



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:08 AM GMT

PDB ID : 3HWK  
Title : Crystal structure of methylcitrate synthase from Mycobacterium tuberculosis  
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)  
Deposited on : 2009-06-17  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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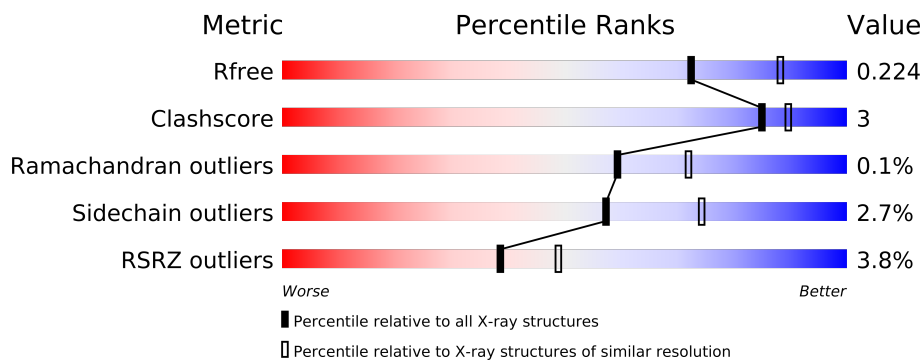
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	414	
1	B	414	
1	C	414	
1	D	414	
1	E	414	
1	F	414	
1	G	414	
1	H	414	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SIN	A	404	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SIN	C	408	-	X
2	SIN	F	412	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23319 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Methylocitrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	2	0
			2826	1780	509	517	20			
1	B	364	Total	C	N	O	S	0	2	0
			2766	1749	487	509	21			
1	C	364	Total	C	N	O	S	0	0	0
			2758	1742	492	504	20			
1	D	365	Total	C	N	O	S	0	1	0
			2795	1764	501	509	21			
1	E	367	Total	C	N	O	S	0	1	0
			2795	1763	499	513	20			
1	F	365	Total	C	N	O	S	0	1	0
			2779	1757	496	506	20			
1	G	364	Total	C	N	O	S	0	0	0
			2770	1749	493	508	20			
1	H	365	Total	C	N	O	S	0	0	0
			2742	1732	492	498	20			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP O08395
A	-19	ALA	-	EXPRESSION TAG	UNP O08395
A	-18	HIS	-	EXPRESSION TAG	UNP O08395
A	-17	HIS	-	EXPRESSION TAG	UNP O08395
A	-16	HIS	-	EXPRESSION TAG	UNP O08395
A	-15	HIS	-	EXPRESSION TAG	UNP O08395
A	-14	HIS	-	EXPRESSION TAG	UNP O08395
A	-13	HIS	-	EXPRESSION TAG	UNP O08395
A	-12	MET	-	EXPRESSION TAG	UNP O08395
A	-11	GLY	-	EXPRESSION TAG	UNP O08395
A	-10	THR	-	EXPRESSION TAG	UNP O08395
A	-9	LEU	-	EXPRESSION TAG	UNP O08395
A	-8	GLU	-	EXPRESSION TAG	UNP O08395

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	EXPRESSION TAG	UNP O08395
A	-6	GLN	-	EXPRESSION TAG	UNP O08395
A	-5	THR	-	EXPRESSION TAG	UNP O08395
A	-4	GLN	-	EXPRESSION TAG	UNP O08395
A	-3	GLY	-	EXPRESSION TAG	UNP O08395
A	-2	PRO	-	EXPRESSION TAG	UNP O08395
A	-1	GLY	-	EXPRESSION TAG	UNP O08395
A	0	SER	-	EXPRESSION TAG	UNP O08395
B	-20	MET	-	EXPRESSION TAG	UNP O08395
B	-19	ALA	-	EXPRESSION TAG	UNP O08395
B	-18	HIS	-	EXPRESSION TAG	UNP O08395
B	-17	HIS	-	EXPRESSION TAG	UNP O08395
B	-16	HIS	-	EXPRESSION TAG	UNP O08395
B	-15	HIS	-	EXPRESSION TAG	UNP O08395
B	-14	HIS	-	EXPRESSION TAG	UNP O08395
B	-13	HIS	-	EXPRESSION TAG	UNP O08395
B	-12	MET	-	EXPRESSION TAG	UNP O08395
B	-11	GLY	-	EXPRESSION TAG	UNP O08395
B	-10	THR	-	EXPRESSION TAG	UNP O08395
B	-9	LEU	-	EXPRESSION TAG	UNP O08395
B	-8	GLU	-	EXPRESSION TAG	UNP O08395
B	-7	ALA	-	EXPRESSION TAG	UNP O08395
B	-6	GLN	-	EXPRESSION TAG	UNP O08395
B	-5	THR	-	EXPRESSION TAG	UNP O08395
B	-4	GLN	-	EXPRESSION TAG	UNP O08395
B	-3	GLY	-	EXPRESSION TAG	UNP O08395
B	-2	PRO	-	EXPRESSION TAG	UNP O08395
B	-1	GLY	-	EXPRESSION TAG	UNP O08395
B	0	SER	-	EXPRESSION TAG	UNP O08395
C	-20	MET	-	EXPRESSION TAG	UNP O08395
C	-19	ALA	-	EXPRESSION TAG	UNP O08395
C	-18	HIS	-	EXPRESSION TAG	UNP O08395
C	-17	HIS	-	EXPRESSION TAG	UNP O08395
C	-16	HIS	-	EXPRESSION TAG	UNP O08395
C	-15	HIS	-	EXPRESSION TAG	UNP O08395
C	-14	HIS	-	EXPRESSION TAG	UNP O08395
C	-13	HIS	-	EXPRESSION TAG	UNP O08395
C	-12	MET	-	EXPRESSION TAG	UNP O08395
C	-11	GLY	-	EXPRESSION TAG	UNP O08395
C	-10	THR	-	EXPRESSION TAG	UNP O08395
C	-9	LEU	-	EXPRESSION TAG	UNP O08395
C	-8	GLU	-	EXPRESSION TAG	UNP O08395

