



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:10 AM GMT

PDB ID : 3O8J
Title : Crystal structure of 2-methylcitrate synthase (PrpC) from *Salmonella typhimurium*
Authors : Chittori, S.; Savithri, H.S.; Murthy, M.R.N.
Deposited on : 2010-08-03
Resolution : 2.41 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
<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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

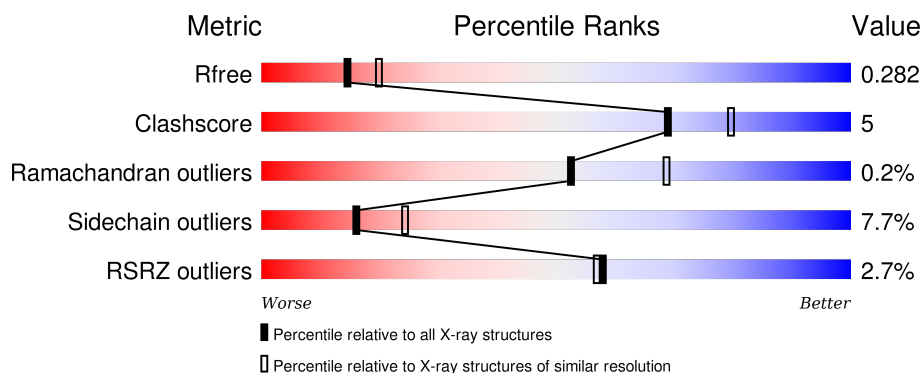
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 $\leq 5\%$. 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	404	<div> <div>2%</div> <div>79% 10% 10%</div> </div>
1	B	404	<div> <div>75% 13% 10%</div> </div>
1	C	404	<div> <div>6%</div> <div>77% 11% 11%</div> </div>
1	D	404	<div> <div>5%</div> <div>74% 12% 11%</div> </div>
1	E	404	<div> <div>0%</div> <div>78% 10% 10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	404	
1	G	404	
1	H	404	
1	I	404	
1	J	404	

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	GOL	A	409	-	-	-	X
2	GOL	B	410	-	-	-	X
2	GOL	E	402	-	-	-	X
2	GOL	F	411	-	-	-	X
2	GOL	G	403	-	-	-	X
2	GOL	H	404	-	-	-	X
2	GOL	J	406	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29229 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 2-methylcitrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2808	1775	494	526	13			
1	B	364	Total	C	N	O	S	0	0	0
			2799	1769	492	526	12			
1	C	360	Total	C	N	O	S	0	0	0
			2769	1750	486	521	12			
1	D	358	Total	C	N	O	S	0	0	0
			2764	1746	486	519	13			
1	E	364	Total	C	N	O	S	0	0	0
			2813	1780	494	526	13			
1	F	364	Total	C	N	O	S	0	0	0
			2816	1781	491	532	12			
1	G	364	Total	C	N	O	S	0	0	0
			2801	1773	492	523	13			
1	H	362	Total	C	N	O	S	0	0	0
			2801	1772	491	525	13			
1	I	362	Total	C	N	O	S	0	0	0
			2799	1769	492	525	13			
1	J	362	Total	C	N	O	S	0	0	0
			2815	1780	494	528	13			

