wwPDB X-ray Structure Validation Summary Report (i)

Nov 1, 2023 – 01:02 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

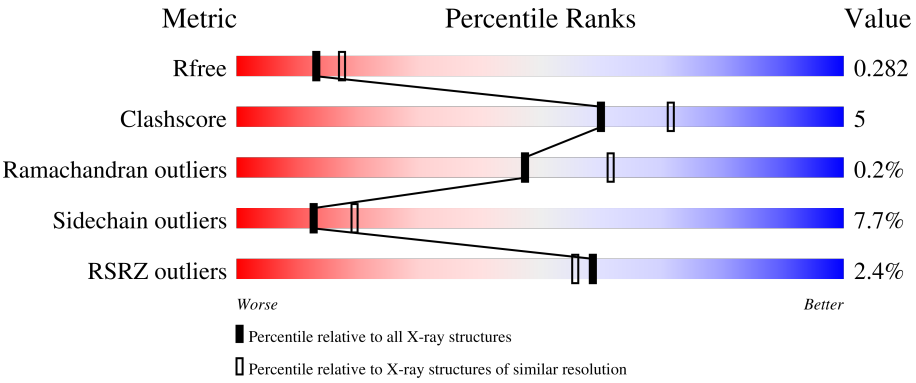
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 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	404	79% 10% 10%
1	B	404	75% 13% • 10%
1	C	404	5% 77% 11% • 11%
1	D	404	4% 74% 12% • 11%
1	E	404	78% 10% • 10%

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Mol	Chain	Length	Quality of chain
1	F	404	2% 77% 10% 10%
1	G	404	2% 77% 13% 10%
1	H	404	1% 78% 11% 10%
1	I	404	1% 75% 13% 10%
1	J	404	4% 78% 10% 10%

2 Entry composition (i)

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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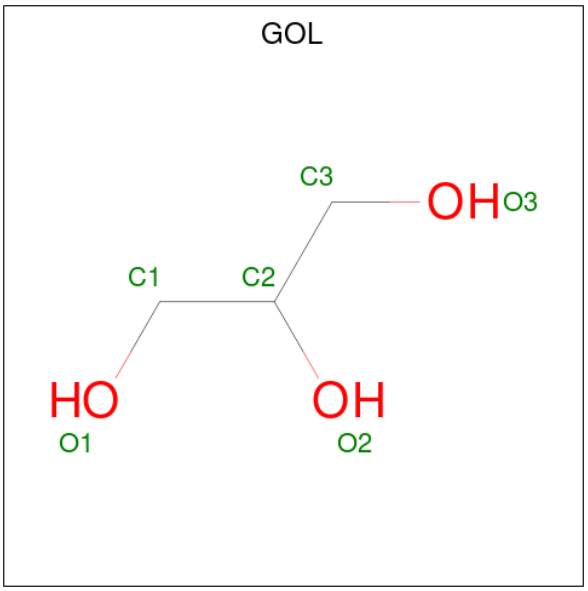
Chain	Residue	Modelled	Actual	Comment	Reference
J	-14	MET	-	expression tag	UNP Q56063
J	-13	ARG	-	expression tag	UNP Q56063
J	-12	GLY	-	expression tag	UNP Q56063
J	-11	SER	-	expression tag	UNP Q56063
J	-10	HIS	-	expression tag	UNP Q56063
J	-9	HIS	-	expression tag	UNP Q56063
J	-8	HIS	-	expression tag	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 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	F	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