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	ALA	-	EXPRESSION TAG	UNP O08395
C	-6	GLN	-	EXPRESSION TAG	UNP O08395
C	-5	THR	-	EXPRESSION TAG	UNP O08395
C	-4	GLN	-	EXPRESSION TAG	UNP O08395
C	-3	GLY	-	EXPRESSION TAG	UNP O08395
C	-2	PRO	-	EXPRESSION TAG	UNP O08395
C	-1	GLY	-	EXPRESSION TAG	UNP O08395
C	0	SER	-	EXPRESSION TAG	UNP O08395
D	-20	MET	-	EXPRESSION TAG	UNP O08395
D	-19	ALA	-	EXPRESSION TAG	UNP O08395
D	-18	HIS	-	EXPRESSION TAG	UNP O08395
D	-17	HIS	-	EXPRESSION TAG	UNP O08395
D	-16	HIS	-	EXPRESSION TAG	UNP O08395
D	-15	HIS	-	EXPRESSION TAG	UNP O08395
D	-14	HIS	-	EXPRESSION TAG	UNP O08395
D	-13	HIS	-	EXPRESSION TAG	UNP O08395
D	-12	MET	-	EXPRESSION TAG	UNP O08395
D	-11	GLY	-	EXPRESSION TAG	UNP O08395
D	-10	THR	-	EXPRESSION TAG	UNP O08395
D	-9	LEU	-	EXPRESSION TAG	UNP O08395
D	-8	GLU	-	EXPRESSION TAG	UNP O08395
D	-7	ALA	-	EXPRESSION TAG	UNP O08395
D	-6	GLN	-	EXPRESSION TAG	UNP O08395
D	-5	THR	-	EXPRESSION TAG	UNP O08395
D	-4	GLN	-	EXPRESSION TAG	UNP O08395
D	-3	GLY	-	EXPRESSION TAG	UNP O08395
D	-2	PRO	-	EXPRESSION TAG	UNP O08395
D	-1	GLY	-	EXPRESSION TAG	UNP O08395
D	0	SER	-	EXPRESSION TAG	UNP O08395
E	-20	MET	-	EXPRESSION TAG	UNP O08395
E	-19	ALA	-	EXPRESSION TAG	UNP O08395
E	-18	HIS	-	EXPRESSION TAG	UNP O08395
E	-17	HIS	-	EXPRESSION TAG	UNP O08395
E	-16	HIS	-	EXPRESSION TAG	UNP O08395
E	-15	HIS	-	EXPRESSION TAG	UNP O08395
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E	-12	MET	-	EXPRESSION TAG	UNP O08395
E	-11	GLY	-	EXPRESSION TAG	UNP O08395
E	-10	THR	-	EXPRESSION TAG	UNP O08395
E	-9	LEU	-	EXPRESSION TAG	UNP O08395
E	-8	GLU	-	EXPRESSION TAG	UNP O08395

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-7	ALA	-	EXPRESSION TAG	UNP O08395
E	-6	GLN	-	EXPRESSION TAG	UNP O08395
E	-5	THR	-	EXPRESSION TAG	UNP O08395
E	-4	GLN	-	EXPRESSION TAG	UNP O08395
E	-3	GLY	-	EXPRESSION TAG	UNP O08395
E	-2	PRO	-	EXPRESSION TAG	UNP O08395
E	-1	GLY	-	EXPRESSION TAG	UNP O08395
E	0	SER	-	EXPRESSION TAG	UNP O08395
F	-20	MET	-	EXPRESSION TAG	UNP O08395
F	-19	ALA	-	EXPRESSION TAG	UNP O08395
F	-18	HIS	-	EXPRESSION TAG	UNP O08395
F	-17	HIS	-	EXPRESSION TAG	UNP O08395
F	-16	HIS	-	EXPRESSION TAG	UNP O08395
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F	-8	GLU	-	EXPRESSION TAG	UNP O08395
F	-7	ALA	-	EXPRESSION TAG	UNP O08395
F	-6	GLN	-	EXPRESSION TAG	UNP O08395
F	-5	THR	-	EXPRESSION TAG	UNP O08395
F	-4	GLN	-	EXPRESSION TAG	UNP O08395
F	-3	GLY	-	EXPRESSION TAG	UNP O08395
F	-2	PRO	-	EXPRESSION TAG	UNP O08395
F	-1	GLY	-	EXPRESSION TAG	UNP O08395
F	0	SER	-	EXPRESSION TAG	UNP O08395
G	-20	MET	-	EXPRESSION TAG	UNP O08395
G	-19	ALA	-	EXPRESSION TAG	UNP O08395
G	-18	HIS	-	EXPRESSION TAG	UNP O08395
G	-17	HIS	-	EXPRESSION TAG	UNP O08395
G	-16	HIS	-	EXPRESSION TAG	UNP O08395
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G	-12	MET	-	EXPRESSION TAG	UNP O08395
G	-11	GLY	-	EXPRESSION TAG	UNP O08395
G	-10	THR	-	EXPRESSION TAG	UNP O08395
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G	-8	GLU	-	EXPRESSION TAG	UNP O08395

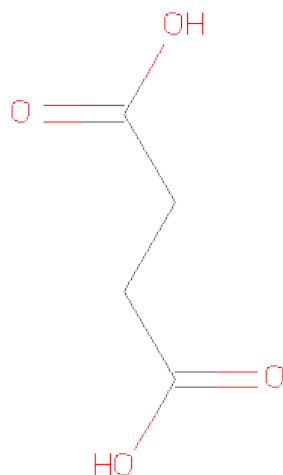
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-7	ALA	-	EXPRESSION TAG	UNP O08395
G	-6	GLN	-	EXPRESSION TAG	UNP O08395
G	-5	THR	-	EXPRESSION TAG	UNP O08395
G	-4	GLN	-	EXPRESSION TAG	UNP O08395
G	-3	GLY	-	EXPRESSION TAG	UNP O08395
G	-2	PRO	-	EXPRESSION TAG	UNP O08395
G	-1	GLY	-	EXPRESSION TAG	UNP O08395
G	0	SER	-	EXPRESSION TAG	UNP O08395
H	-20	MET	-	EXPRESSION TAG	UNP O08395
H	-19	ALA	-	EXPRESSION TAG	UNP O08395
H	-18	HIS	-	EXPRESSION TAG	UNP O08395
H	-17	HIS	-	EXPRESSION TAG	UNP O08395
H	-16	HIS	-	EXPRESSION TAG	UNP O08395
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H	-10	THR	-	EXPRESSION TAG	UNP O08395
H	-9	LEU	-	EXPRESSION TAG	UNP O08395
H	-8	GLU	-	EXPRESSION TAG	UNP O08395
H	-7	ALA	-	EXPRESSION TAG	UNP O08395
H	-6	GLN	-	EXPRESSION TAG	UNP O08395
H	-5	THR	-	EXPRESSION TAG	UNP O08395
H	-4	GLN	-	EXPRESSION TAG	UNP O08395
H	-3	GLY	-	EXPRESSION TAG	UNP O08395
H	-2	PRO	-	EXPRESSION TAG	UNP O08395
H	-1	GLY	-	EXPRESSION TAG	UNP O08395
H	0	SER	-	EXPRESSION TAG	UNP O08395