There are 150 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP Q56063
A	-13	ARG	-	EXPRESSION TAG	UNP Q56063
A	-12	GLY	-	EXPRESSION TAG	UNP Q56063
A	-11	SER	-	EXPRESSION TAG	UNP Q56063
A	-10	HIS	-	EXPRESSION TAG	UNP Q56063
A	-9	HIS	-	EXPRESSION TAG	UNP Q56063
A	-8	HIS	-	EXPRESSION TAG	UNP Q56063
A	-7	HIS	-	EXPRESSION TAG	UNP Q56063
A	-6	HIS	-	EXPRESSION TAG	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q56063
A	-4	GLY	-	EXPRESSION TAG	UNP Q56063
A	-3	MET	-	EXPRESSION TAG	UNP Q56063
A	-2	ALA	-	EXPRESSION TAG	UNP Q56063
A	-1	SER	-	EXPRESSION TAG	UNP Q56063
A	0	HIS	-	EXPRESSION TAG	UNP Q56063
B	-14	MET	-	EXPRESSION TAG	UNP Q56063
B	-13	ARG	-	EXPRESSION TAG	UNP Q56063
B	-12	GLY	-	EXPRESSION TAG	UNP Q56063
B	-11	SER	-	EXPRESSION TAG	UNP Q56063
B	-10	HIS	-	EXPRESSION TAG	UNP Q56063
B	-9	HIS	-	EXPRESSION TAG	UNP Q56063
B	-8	HIS	-	EXPRESSION TAG	UNP Q56063
B	-7	HIS	-	EXPRESSION TAG	UNP Q56063
B	-6	HIS	-	EXPRESSION TAG	UNP Q56063
B	-5	HIS	-	EXPRESSION TAG	UNP Q56063
B	-4	GLY	-	EXPRESSION TAG	UNP Q56063
B	-3	MET	-	EXPRESSION TAG	UNP Q56063
B	-2	ALA	-	EXPRESSION TAG	UNP Q56063
B	-1	SER	-	EXPRESSION TAG	UNP Q56063
B	0	HIS	-	EXPRESSION TAG	UNP Q56063
C	-14	MET	-	EXPRESSION TAG	UNP Q56063
C	-13	ARG	-	EXPRESSION TAG	UNP Q56063
C	-12	GLY	-	EXPRESSION TAG	UNP Q56063
C	-11	SER	-	EXPRESSION TAG	UNP Q56063
C	-10	HIS	-	EXPRESSION TAG	UNP Q56063
C	-9	HIS	-	EXPRESSION TAG	UNP Q56063
C	-8	HIS	-	EXPRESSION TAG	UNP Q56063
C	-7	HIS	-	EXPRESSION TAG	UNP Q56063
C	-6	HIS	-	EXPRESSION TAG	UNP Q56063
C	-5	HIS	-	EXPRESSION TAG	UNP Q56063
C	-4	GLY	-	EXPRESSION TAG	UNP Q56063
C	-3	MET	-	EXPRESSION TAG	UNP Q56063
C	-2	ALA	-	EXPRESSION TAG	UNP Q56063
C	-1	SER	-	EXPRESSION TAG	UNP Q56063
C	0	HIS	-	EXPRESSION TAG	UNP Q56063
D	-14	MET	-	EXPRESSION TAG	UNP Q56063
D	-13	ARG	-	EXPRESSION TAG	UNP Q56063
D	-12	GLY	-	EXPRESSION TAG	UNP Q56063
D	-11	SER	-	EXPRESSION TAG	UNP Q56063
D	-10	HIS	-	EXPRESSION TAG	UNP Q56063
D	-9	HIS	-	EXPRESSION TAG	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	HIS	-	EXPRESSION TAG	UNP Q56063
D	-7	HIS	-	EXPRESSION TAG	UNP Q56063
D	-6	HIS	-	EXPRESSION TAG	UNP Q56063
D	-5	HIS	-	EXPRESSION TAG	UNP Q56063
D	-4	GLY	-	EXPRESSION TAG	UNP Q56063
D	-3	MET	-	EXPRESSION TAG	UNP Q56063
D	-2	ALA	-	EXPRESSION TAG	UNP Q56063
D	-1	SER	-	EXPRESSION TAG	UNP Q56063
D	0	HIS	-	EXPRESSION TAG	UNP Q56063
E	-14	MET	-	EXPRESSION TAG	UNP Q56063
E	-13	ARG	-	EXPRESSION TAG	UNP Q56063
E	-12	GLY	-	EXPRESSION TAG	UNP Q56063
E	-11	SER	-	EXPRESSION TAG	UNP Q56063
E	-10	HIS	-	EXPRESSION TAG	UNP Q56063
E	-9	HIS	-	EXPRESSION TAG	UNP Q56063
E	-8	HIS	-	EXPRESSION TAG	UNP Q56063
E	-7	HIS	-	EXPRESSION TAG	UNP Q56063
E	-6	HIS	-	EXPRESSION TAG	UNP Q56063
E	-5	HIS	-	EXPRESSION TAG	UNP Q56063
E	-4	GLY	-	EXPRESSION TAG	UNP Q56063
E	-3	MET	-	EXPRESSION TAG	UNP Q56063
E	-2	ALA	-	EXPRESSION TAG	UNP Q56063
E	-1	SER	-	EXPRESSION TAG	UNP Q56063
E	0	HIS	-	EXPRESSION TAG	UNP Q56063
F	-14	MET	-	EXPRESSION TAG	UNP Q56063
F	-13	ARG	-	EXPRESSION TAG	UNP Q56063
F	-12	GLY	-	EXPRESSION TAG	UNP Q56063
F	-11	SER	-	EXPRESSION TAG	UNP Q56063
F	-10	HIS	-	EXPRESSION TAG	UNP Q56063
F	-9	HIS	-	EXPRESSION TAG	UNP Q56063
F	-8	HIS	-	EXPRESSION TAG	UNP Q56063
F	-7	HIS	-	EXPRESSION TAG	UNP Q56063
F	-6	HIS	-	EXPRESSION TAG	UNP Q56063
F	-5	HIS	-	EXPRESSION TAG	UNP Q56063
F	-4	GLY	-	EXPRESSION TAG	UNP Q56063
F	-3	MET	-	EXPRESSION TAG	UNP Q56063
F	-2	ALA	-	EXPRESSION TAG	UNP Q56063
F	-1	SER	-	EXPRESSION TAG	UNP Q56063
F	0	HIS	-	EXPRESSION TAG	UNP Q56063
G	-14	MET	-	EXPRESSION TAG	UNP Q56063
G	-13	ARG	-	EXPRESSION TAG	UNP Q56063
G	-12	GLY	-	EXPRESSION TAG	UNP Q56063

