UNP A0A1I4B681
I	388	PRO	-	expression tag	UNP A0A1I4B681
I	389	ARG	-	expression tag	UNP A0A1I4B681
I	390	LEU	-	expression tag	UNP A0A1I4B681
I	391	GLU	-	expression tag	UNP A0A1I4B681
I	392	HIS	-	expression tag	UNP A0A1I4B681
I	393	HIS	-	expression tag	UNP A0A1I4B681
I	394	HIS	-	expression tag	UNP A0A1I4B681
I	395	HIS	-	expression tag	UNP A0A1I4B681
I	396	HIS	-	expression tag	UNP A0A1I4B681
I	397	HIS	-	expression tag	UNP A0A1I4B681
J	386	LEU	-	expression tag	UNP A0A1I4B681
J	387	VAL	-	expression tag	UNP A0A1I4B681
J	388	PRO	-	expression tag	UNP A0A1I4B681
J	389	ARG	-	expression tag	UNP A0A1I4B681
J	390	LEU	-	expression tag	UNP A0A1I4B681
J	391	GLU	-	expression tag	UNP A0A1I4B681
J	392	HIS	-	expression tag	UNP A0A1I4B681
J	393	HIS	-	expression tag	UNP A0A1I4B681
J	394	HIS	-	expression tag	UNP A0A1I4B681
J	395	HIS	-	expression tag	UNP A0A1I4B681
J	396	HIS	-	expression tag	UNP A0A1I4B681
J	397	HIS	-	expression tag	UNP A0A1I4B681
K	386	LEU	-	expression tag	UNP A0A1I4B681
K	387	VAL	-	expression tag	UNP A0A1I4B681
K	388	PRO	-	expression tag	UNP A0A1I4B681
K	389	ARG	-	expression tag	UNP A0A1I4B681
K	390	LEU	-	expression tag	UNP A0A1I4B681
K	391	GLU	-	expression tag	UNP A0A1I4B681
K	392	HIS	-	expression tag	UNP A0A1I4B681
K	393	HIS	-	expression tag	UNP A0A1I4B681
K	394	HIS	-	expression tag	UNP A0A1I4B681
K	395	HIS	-	expression tag	UNP A0A1I4B681
K	396	HIS	-	expression tag	UNP A0A1I4B681

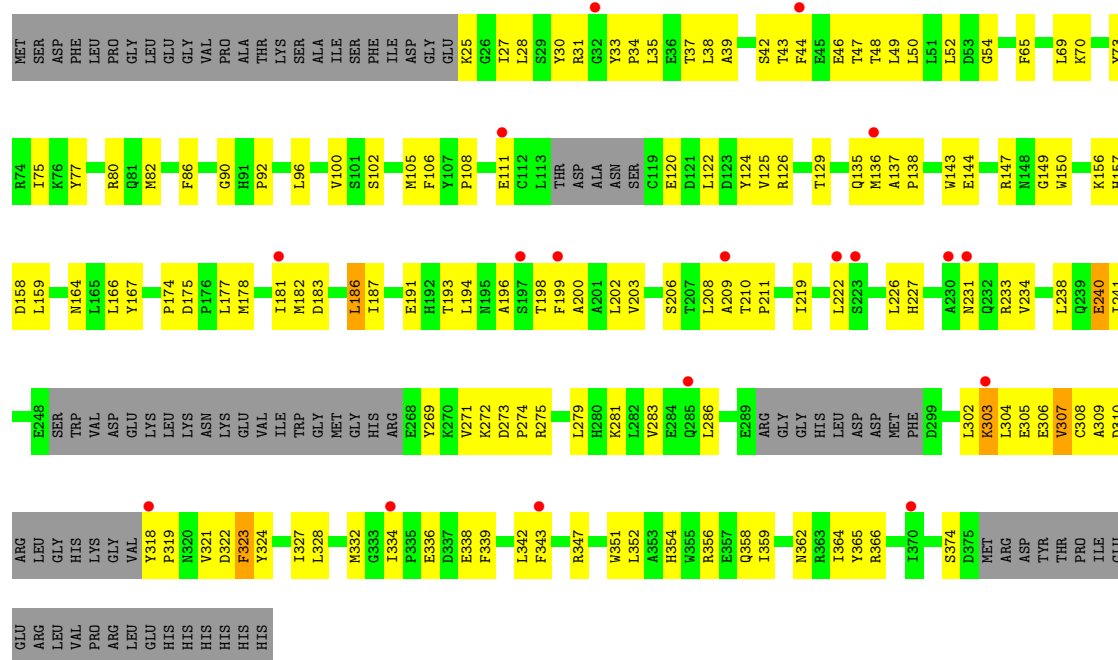
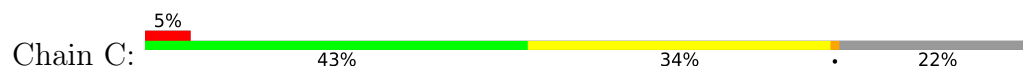
Continued on next page...