- Molecule 2 is SUCCINIC ACID (three-letter code: SIN) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	4	4		
2	A	1	Total	C	O	0	0
			8	4	4		
2	A	1	Total	C	O	0	0
			8	4	4		
2	A	1	Total	C	O	0	0
			8	4	4		
2	B	1	Total	C	O	0	0
			8	4	4		
2	B	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		
2	D	1	Total	C	O	0	0
			8	4	4		
2	D	1	Total	C	O	0	0
			8	4	4		
2	E	1	Total	C	O	0	0
			8	4	4		
2	F	1	Total	C	O	0	0
			8	4	4		
2	F	1	Total	C	O	0	0
			8	4	4		
2	G	1	Total	C	O	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	C	O	0	0
			8	4	4		
2	H	1	Total	C	O	0	0
			8	4	4		

- Molecule 3 is water.

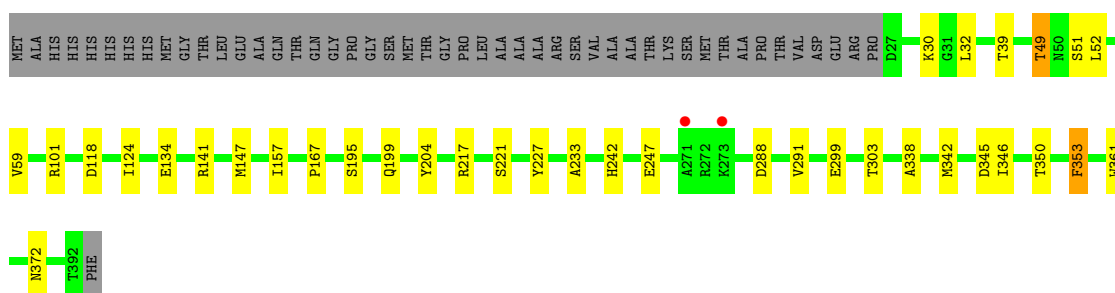
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	172	Total	O		0	0
			172	172			
3	B	126	Total	O		0	0
			126	126			
3	C	96	Total	O		0	0
			96	96			
3	D	156	Total	O		0	0
			156	156			
3	E	89	Total	O		0	0
			89	89			
3	F	123	Total	O		0	0
			123	123			
3	G	127	Total	O		0	0
			127	127			
3	H	71	Total	O		0	0
			71	71			

### 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.

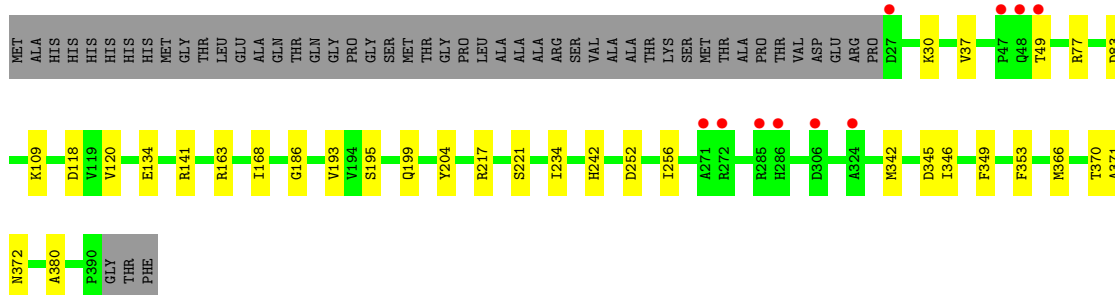
- Molecule 1: Methylcitrate synthase

Chain A:



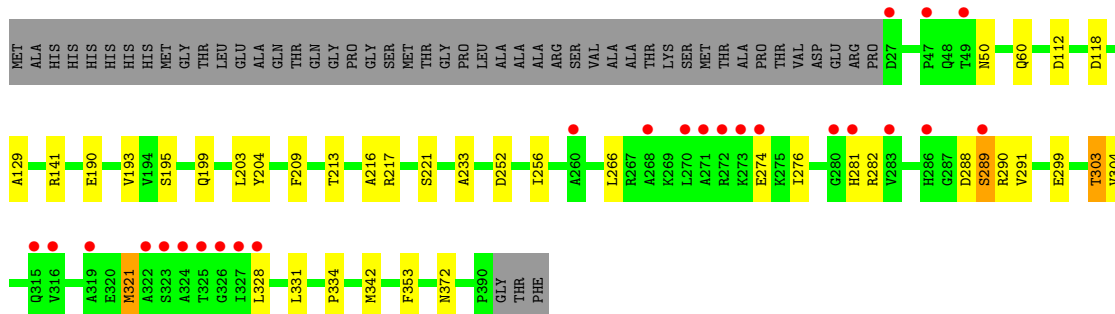
- Molecule 1: Methylcitrate synthase

Chain B:



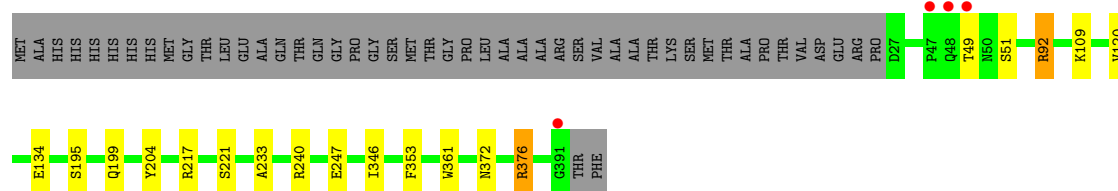
- Molecule 1: Methylcitrate synthase

Chain C:



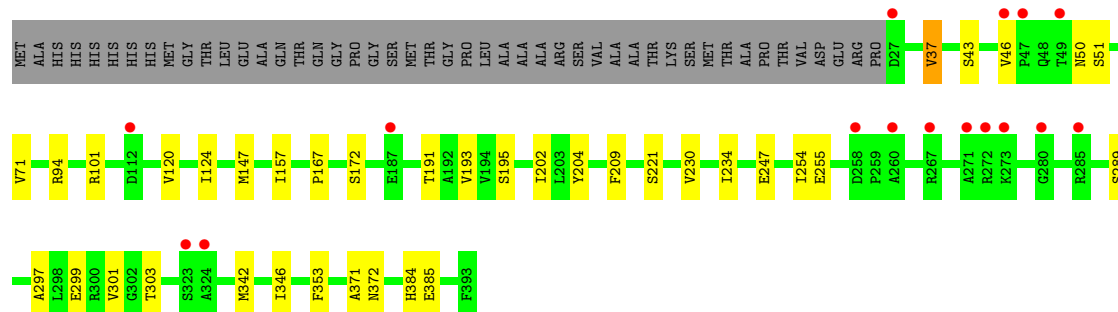
- Molecule 1: Methylcitrate synthase

Chain D:



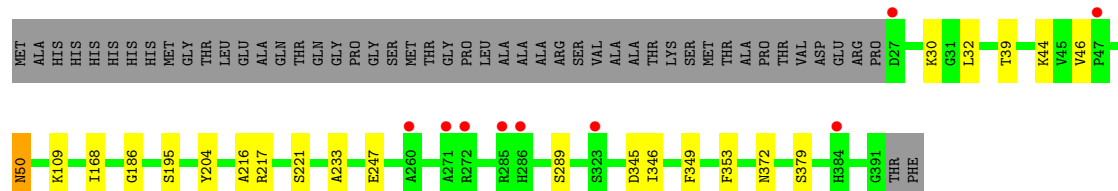
- Molecule 1: Methylcitrate synthase

Chain E:



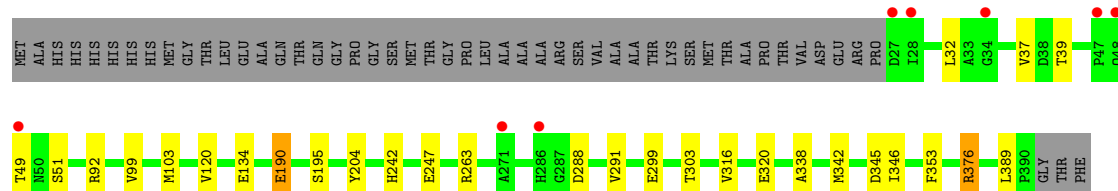
- Molecule 1: Methylcitrate synthase

Chain F:



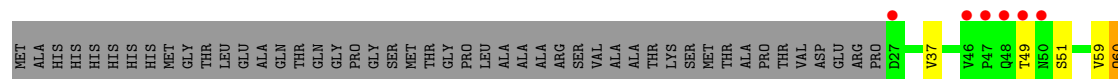
- Molecule 1: Methylcitrate synthase

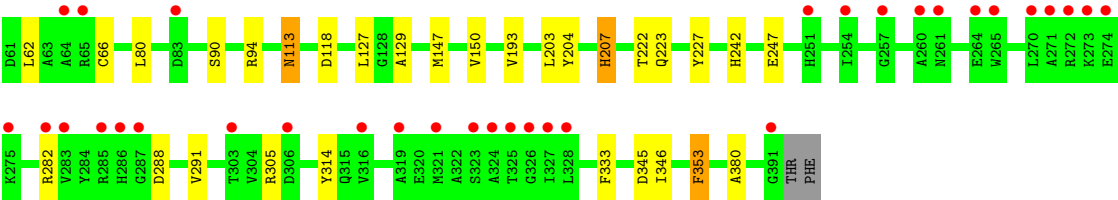
Chain G:



- Molecule 1: Methylcitrate synthase

Chain H:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.58Å 179.68Å 193.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.30 19.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.91-2.30) 99.8 (19.91-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.04 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.186 , 0.228 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	8613 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 22.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 172139 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	23319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.56	0/2886	0.63	1/3915 (0.0%)
1	B	0.55	0/2829	0.60	1/3846 (0.0%)
1	C	0.55	0/2818	0.62	0/3831
1	D	0.58	0/2858	0.64	1/3878 (0.0%)
1	E	0.52	0/2859	0.61	0/3885
1	F	0.52	0/2842	0.60	1/3860 (0.0%)
1	G	0.54	0/2830	0.60	0/3845
1	H	0.53	0/2802	0.58	0/3810
All	All	0.54	0/22724	0.61	4/30870 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	D	217	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	217	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	217	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2826	0	2813	26	0
1	B	2766	0	2720	18	0
1	C	2758	0	2714	20	0
1	D	2795	0	2778	10	0
1	E	2795	0	2743	21	0
1	F	2779	0	2756	11	0
1	G	2770	0	2733	15	0
1	H	2742	0	2685	22	0
2	A	32	0	16	2	0
2	B	16	0	8	0	0
2	C	16	0	8	2	0
2	D	16	0	8	0	0
2	E	8	0	4	0	0
2	F	16	0	8	0	0
2	G	16	0	8	0	0
2	H	8	0	4	0	0
3	A	172	0	0	0	0
3	B	126	0	0	1	0
3	C	96	0	0	1	0
3	D	156	0	0	0	0
3	E	89	0	0	0	0
3	F	123	0	0	1	0
3	G	127	0	0	2	0
3	H	71	0	0	0	0
All	All	23319	0	22006	122	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (122) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:THR:HG22	1:A:51:SER:HB2	1.42	0.98
1:A:141:ARG:HB3	2:A:404:SIN:H31	1.46	0.95
1:C:141:ARG:HB3	2:C:408:SIN:H22	1.53	0.91
1:A:49:THR:CG2	1:A:51:SER:HB2	2.05	0.86
1:C:282:ARG:HG2	1:D:376:ARG:HG3	1.63	0.80
1:A:141:ARG:HB3	2:A:404:SIN:C3	2.18	0.72
1:C:266:LEU:HD21	1:C:321:MET:HG2	1.71	0.71
1:C:141:ARG:CB	2:C:408:SIN:H22	2.23	0.67
1:C:288:ASP:HB3	1:C:291:VAL:HG23	1.76	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:147:MET:HE1	1:H:227:TYR:HA	1.79	0.65
1:F:50:ASN:O	1:F:289:SER:HB3	1.99	0.62
1:E:46:VAL:HG22	1:E:51:SER:O	2.00	0.62
3:C:763:HOH:O	1:D:240:ARG:HD3	2.00	0.62
1:E:147:MET:HE2	1:E:230:VAL:HG11	1.82	0.61
1:F:168:ILE:HD13	1:F:186:GLY:HA2	1.83	0.61
1:G:39:THR:HG22	1:H:380:ALA:HB3	1.83	0.60
1:E:124:ILE:HD12	1:E:147:MET:HE3	1.84	0.59
1:C:331:LEU:O	1:C:334:PRO:HD2	2.03	0.59
1:A:299:GLU:O	1:A:303:THR:HG23	2.03	0.58
1:A:195:SER:O	1:A:199:GLN:HG3	2.04	0.58
1:A:247:GLU:HG3	1:A:346:ILE:HG22	1.85	0.58
1:H:247:GLU:HG3	1:H:346:ILE:HG22	1.85	0.58
1:H:288:ASP:HB3	1:H:291:VAL:HG23	1.84	0.58
1:E:157:ILE:HG12	1:E:167:PRO:HB3	1.85	0.57
1:G:299:GLU:O	1:G:303:THR:HG23	2.03	0.57
1:G:288:ASP:HB3	1:G:291:VAL:HG23	1.86	0.57
1:B:168:ILE:HD13	1:B:186:GLY:HA2	1.86	0.57
1:F:247:GLU:HG3	1:F:346:ILE:HG22	1.88	0.56
1:C:195:SER:O	1:C:199:GLN:HG3	2.06	0.56
1:E:384[B]:HIS:HD2	1:E:385:GLU:O	1.89	0.55
1:B:366:MET:O	1:B:370:THR:HG23	2.07	0.54
1:G:49:THR:HG23	1:G:51:SER:HB2	1.89	0.54
1:G:338:ALA:O	1:G:342:MET:HG3	2.08	0.54
1:C:274:GLU:O	1:C:276:ILE:HD12	2.07	0.54
1:B:109:LYS:HE3	3:G:856:HOH:O	2.07	0.53
1:A:134:GLU:OE1	1:B:118:ASP:OD2	2.25	0.53
1:E:247:GLU:HG3	1:E:346:ILE:HG22	1.91	0.53
1:C:209:PHE:O	1:D:376:ARG:HD3	2.09	0.53
1:D:247:GLU:HG3	1:D:346:ILE:HG22	1.90	0.53
1:E:37:VAL:CG2	1:F:32:LEU:HD21	2.38	0.53
1:C:50:ASN:O	1:C:289:SER:HB3	2.09	0.52
1:C:203:LEU:HD22	1:C:290:ARG:HB3	1.91	0.52
1:A:221:SER:HA	1:A:372:ASN:OD1	2.09	0.52
1:G:376:ARG:HG3	1:H:282:ARG:HG2	1.92	0.52
1:A:124:ILE:HG23	1:A:147:MET:CE	2.39	0.52
1:F:44:LYS:HE2	1:F:46:VAL:HG22	1.91	0.52
1:C:129:ALA:O	1:E:101:ARG:HD2	2.10	0.51
1:E:147:MET:CE	1:E:230:VAL:HG11	2.40	0.51
1:E:50:ASN:O	1:E:289:SER:HB3	2.11	0.51
1:E:71:VAL:HG21	1:E:202:ILE:HG12	1.92	0.51
1:H:314:TYR:CE2	1:H:333:PHE:CD2	2.99	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:32:LEU:HD21	1:B:37:VAL:HG22	1.93	0.50
1:H:59:VAL:CG1	1:H:203:LEU:HD23	2.41	0.50
1:C:299:GLU:O	1:C:303:THR:HG23	2.10	0.50
1:A:32:LEU:CD2	1:B:37:VAL:HG22	2.41	0.50
1:H:90:SER:O	1:H:94:ARG:HG3	2.11	0.50
1:B:193:VAL:HG13	1:B:342:MET:HG2	1.94	0.50
1:E:193:VAL:HG13	1:E:342:MET:HG2	1.94	0.49
1:B:252:ASP:O	1:B:256:ILE:HG13	2.13	0.49
1:A:124:ILE:HG23	1:A:147:MET:HE3	1.94	0.49
1:E:297:ALA:O	1:E:301:VAL:HG23	2.13	0.49
1:D:221:SER:HA	1:D:372:ASN:OD1	2.13	0.48
1:E:299:GLU:O	1:E:303:THR:HG23	2.13	0.48
1:H:49:THR:HG23	1:H:51:SER:HB3	1.95	0.48
1:E:221:SER:HA	1:E:372:ASN:OD1	2.13	0.48
1:C:213:THR:O	1:C:217:ARG:HG3	2.14	0.48
1:H:193:VAL:HG21	1:H:305:ARG:HH21	1.77	0.48
1:A:288:ASP:HB3	1:A:291:VAL:HG23	1.95	0.48
1:A:32:LEU:HD21	1:B:37:VAL:CG2	2.44	0.47
1:A:49:THR:HG22	1:A:51:SER:CB	2.30	0.47
1:A:118:ASP:OD2	1:B:134:GLU:OE1	2.31	0.47
1:D:195:SER:O	1:D:199:GLN:HG3	2.15	0.47
1:B:346:ILE:HA	1:B:349:PHE:CE1	2.50	0.47
1:E:37:VAL:HG23	1:F:32:LEU:HD21	1.97	0.47
1:H:113:ASN:OD1	1:H:113:ASN:N	2.48	0.47
1:A:338:ALA:O	1:A:342:MET:HG3	2.15	0.46
1:A:233:ALA:HB1	1:A:361:TRP:CE2	2.50	0.46
1:C:288:ASP:HB3	1:C:291:VAL:CG2	2.44	0.45
1:D:109:LYS:HE3	3:F:816:HOH:O	2.15	0.45
1:C:193:VAL:HG13	1:C:342:MET:HG2	1.97	0.45
1:H:62:LEU:O	1:H:66:CYS:HB2	2.16	0.45
1:H:59:VAL:HG12	1:H:203:LEU:HD23	1.99	0.45
1:B:221:SER:HA	1:B:372:ASN:OD1	2.16	0.45
1:A:39:THR:HA	1:B:380:ALA:O	2.18	0.44
1:B:120:VAL:HG12	1:B:234:ILE:HD13	2.00	0.44
1:B:163:ARG:NH1	3:B:692:HOH:O	2.48	0.44
1:B:195:SER:O	1:B:199:GLN:HG3	2.17	0.43
1:E:50:ASN:O	1:E:289:SER:CB	2.66	0.43
1:G:92:ARG:NH1	3:G:439:HOH:O	2.51	0.43
1:A:30:LYS:NZ	1:B:371:ALA:O	2.50	0.43
1:C:118:ASP:OD2	1:D:134:GLU:OE1	2.36	0.43
1:H:353:PHE:HD1	1:H:353:PHE:O	2.02	0.43
1:G:190:GLU:HG3	1:G:190:GLU:H	1.58	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:233:ALA:HB1	1:D:361:TRP:CE2	2.53	0.43
1:E:209:PHE:CE2	1:F:379:SER:HB3	2.53	0.43
1:D:92:ARG:HA	1:D:92:ARG:HD3	1.77	0.43
1:H:127:LEU:HD11	1:H:150:VAL:HG11	2.01	0.43
1:F:221:SER:HA	1:F:372:ASN:OD1	2.19	0.43
1:H:288:ASP:HB3	1:H:291:VAL:CG2	2.48	0.43
1:G:99:VAL:HB	1:G:103:MET:HB3	2.01	0.42
1:G:389:LEU:HD12	1:H:80:LEU:HD11	2.01	0.42
1:A:147:MET:HE1	1:A:227:TYR:HA	2.01	0.42
1:G:134:GLU:OE1	1:H:118:ASP:OD2	2.37	0.42
1:E:371:ALA:O	1:F:30:LYS:NZ	2.52	0.42
1:H:222:THR:O	1:H:223:GLN:HB2	2.20	0.42
1:F:216:ALA:HB2	1:F:233:ALA:HB2	2.01	0.42
1:A:157:ILE:HG12	1:A:167:PRO:HB3	2.02	0.42
1:B:77:ARG:HD3	1:B:141:ARG:NH1	2.35	0.42
1:C:221:SER:HA	1:C:372:ASN:OD1	2.20	0.42
1:A:350:THR:O	1:A:353:PHE:HB3	2.20	0.42
1:F:346:ILE:HA	1:F:349:PHE:CE1	2.56	0.41
1:H:60:GLN:HG3	1:H:60:GLN:H	1.55	0.41
1:E:120:VAL:HG12	1:E:234:ILE:HD13	2.02	0.41
1:C:216:ALA:HB2	1:C:233:ALA:HB2	2.03	0.41
1:G:316:VAL:O	1:G:320:GLU:HG2	2.20	0.41
1:G:247:GLU:HG3	1:G:346:ILE:HG22	2.03	0.41
1:E:94:ARG:HD3	1:E:172:SER:O	2.20	0.41
1:A:52:LEU:HG	1:A:59:VAL:HG21	2.03	0.41
1:C:252:ASP:O	1:C:256:ILE:HD12	2.21	0.40
1:G:32:LEU:HD21	1:H:37:VAL:HG22	2.03	0.40
1:G:288:ASP:HB3	1:G:291:VAL:CG2	2.50	0.40
1:A:101:ARG:HD2	1:H:129:ALA:O	2.20	0.40