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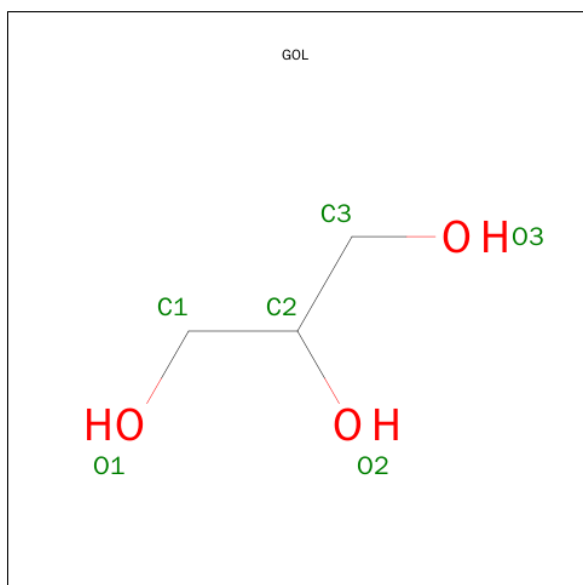
Chain	Residue	Modelled	Actual	Comment	Reference
G	-11	SER	-	EXPRESSION TAG	UNP Q56063
G	-10	HIS	-	EXPRESSION TAG	UNP Q56063
G	-9	HIS	-	EXPRESSION TAG	UNP Q56063
G	-8	HIS	-	EXPRESSION TAG	UNP Q56063
G	-7	HIS	-	EXPRESSION TAG	UNP Q56063
G	-6	HIS	-	EXPRESSION TAG	UNP Q56063
G	-5	HIS	-	EXPRESSION TAG	UNP Q56063
G	-4	GLY	-	EXPRESSION TAG	UNP Q56063
G	-3	MET	-	EXPRESSION TAG	UNP Q56063
G	-2	ALA	-	EXPRESSION TAG	UNP Q56063
G	-1	SER	-	EXPRESSION TAG	UNP Q56063
G	0	HIS	-	EXPRESSION TAG	UNP Q56063
H	-14	MET	-	EXPRESSION TAG	UNP Q56063
H	-13	ARG	-	EXPRESSION TAG	UNP Q56063
H	-12	GLY	-	EXPRESSION TAG	UNP Q56063
H	-11	SER	-	EXPRESSION TAG	UNP Q56063
H	-10	HIS	-	EXPRESSION TAG	UNP Q56063
H	-9	HIS	-	EXPRESSION TAG	UNP Q56063
H	-8	HIS	-	EXPRESSION TAG	UNP Q56063
H	-7	HIS	-	EXPRESSION TAG	UNP Q56063
H	-6	HIS	-	EXPRESSION TAG	UNP Q56063
H	-5	HIS	-	EXPRESSION TAG	UNP Q56063
H	-4	GLY	-	EXPRESSION TAG	UNP Q56063
H	-3	MET	-	EXPRESSION TAG	UNP Q56063
H	-2	ALA	-	EXPRESSION TAG	UNP Q56063
H	-1	SER	-	EXPRESSION TAG	UNP Q56063
H	0	HIS	-	EXPRESSION TAG	UNP Q56063
I	-14	MET	-	EXPRESSION TAG	UNP Q56063
I	-13	ARG	-	EXPRESSION TAG	UNP Q56063
I	-12	GLY	-	EXPRESSION TAG	UNP Q56063
I	-11	SER	-	EXPRESSION TAG	UNP Q56063
I	-10	HIS	-	EXPRESSION TAG	UNP Q56063
I	-9	HIS	-	EXPRESSION TAG	UNP Q56063
I	-8	HIS	-	EXPRESSION TAG	UNP Q56063
I	-7	HIS	-	EXPRESSION TAG	UNP Q56063
I	-6	HIS	-	EXPRESSION TAG	UNP Q56063
I	-5	HIS	-	EXPRESSION TAG	UNP Q56063
I	-4	GLY	-	EXPRESSION TAG	UNP Q56063
I	-3	MET	-	EXPRESSION TAG	UNP Q56063
I	-2	ALA	-	EXPRESSION TAG	UNP Q56063
I	-1	SER	-	EXPRESSION TAG	UNP Q56063
I	0	HIS	-	EXPRESSION TAG	UNP Q56063