Continued from previous page...

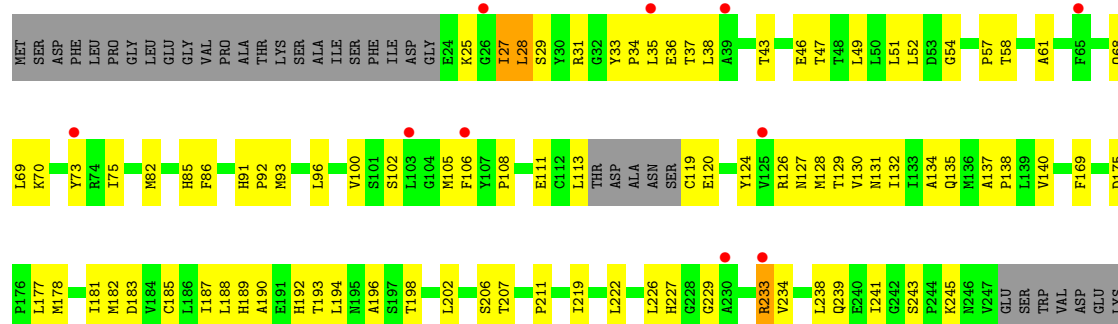
Chain	Residue	Modelled	Actual	Comment	Reference
K	397	HIS	-	expression tag	UNP A0A1I4B681
L	386	LEU	-	expression tag	UNP A0A1I4B681
L	387	VAL	-	expression tag	UNP A0A1I4B681
L	388	PRO	-	expression tag	UNP A0A1I4B681
L	389	ARG	-	expression tag	UNP A0A1I4B681
L	390	LEU	-	expression tag	UNP A0A1I4B681
L	391	GLU	-	expression tag	UNP A0A1I4B681
L	392	HIS	-	expression tag	UNP A0A1I4B681
L	393	HIS	-	expression tag	UNP A0A1I4B681
L	394	HIS	-	expression tag	UNP A0A1I4B681
L	395	HIS	-	expression tag	UNP A0A1I4B681
L	396	HIS	-	expression tag	UNP A0A1I4B681
L	397	HIS	-	expression tag	UNP A0A1I4B681