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	366/414 (88%)	358 (98%)	8 (2%)	0	100	100
1	B	364/414 (88%)	354 (97%)	10 (3%)	0	100	100
1	C	362/414 (87%)	353 (98%)	9 (2%)	0	100	100
1	D	364/414 (88%)	354 (97%)	10 (3%)	0	100	100
1	E	366/414 (88%)	355 (97%)	11 (3%)	0	100	100
1	F	364/414 (88%)	355 (98%)	8 (2%)	1 (0%)	50	60
1	G	362/414 (87%)	353 (98%)	9 (2%)	0	100	100
1	H	363/414 (88%)	344 (95%)	18 (5%)	1 (0%)	50	60
All	All	2911/3312 (88%)	2826 (97%)	83 (3%)	2 (0%)	59	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	207	HIS
1	F	50	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	292/328 (89%)	287 (98%)	5 (2%)	73	87
1	B	282/328 (86%)	275 (98%)	7 (2%)	60	77
1	C	280/328 (85%)	269 (96%)	11 (4%)	43	57
1	D	287/328 (88%)	280 (98%)	7 (2%)	61	79
1	E	284/328 (87%)	276 (97%)	8 (3%)	56	73
1	F	284/328 (87%)	278 (98%)	6 (2%)	66	83
1	G	283/328 (86%)	273 (96%)	10 (4%)	48	63
1	H	274/328 (84%)	267 (97%)	7 (3%)	59	76
All	All	2266/2624 (86%)	2205 (97%)	61 (3%)	57	74