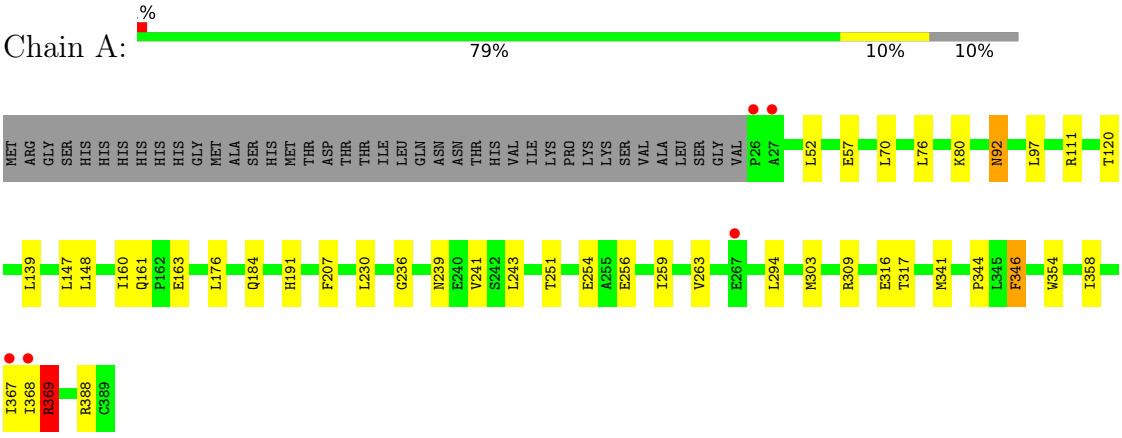
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	145	Total O 145 145	0	0
3	B	119	Total O 119 119	0	0
3	C	84	Total O 84 84	0	0
3	D	96	Total O 96 96	0	0
3	E	146	Total O 146 146	0	0
3	F	113	Total O 113 113	0	0
3	G	106	Total O 106 106	0	0
3	H	126	Total O 126 126	0	0
3	I	131	Total O 131 131	0	0
3	J	112	Total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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

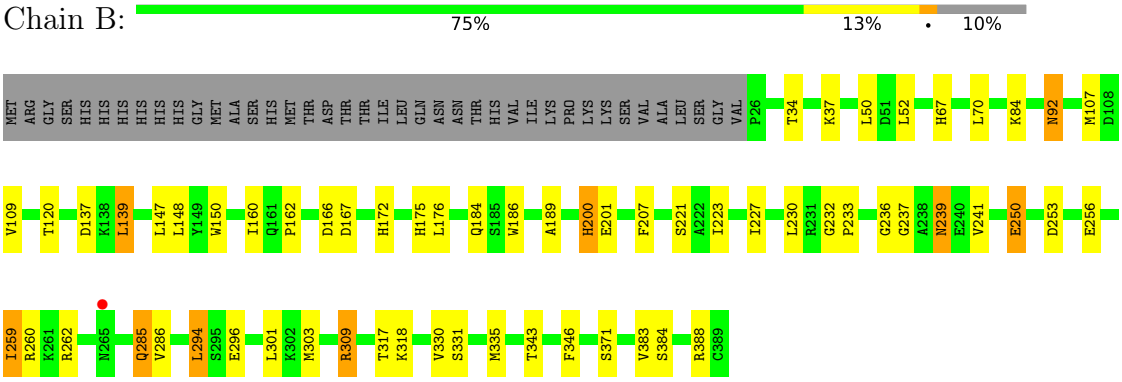
- Molecule 1: 2-methylcitrate synthase

Chain A:



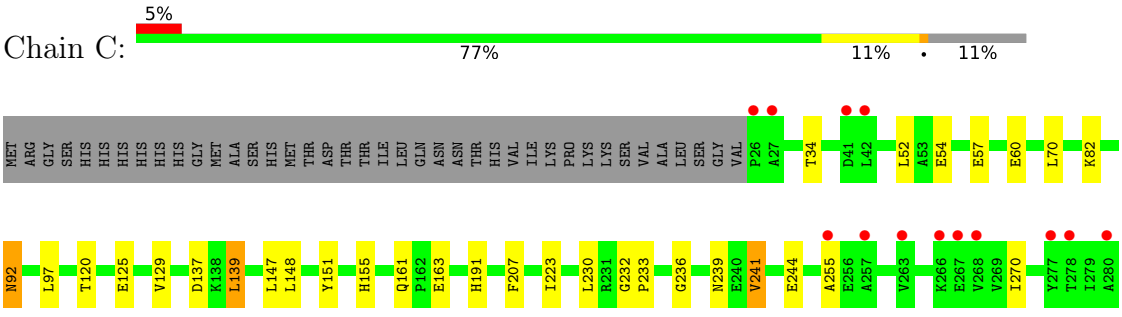
- Molecule 1: 2-methylcitrate synthase

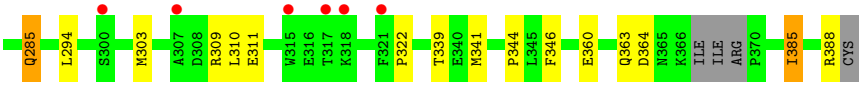
Chain B:



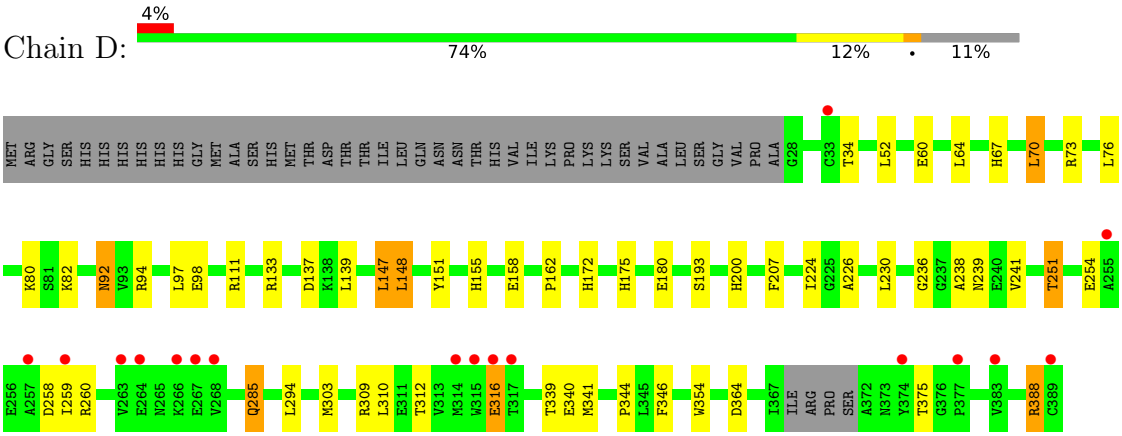
- Molecule 1: 2-methylcitrate synthase

Chain C:

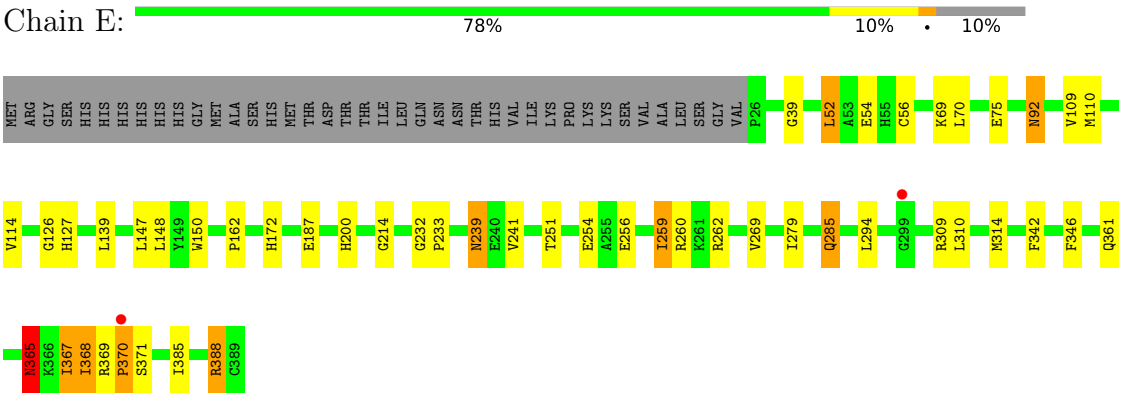




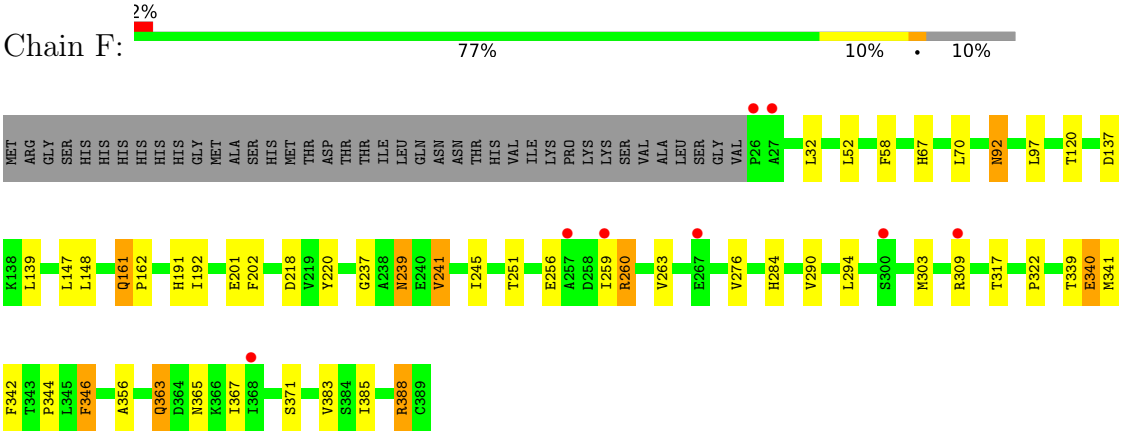
• Molecule 1: 2-methylcitrate synthase



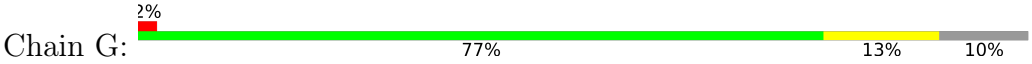
• Molecule 1: 2-methylcitrate synthase

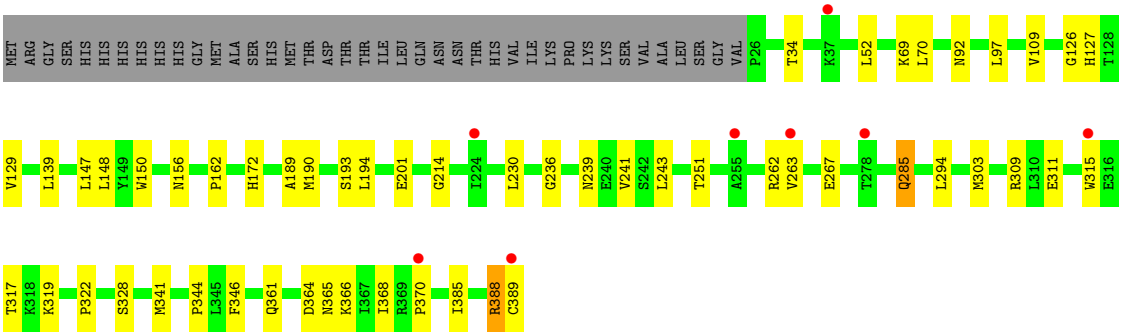


• Molecule 1: 2-methylcitrate synthase

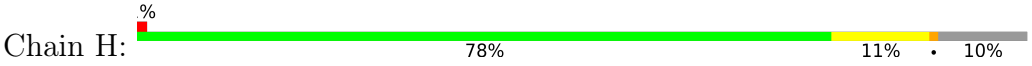


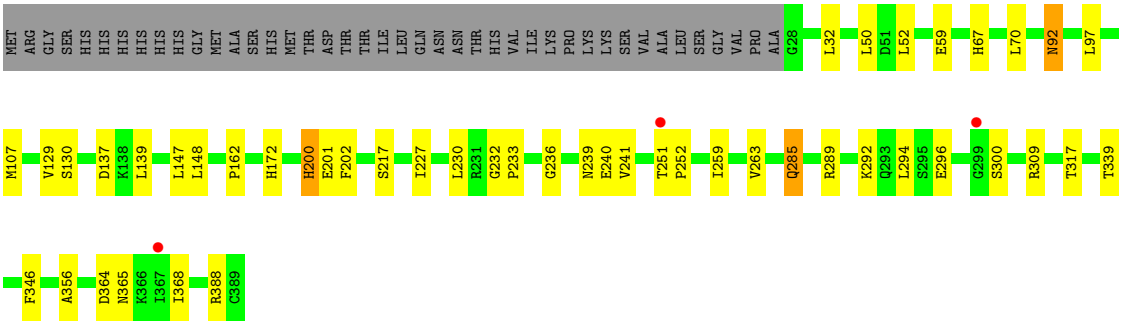
• Molecule 1: 2-methylcitrate synthase



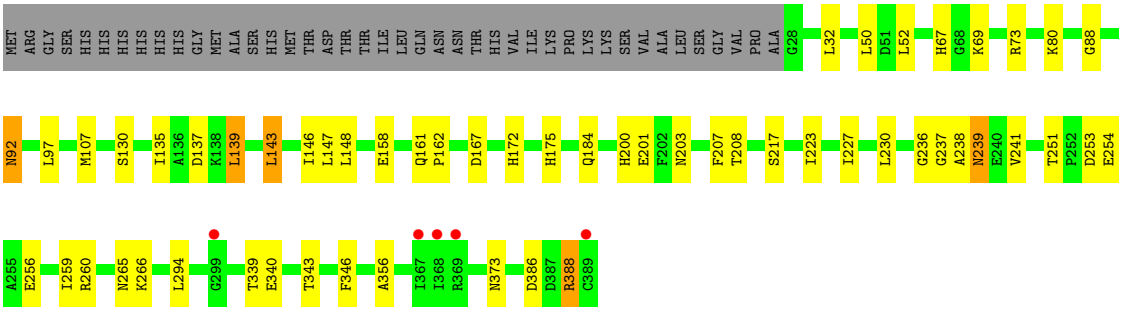


• Molecule 1: 2-methylcitrate synthase

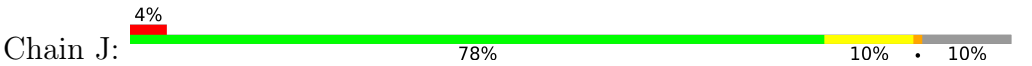


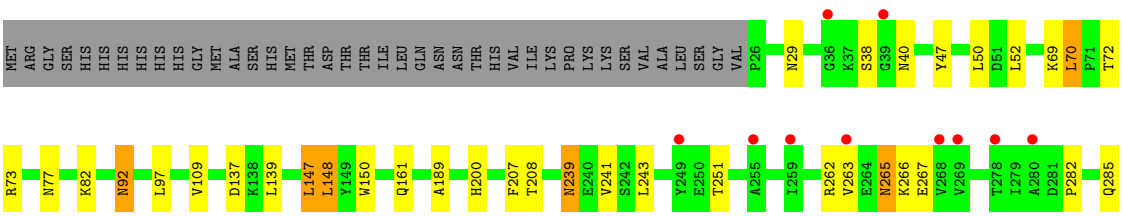


• Molecule 1: 2-methylcitrate synthase



• Molecule 1: 2-methylcitrate synthase






L294
R309
L310
V313
M314
W315
E316
T317
K318
K319
A329
T339
F346
Q361
K366
I367
I368
ARG
PRO
S371
E378
R388
C389

4 Data and refinement statistics (i)

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) 91.0 (49.51-2.