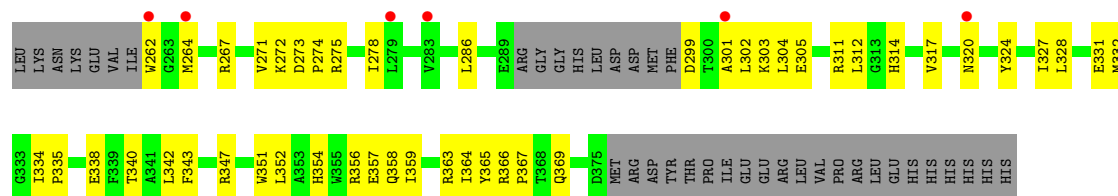


• Molecule 1: Citrate synthase

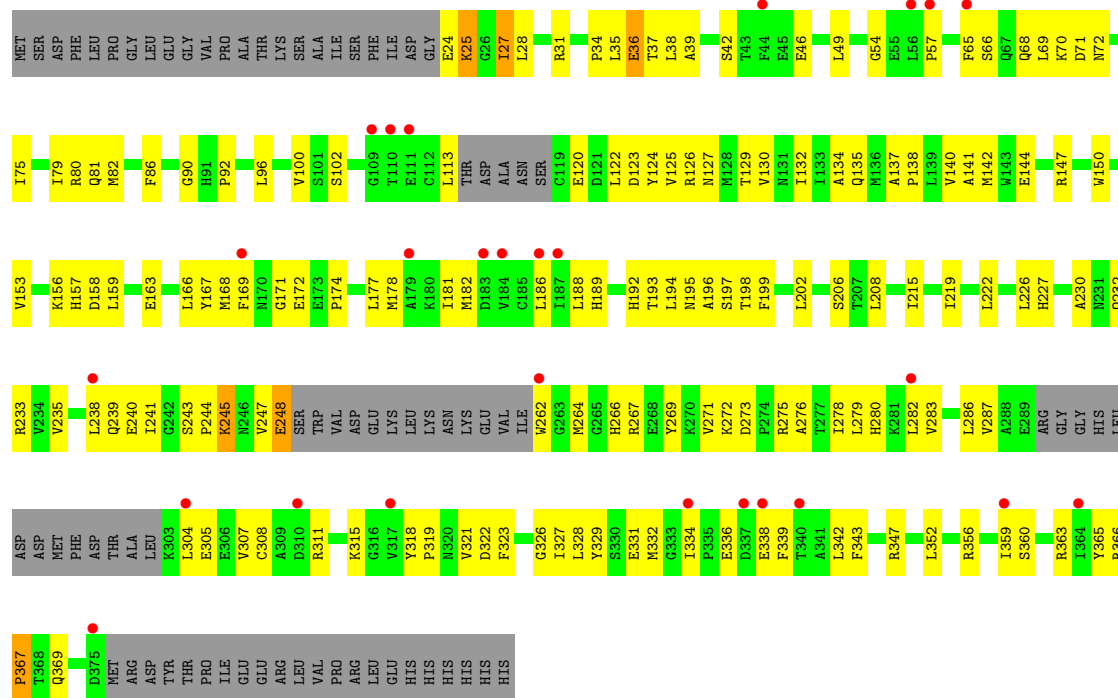
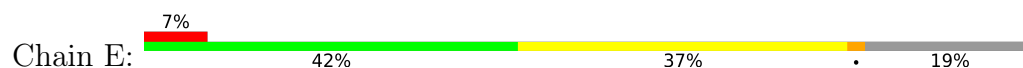