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	MET	-	EXPRESSION TAG	UNP Q56063
J	-13	ARG	-	EXPRESSION TAG	UNP Q56063
J	-12	GLY	-	EXPRESSION TAG	UNP Q56063
J	-11	SER	-	EXPRESSION TAG	UNP Q56063
J	-10	HIS	-	EXPRESSION TAG	UNP Q56063
J	-9	HIS	-	EXPRESSION TAG	UNP Q56063
J	-8	HIS	-	EXPRESSION TAG	UNP Q56063
J	-7	HIS	-	EXPRESSION TAG	UNP Q56063
J	-6	HIS	-	EXPRESSION TAG	UNP Q56063
J	-5	HIS	-	EXPRESSION TAG	UNP Q56063
J	-4	GLY	-	EXPRESSION TAG	UNP Q56063
J	-3	MET	-	EXPRESSION TAG	UNP Q56063
J	-2	ALA	-	EXPRESSION TAG	UNP Q56063
J	-1	SER	-	EXPRESSION TAG	UNP Q56063
J	0	HIS	-	EXPRESSION TAG	UNP Q56063

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		

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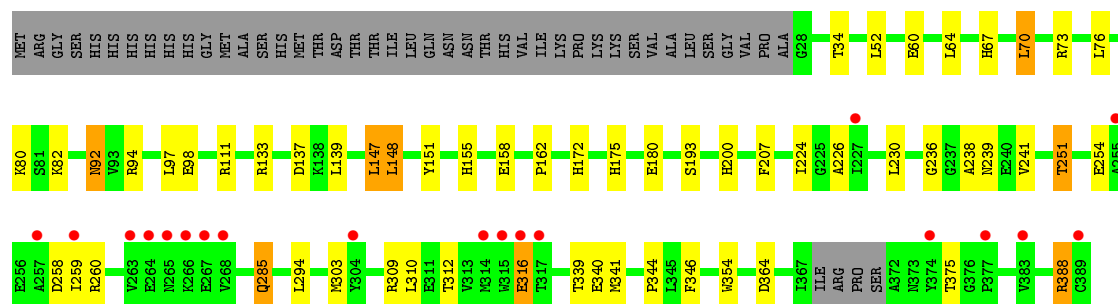
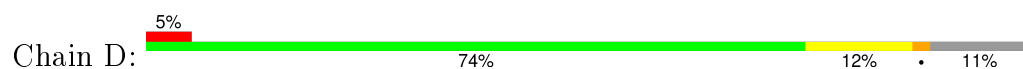
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