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	THR
1	A	204	TYR
1	A	242	HIS
1	A	345	ASP
1	A	353	PHE
1	B	30	LYS
1	B	49	THR
1	B	83	ASP
1	B	204	TYR
1	B	242	HIS
1	B	345	ASP
1	B	353	PHE
1	C	60	GLN
1	C	112	ASP
1	C	190	GLU
1	C	204	TYR
1	C	281	HIS
1	C	289	SER
1	C	303	THR
1	C	304	VAL
1	C	321	MET
1	C	328	LEU
1	C	353	PHE
1	D	49	THR
1	D	51	SER
1	D	92	ARG
1	D	120	VAL
1	D	204	TYR
1	D	353	PHE
1	D	376	ARG
1	E	37	VAL
1	E	43	SER
1	E	191	THR
1	E	195	SER
1	E	204	TYR
1	E	254	ILE
1	E	255	GLU
1	E	353	PHE
1	F	39	THR
1	F	109	LYS
1	F	195	SER
1	F	204	TYR
1	F	345	ASP

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Mol	Chain	Res	Type
1	F	353	PHE
1	G	37	VAL
1	G	120	VAL
1	G	190	GLU
1	G	195	SER
1	G	204	TYR
1	G	242	HIS
1	G	263	ARG
1	G	345	ASP
1	G	353	PHE
1	G	376	ARG
1	H	60	GLN
1	H	113	ASN
1	H	204	TYR
1	H	207	HIS
1	H	242	HIS
1	H	345	ASP
1	H	353	PHE

Some 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 chains 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 ⓘ

16 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	SIN	A	401	-	7,7,7	1.08	0	8,8,8	1.87	3 (37%)
2	SIN	A	402	-	7,7,7	0.94	0	8,8,8	1.67	2 (25%)
2	SIN	A	403	-	7,7,7	0.97	0	8,8,8	1.46	2 (25%)
2	SIN	A	404	-	7,7,7	0.90	0	8,8,8	1.73	1 (12%)
2	SIN	B	405	-	7,7,7	1.02	0	8,8,8	1.63	2 (25%)
2	SIN	B	406	-	7,7,7	0.98	0	8,8,8	1.56	2 (25%)
2	SIN	C	407	-	7,7,7	1.01	0	8,8,8	1.52	1 (12%)
2	SIN	C	408	-	7,7,7	0.89	0	8,8,8	1.59	2 (25%)
2	SIN	D	409	-	7,7,7	0.82	0	8,8,8	1.60	1 (12%)
2	SIN	D	410	-	7,7,7	0.91	0	8,8,8	1.48	1 (12%)
2	SIN	E	416	-	7,7,7	0.94	0	8,8,8	1.61	2 (25%)
2	SIN	F	411	-	7,7,7	1.02	0	8,8,8	1.42	1 (12%)
2	SIN	F	412	-	7,7,7	0.92	0	8,8,8	1.55	2 (25%)
2	SIN	G	413	-	7,7,7	1.08	0	8,8,8	1.30	1 (12%)
2	SIN	G	414	-	7,7,7	0.99	0	8,8,8	1.58	2 (25%)
2	SIN	H	415	-	7,7,7	0.97	0	8,8,8	1.66	3 (37%)

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	SIN	A	401	-	-	0/5/5/5	0/0/0/0
2	SIN	A	402	-	-	0/5/5/5	0/0/0/0
2	SIN	A	403	-	-	0/5/5/5	0/0/0/0
2	SIN	A	404	-	-	0/5/5/5	0/0/0/0
2	SIN	B	405	-	-	0/5/5/5	0/0/0/0
2	SIN	B	406	-	-	0/5/5/5	0/0/0/0
2	SIN	C	407	-	-	0/5/5/5	0/0/0/0
2	SIN	C	408	-	-	0/5/5/5	0/0/0/0
2	SIN	D	409	-	-	0/5/5/5	0/0/0/0
2	SIN	D	410	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SIN	E	416	-	-	0/5/5/5	0/0/0/0
2	SIN	F	411	-	-	0/5/5/5	0/0/0/0
2	SIN	F	412	-	-	0/5/5/5	0/0/0/0
2	SIN	G	413	-	-	0/5/5/5	0/0/0/0
2	SIN	G	414	-	-	0/5/5/5	0/0/0/0
2	SIN	H	415	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SIN	O4-C4-O3	-3.02	115.62	123.30
2	A	401	SIN	O4-C4-C3	2.77	123.99	114.22
2	A	404	SIN	O2-C1-C2	2.71	123.80	114.22
2	F	412	SIN	O2-C1-O1	-2.70	116.44	123.30
2	B	405	SIN	O2-C1-O1	-2.67	116.50	123.30
2	E	416	SIN	O4-C4-C3	2.61	123.43	114.22
2	C	408	SIN	C3-C2-C1	-2.56	108.79	113.53
2	F	411	SIN	O2-C1-C2	2.45	122.88	114.22
2	D	410	SIN	O2-C1-C2	2.44	122.86	114.22
2	A	401	SIN	O2-C1-O1	-2.41	117.16	123.30
2	D	409	SIN	O4-C4-C3	2.37	122.59	114.22
2	B	405	SIN	O4-C4-C3	2.36	122.56	114.22
2	A	403	SIN	O2-C1-C2	2.31	122.37	114.22
2	C	408	SIN	C2-C3-C4	-2.27	109.32	113.53
2	B	406	SIN	O2-C1-O1	-2.24	117.59	123.30
2	H	415	SIN	O4-C4-C3	2.23	122.09	114.22
2	G	414	SIN	O2-C1-O1	-2.23	117.63	123.30
2	E	416	SIN	O4-C4-O3	-2.20	117.71	123.30
2	A	402	SIN	C3-C2-C1	-2.19	109.47	113.53
2	B	406	SIN	O2-C1-C2	2.16	121.85	114.22
2	C	407	SIN	O4-C4-O3	-2.16	117.81	123.30
2	A	402	SIN	O4-C4-C3	2.12	121.72	114.22
2	H	415	SIN	C3-C2-C1	-2.08	109.67	113.53
2	G	413	SIN	O4-C4-C3	2.08	121.56	114.22
2	G	414	SIN	O4-C4-C3	2.07	121.52	114.22
2	H	415	SIN	O2-C1-O1	-2.04	118.12	123.30
2	F	412	SIN	O4-C4-C3	2.03	121.38	114.22
2	A	403	SIN	O2-C1-O1	-2.02	118.15	123.30