• Molecule 1: Citrate synthase

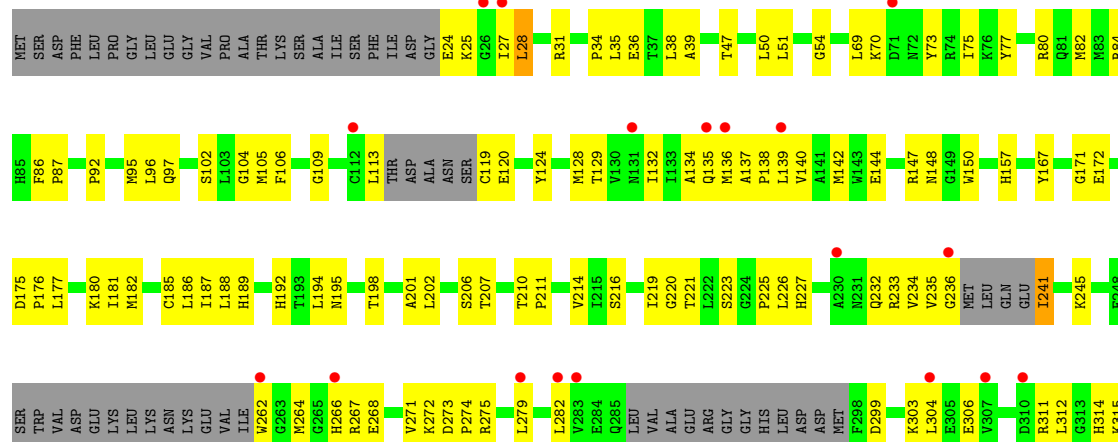


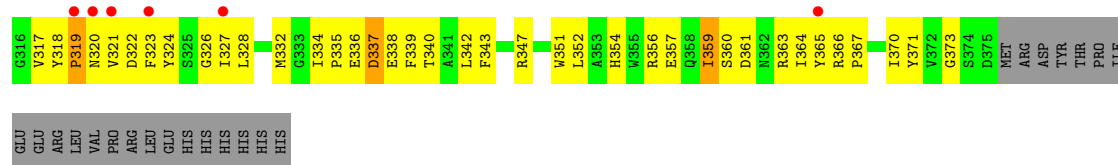


• Molecule 1: Citrate synthase

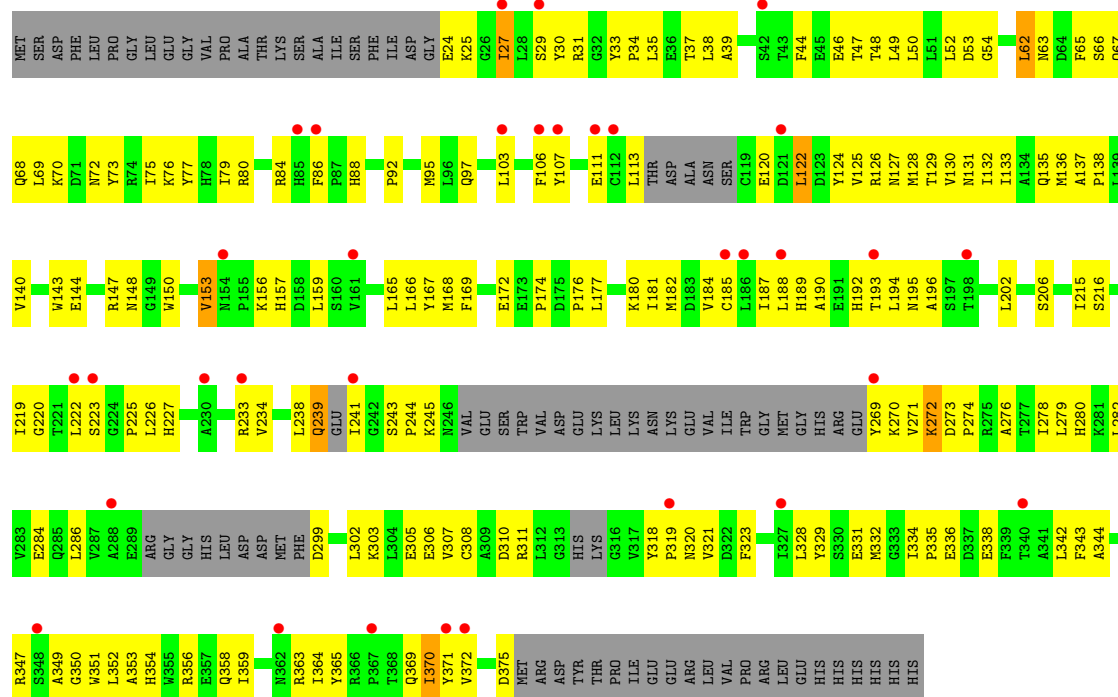


• Molecule 1: Citrate synthase

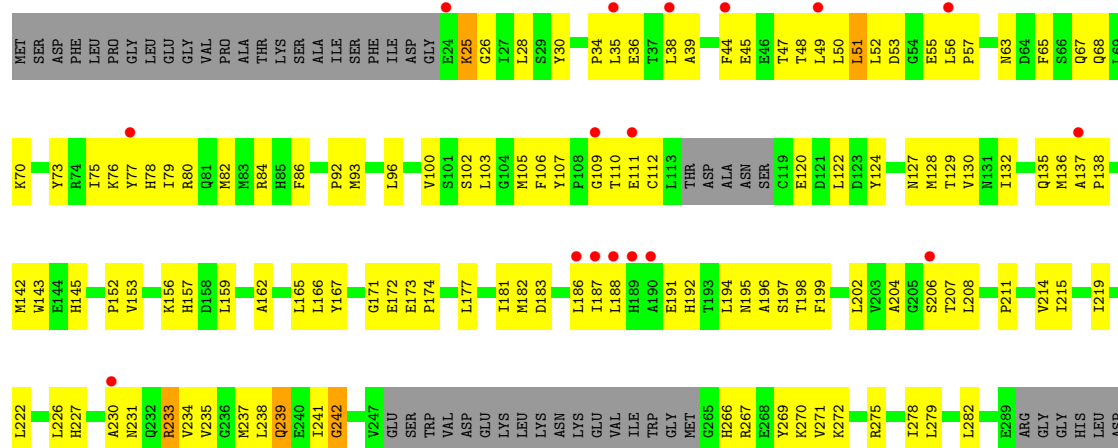


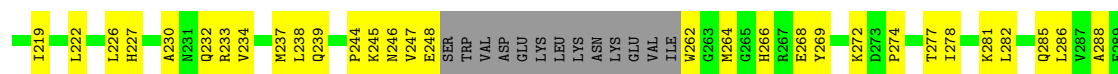
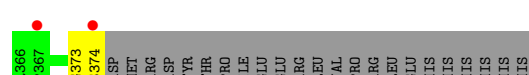


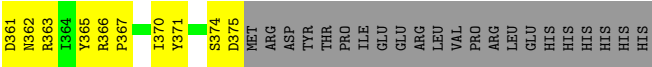
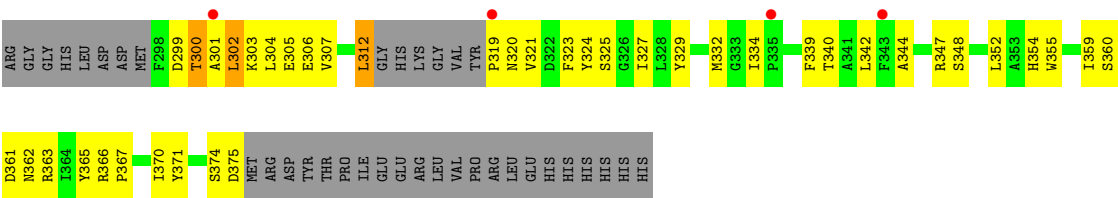
● Molecule 1: Citrate synthase



● Molecule 1: Citrate synthase







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	155.69Å 96.61Å 203.10Å 90.00° 110.41° 90.00°	Depositor
Resolution (Å)	48.31 – 3.20 48.31 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.31-3.20) 99.0 (48.31-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2-3874	Depositor
R, R_{free}	0.282 , 0.325 0.324 , 0.323	Depositor DCC
R_{free} test set	4638 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	114.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 136.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30057	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.13% 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 [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	0.90	0/2615	1.15	0/3547