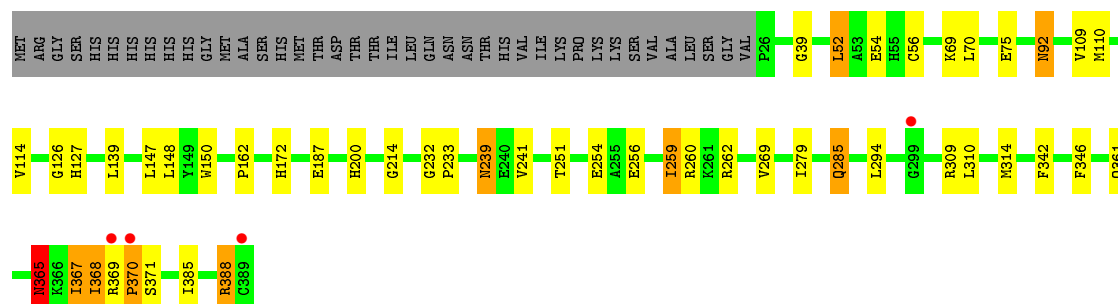
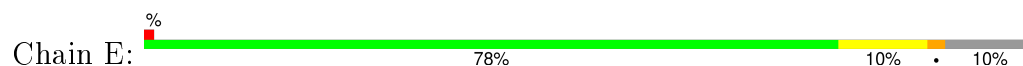
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	119	Total	O	0	0
			119	119		
3	C	84	Total	O	0	0
			84	84		
3	D	96	Total	O	0	0
			96	96		
3	E	146	Total	O	0	0
			146	146		
3	F	113	Total	O	0	0
			113	113		
3	G	106	Total	O	0	0
			106	106		
3	H	126	Total	O	0	0
			126	126		
3	I	131	Total	O	0	0
			131	131		
3	J	112	Total	O	0	0
			112	112		



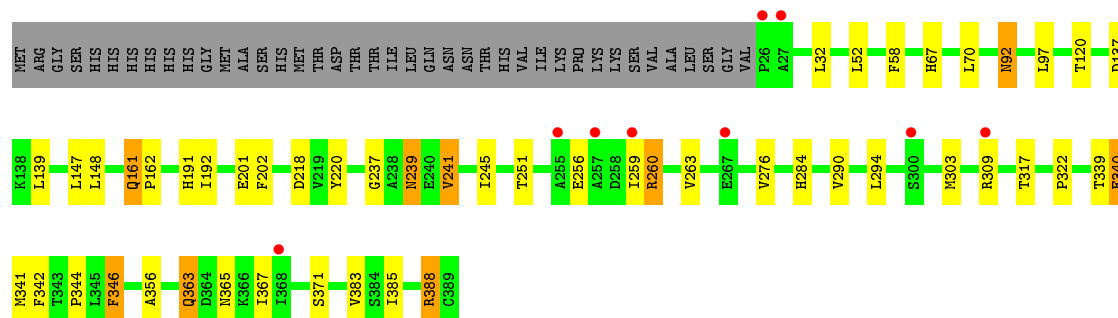
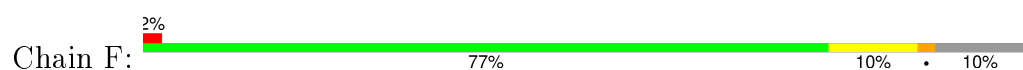
- Molecule 1: 2-methylcitrate synthase



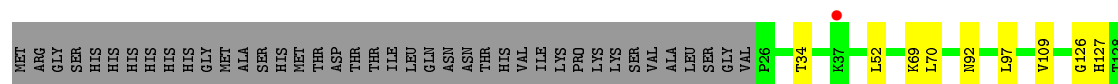
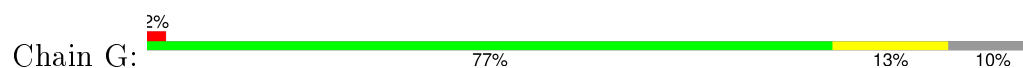
- Molecule 1: 2-methylcitrate synthase



- Molecule 1: 2-methylcitrate synthase



- Molecule 1: 2-methylcitrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.07Å 118.16Å 120.66Å 60.84° 67.77° 81.92°	Depositor
Resolution (Å)	50.00 – 2.41 49.51 – 2.41	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.41) 77.4 (49.51-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.09 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.218 , 0.282 0.220 , 0.282	Depositor DCC
R_{free} test set	7252 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 144957 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29229	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL