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	366/414 (88%)	-0.40	2 (0%) 88 94	19, 28, 47, 58	0
1	B	364/414 (87%)	-0.27	10 (2%) 52 62	18, 30, 56, 68	0
1	C	364/414 (87%)	0.05	25 (6%) 17 24	19, 32, 66, 71	0
1	D	365/414 (88%)	-0.34	4 (1%) 77 85	17, 27, 46, 57	0
1	E	367/414 (88%)	-0.04	16 (4%) 33 43	21, 36, 62, 74	0
1	F	365/414 (88%)	-0.25	9 (2%) 54 65	19, 30, 55, 69	0
1	G	364/414 (87%)	-0.20	8 (2%) 59 69	20, 31, 56, 62	0
1	H	365/414 (88%)	0.26	39 (10%) 6 10	25, 39, 68, 77	0
All	All	2920/3312 (88%)	-0.15	113 (3%) 38 48	17, 31, 60, 77	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	47	PRO	5.9
1	C	326	GLY	5.7
1	H	260	ALA	5.2
1	H	324	ALA	5.0
1	H	325	THR	5.0
1	E	271	ALA	4.8
1	C	327	ILE	4.8
1	H	271	ALA	4.8
1	E	260	ALA	4.8
1	C	281	HIS	4.7
1	D	47	PRO	4.5
1	C	271	ALA	4.3
1	H	327	ILE	4.3
1	C	268	ALA	4.2
1	H	286	HIS	4.2
1	H	48	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	THR	4.0
1	D	48	GLN	3.9
1	H	254	ILE	3.9
1	H	47	PRO	3.9
1	E	47	PRO	3.8
1	C	325	THR	3.8
1	H	272	ARG	3.7
1	C	286	HIS	3.7
1	B	286	HIS	3.7
1	C	319	ALA	3.6
1	B	48	GLN	3.6
1	H	64	ALA	3.6
1	H	49	THR	3.6
1	H	323	SER	3.6
1	C	322	ALA	3.6
1	E	280	GLY	3.5
1	C	328	LEU	3.4
1	G	49	THR	3.4
1	C	260	ALA	3.4
1	C	280	GLY	3.4
1	H	326	GLY	3.4
1	F	286	HIS	3.4
1	B	47	PRO	3.4
1	E	272	ARG	3.4
1	H	257	GLY	3.4
1	G	286	HIS	3.3
1	H	287	GLY	3.2
1	G	48	GLN	3.2
1	C	270	LEU	3.1
1	C	315	GLN	3.1
1	B	271	ALA	3.1
1	C	273	LYS	3.0
1	H	283	VAL	3.0
1	C	27	ASP	3.0
1	C	283	VAL	3.0
1	E	49	THR	3.0
1	C	324	ALA	2.9
1	D	391	GLY	2.9
1	G	271	ALA	2.9
1	C	274	GLU	2.9
1	C	323	SER	2.9
1	H	391	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	260	ALA	2.8
1	E	46	VAL	2.8
1	B	272	ARG	2.8
1	H	27	ASP	2.8
1	D	49	THR	2.7
1	H	303	THR	2.7
1	B	324	ALA	2.7
1	H	273	LYS	2.7
1	G	27	ASP	2.7
1	F	272	ARG	2.7
1	H	265	TRP	2.6
1	E	323	SER	2.6
1	F	47	PRO	2.6
1	H	83	ASP	2.6
1	H	261	ASN	2.6
1	E	258	ASP	2.6
1	C	47	PRO	2.6
1	H	321	MET	2.6
1	E	27	ASP	2.6
1	C	316	VAL	2.5
1	H	274	GLU	2.5
1	E	285	ARG	2.5
1	E	324	ALA	2.4
1	C	289	SER	2.4
1	H	270	LEU	2.4
1	H	251	HIS	2.4
1	H	46	VAL	2.4
1	C	49	THR	2.4
1	F	384	HIS	2.4
1	H	316	VAL	2.4
1	E	112	ASP	2.4
1	B	285	ARG	2.4
1	H	282	ARG	2.4
1	F	271	ALA	2.3
1	B	27	ASP	2.3
1	C	272	ARG	2.3
1	H	65	ARG	2.3
1	F	323	SER	2.3
1	H	285	ARG	2.3
1	H	275	LYS	2.3
1	A	271	ALA	2.2
1	A	273	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	306	ASP	2.2
1	G	28	ILE	2.2
1	G	34	GLY	2.2
1	F	285	ARG	2.1
1	H	264	GLU	2.1
1	B	306	ASP	2.1
1	H	50	ASN	2.1
1	E	273	LYS	2.1
1	H	328	LEU	2.1
1	E	267	ARG	2.1
1	E	187	GLU	2.1
1	H	319	ALA	2.0
1	F	27	ASP	2.0

## 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SIN	C	408	8/8	0.22	4.40	50,54,59,60	0
2	SIN	A	404	8/8	0.20	2.60	58,61,64,64	0
2	SIN	F	412	8/8	0.17	2.15	52,52,54,54	0
2	SIN	D	410	8/8	0.18	1.70	51,53,54,54	0
2	SIN	G	414	8/8	0.19	1.22	54,57,58,59	0
2	SIN	A	403	8/8	0.16	0.87	60,61,63,64	0
2	SIN	B	406	8/8	0.14	0.31	48,51,52,52	0
2	SIN	H	415	8/8	0.12	0.27	42,43,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SIN	F	411	8/8	0.09	-0.25	28,30,33,34	0
2	SIN	C	407	8/8	0.11	-0.37	33,34,35,37	0
2	SIN	E	416	8/8	0.08	-0.71	37,38,38,39	0
2	SIN	G	413	8/8	0.08	-0.87	29,31,33,33	0
2	SIN	B	405	8/8	0.07	-0.92	25,29,31,32	0
2	SIN	A	401	8/8	0.07	-1.50	25,27,27,28	0
2	SIN	A	402	8/8	0.08	-1.58	29,32,35,36	0
2	SIN	D	409	8/8	0.06	-1.90	25,26,26,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.