1	B	0.89	0/2640	1.17	0/3580
1	C	0.87	0/2494	1.18	0/3385
1	D	0.89	0/2611	1.18	0/3542
1	E	0.90	0/2592	1.16	0/3515
1	F	0.87	0/2568	1.18	2/3482 (0.1%)
1	G	0.92	0/2510	1.16	1/3404 (0.0%)
1	H	0.90	0/2539	1.16	1/3444 (0.0%)
1	I	0.87	0/2498	1.17	0/3384
1	J	0.90	0/2622	1.16	0/3557
1	K	0.89	0/2487	1.17	1/3372 (0.0%)
1	L	0.89	0/2561	1.15	0/3474
All	All	0.89	0/30737	1.17	5/41686 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	109	GLY	CA-C-O	-5.75	118.17	122.37
1	F	319	PRO	CB-CA-C	-5.24	102.92	111.56
1	G	364	ILE	N-CA-C	-5.20	108.43	113.53
1	K	137	ALA	N-CA-C	-5.10	106.62	113.25
1	F	211	PRO	N-CA-C	-5.03	106.25	113.75

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	2555	0	2508	138	0
1	B	2580	0	2527	155	0
1	C	2441	0	2391	133	0
1	D	2552	0	2503	136	0
1	E	2533	0	2482	155	0
1	F	2509	0	2452	169	0
1	G	2457	0	2415	160	0
1	H	2484	0	2443	160	0
1	I	2446	0	2402	165	0
1	J	2563	0	2507	149	0
1	K	2433	0	2377	157	0
1	L	2504	0	2452	178	0
All	All	30057	0	29459	1761	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 30.