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	0.46	0/2876	0.58	0/3907
1	B	0.45	0/2867	0.57	0/3894
1	C	0.39	0/2836	0.55	0/3852
1	D	0.39	0/2829	0.55	0/3840
1	E	0.43	0/2881	0.59	0/3912
1	F	0.44	0/2884	0.57	0/3919
1	G	0.44	0/2869	0.58	0/3898
1	H	0.44	0/2868	0.58	0/3895
1	I	0.43	0/2866	0.58	0/3892
1	J	0.43	0/2881	0.58	0/3907
All	All	0.43	0/28657	0.57	0/38916

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	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	365	ASN	Peptide

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	2808	0	2703	24	0
1	B	2799	0	2679	41	0
1	C	2769	0	2653	22	0
1	D	2764	0	2653	29	0
1	E	2813	0	2726	32	0
1	F	2816	0	2713	27	0
1	G	2801	0	2696	23	0
1	H	2801	0	2705	21	0
1	I	2799	0	2701	27	0
1	J	2815	0	2745	22	0
2	A	6	0	8	0	0
2	B	6	0	8	1	0
2	C	6	0	8	1	0
2	E	12	0	16	1	0
2	F	12	0	16	0	0
2	G	6	0	8	0	0
2	H	6	0	8	1	0
2	I	6	0	8	2	0
2	J	6	0	8	0	0
3	A	145	0	0	1	0
3	B	119	0	0	1	0
3	C	84	0	0	2	0
3	D	96	0	0	0	0
3	E	146	0	0	0	0
3	F	113	0	0	1	0
3	G	106	0	0	1	0
3	H	126	0	0	4	0
3	I	131	0	0	1	0
3	J	112	0	0	2	0
All	All	29229	0	27062	251	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 251 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:E:361:GLN:HE21	1:E:365:ASN:HB2	1.29	0.95
1:F:58:PHE:H	1:F:191:HIS:HD2	1.22	0.87
1:C:207:PHE:HE2	1:D:207:PHE:HE2	1.22	0.86
1:A:230:LEU:O	1:A:236:GLY:HA3	1.76	0.85
1:E:361:GLN:HE21	1:E:365:ASN:CB	1.92	0.81

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	362/404 (90%)	350 (97%)	10 (3%)	2 (1%)	30	41
1	B	362/404 (90%)	351 (97%)	11 (3%)	0	100	100
1	C	356/404 (88%)	349 (98%)	7 (2%)	0	100	100
1	D	354/404 (88%)	346 (98%)	7 (2%)	1 (0%)	46	62
1	E	362/404 (90%)	346 (96%)	14 (4%)	2 (1%)	30	41
1	F	362/404 (90%)	355 (98%)	6 (2%)	1 (0%)	46	62
1	G	362/404 (90%)	348 (96%)	14 (4%)	0	100	100
1	H	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	46	62
1	I	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	46	62
1	J	358/404 (89%)	349 (98%)	9 (2%)	0	100	100
All	All	3598/4040 (89%)	3492 (97%)	98 (3%)	8 (0%)	52	69

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ILE
1	A	369	ARG
1	E	370	PRO

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Mol	Chain	Res	Type
1	I	238	ALA
1	F	365	ASN

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	289/339 (85%)	271 (94%)	18 (6%)	23	35
1	B	285/339 (84%)	264 (93%)	21 (7%)	17	26
1	C	284/339 (84%)	264 (93%)	20 (7%)	19	29
1	D	284/339 (84%)	258 (91%)	26 (9%)	11	16
1	E	292/339 (86%)	273 (94%)	19 (6%)	21	32
1	F	292/339 (86%)	268 (92%)	24 (8%)	14	21
1	G	287/339 (85%)	265 (92%)	22 (8%)	16	24
1	H	290/339 (86%)	267 (92%)	23 (8%)	15	23
1	I	290/339 (86%)	261 (90%)	29 (10%)	9	13
1	J	296/339 (87%)	275 (93%)	21 (7%)	18	28
All	All	2889/3390 (85%)	2666 (92%)	223 (8%)	16	24

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	346	PHE
1	F	346	PHE
1	J	70	LEU
1	E	388	ARG
1	F	239	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	246	GLN

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Mol	Chain	Res	Type
1	F	247	GLN
1	J	239	ASN
1	E	285	GLN
1	F	161	GLN