The worst 5 of 1761 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:F:264:MET:HA	1:F:319:PRO:HB3	1.34	1.05
1:A:28:LEU:HD12	1:A:35:LEU:HB2	1.42	1.02
1:A:334:ILE:HG21	1:A:342:LEU:HD11	1.42	0.99
1:K:266:HIS:HB3	1:K:269:TYR:HB2	1.45	0.98
1:I:233:ARG:HB2	1:I:323:PHE:HA	1.47	0.96

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	A	316/397 (80%)	297 (94%)	19 (6%)	0	100	100
1	B	319/397 (80%)	292 (92%)	27 (8%)	0	100	100
1	C	301/397 (76%)	283 (94%)	18 (6%)	0	100	100
1	D	316/397 (80%)	300 (95%)	16 (5%)	0	100	100
1	E	313/397 (79%)	297 (95%)	15 (5%)	1 (0%)	36	68
1	F	308/397 (78%)	284 (92%)	24 (8%)	0	100	100
1	G	301/397 (76%)	282 (94%)	19 (6%)	0	100	100
1	H	305/397 (77%)	283 (93%)	21 (7%)	1 (0%)	36	68
1	I	297/397 (75%)	280 (94%)	16 (5%)	1 (0%)	36	68
1	J	318/397 (80%)	299 (94%)	19 (6%)	0	100	100
1	K	295/397 (74%)	280 (95%)	15 (5%)	0	100	100
1	L	307/397 (77%)	286 (93%)	21 (7%)	0	100	100
All	All	3696/4764 (78%)	3463 (94%)	230 (6%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	242	GLY
1	I	108	PRO
1	E	367	PRO

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	275/340 (81%)	270 (98%)	5 (2%)	51	74
1	B	278/340 (82%)	265 (95%)	13 (5%)	23	57
1	C	265/340 (78%)	257 (97%)	8 (3%)	36	66
1	D	275/340 (81%)	270 (98%)	5 (2%)	51	74
1	E	273/340 (80%)	268 (98%)	5 (2%)	51	74
1	F	270/340 (79%)	264 (98%)	6 (2%)	45	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	266/340 (78%)	256 (96%)	10 (4%)	29	62
1	H	269/340 (79%)	261 (97%)	8 (3%)	36	66
1	I	264/340 (78%)	255 (97%)	9 (3%)	32	64
1	J	275/340 (81%)	266 (97%)	9 (3%)	33	65
1	K	262/340 (77%)	258 (98%)	4 (2%)	57	76
1	L	271/340 (80%)	261 (96%)	10 (4%)	30	63
All	All	3243/4080 (80%)	3151 (97%)	92 (3%)	38	68

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	239	GLN
1	J	107	TYR
1	H	358	GLN
1	I	271	VAL
1	J	245	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	192	HIS
1	I	362	ASN
1	H	239	GLN
1	I	131	ASN
1	J	227	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 oligosaccharides 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	324/397 (81%)	0.65	23 (7%)	22	14	86, 118, 157, 237	0
1	B	327/397 (82%)	0.65	27 (8%)	17	11	84, 114, 187, 280	0
1	C	311/397 (78%)	0.62	18 (5%)	29	18	89, 135, 208, 286	0
1	D	324/397 (81%)	0.58	16 (4%)	35	22	85, 117, 172, 218	0
1	E	321/397 (80%)	0.62	26 (8%)	18	11	85, 116, 171, 259	0
1	F	318/397 (80%)	0.58	24 (7%)	20	13	30, 122, 183, 255	0
1	G	313/397 (78%)	0.84	33 (10%)	11	8	96, 127, 207, 286	0
1	H	315/397 (79%)	0.74	24 (7%)	20	13	89, 140, 207, 271	0
1	I	311/397 (78%)	0.52	12 (3%)	43	27	94, 135, 209, 262	0
1	J	326/397 (82%)	0.67	25 (7%)	19	13	96, 131, 187, 285	0
1	K	309/397 (77%)	0.70	27 (8%)	16	11	92, 132, 205, 241	0
1	L	317/397 (79%)	0.64	11 (3%)	47	29	30, 147, 209, 288	0
All	All	3816/4764 (80%)	0.65	266 (6%)	22	14	30, 128, 199, 288	0

The worst 5 of 266 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	SER	8.3
1	B	370	ILE	6.4
1	J	304	LEU	5.8
1	F	319	PRO	5.4
1	E	44	PHE	5.2

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.