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 ⓘ

11 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	GOL	A	409	-	5,5,5	0.33	0	5,5,5	0.23	0
2	GOL	B	410	-	5,5,5	0.23	0	5,5,5	0.44	0
2	GOL	C	401	-	5,5,5	0.36	0	5,5,5	0.37	0
2	GOL	E	402	-	5,5,5	0.32	0	5,5,5	0.15	0
2	GOL	E	408	-	5,5,5	0.31	0	5,5,5	0.32	0
2	GOL	F	407	-	5,5,5	0.31	0	5,5,5	0.42	0
2	GOL	F	411	-	5,5,5	0.31	0	5,5,5	0.67	0
2	GOL	G	403	-	5,5,5	0.40	0	5,5,5	0.39	0
2	GOL	H	404	-	5,5,5	0.27	0	5,5,5	0.28	0
2	GOL	I	405	-	5,5,5	0.36	0	5,5,5	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	J	406	-	5,5,5	0.32	0	5,5,5	0.35	0

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	GOL	A	409	-	-	0/4/4/4	0/0/0/0
2	GOL	B	410	-	-	0/4/4/4	0/0/0/0
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
2	GOL	E	402	-	-	0/4/4/4	0/0/0/0
2	GOL	E	408	-	-	0/4/4/4	0/0/0/0
2	GOL	F	407	-	-	0/4/4/4	0/0/0/0
2	GOL	F	411	-	-	0/4/4/4	0/0/0/0
2	GOL	G	403	-	-	0/4/4/4	0/0/0/0
2	GOL	H	404	-	-	0/4/4/4	0/0/0/0
2	GOL	I	405	-	-	0/4/4/4	0/0/0/0
2	GOL	J	406	-	-	0/4/4/4	0/0/0/0

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.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	410	GOL	1	0
2	C	401	GOL	1	0
2	E	408	GOL	1	0
2	H	404	GOL	1	0
2	I	405	GOL	2	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	364/404 (90%)	-0.20	7 (1%) 70 69	22, 36, 53, 63	1 (0%)
1	B	364/404 (90%)	-0.13	1 (0%) 94 94	23, 36, 63, 70	1 (0%)
1	C	360/404 (89%)	0.17	23 (6%) 23 22	27, 47, 72, 77	1 (0%)
1	D	358/404 (88%)	0.19	19 (5%) 30 29	25, 46, 74, 84	1 (0%)
1	E	364/404 (90%)	-0.26	4 (1%) 82 82	24, 37, 58, 68	1 (0%)
1	F	364/404 (90%)	-0.09	9 (2%) 61 60	24, 39, 57, 66	1 (0%)
1	G	364/404 (90%)	0.02	9 (2%) 61 60	23, 37, 66, 75	2 (0%)
1	H	362/404 (89%)	-0.23	3 (0%) 87 87	24, 36, 54, 63	1 (0%)
1	I	362/404 (89%)	-0.16	5 (1%) 78 77	23, 37, 57, 64	1 (0%)
1	J	362/404 (89%)	0.10	19 (5%) 31 30	23, 39, 70, 80	1 (0%)
All	All	3624/4040 (89%)	-0.06	99 (2%) 58 57	22, 39, 66, 84	11 (0%)

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ILE	8.5
1	G	370	PRO	7.0
1	E	370	PRO	5.0
1	J	255	ALA	5.0
1	D	267	GLU	4.9

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	F	411	6/6	0.77	0.20	9.35	53,55,56,56	0
2	GOL	B	410	6/6	0.79	0.26	5.56	57,59,60,60	0
2	GOL	G	403	6/6	0.82	0.24	4.72	56,58,60,60	0
2	GOL	E	402	6/6	0.81	0.18	4.06	59,61,62,62	0
2	GOL	J	406	6/6	0.86	0.21	3.10	61,61,62,63	0
2	GOL	H	404	6/6	0.85	0.19	3.03	49,49,50,52	0
2	GOL	A	409	6/6	0.92	0.18	2.02	54,55,55,56	0
2	GOL	C	401	6/6	0.81	0.23	1.69	64,66,67,68	0
2	GOL	I	405	6/6	0.85	0.19	1.61	53,56,57,57	0
2	GOL	F	407	6/6	0.85	0.20	0.95	63,64,64,64	0
2	GOL	E	408	6/6	0.90	0.19	-0.16	65,66,66,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.