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	7257 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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: 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 (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	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%)	25	35
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%)	41	54
1	E	362/404 (90%)	346 (96%)	14 (4%)	2 (1%)	25	35
1	F	362/404 (90%)	355 (98%)	6 (2%)	1 (0%)	41	54
1	G	362/404 (90%)	348 (96%)	14 (4%)	0	100	100
1	H	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	41	54
1	I	360/404 (89%)	349 (97%)	10 (3%)	1 (0%)	41	54
1	J	358/404 (89%)	349 (98%)	9 (2%)	0	100	100
All	All	3598/4040 (89%)	3492 (97%)	98 (3%)	8 (0%)	47	61

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	289/339 (85%)	271 (94%)	18 (6%)	18 28
1	B	285/339 (84%)	264 (93%)	21 (7%)	13 21
1	C	284/339 (84%)	264 (93%)	20 (7%)	15 23
1	D	284/339 (84%)	258 (91%)	26 (9%)	9 13
1	E	292/339 (86%)	273 (94%)	19 (6%)	17 26
1	F	292/339 (86%)	268 (92%)	24 (8%)	11 16
1	G	287/339 (85%)	265 (92%)	22 (8%)	13 19
1	H	290/339 (86%)	267 (92%)	23 (8%)	12 18
1	I	290/339 (86%)	261 (90%)	29 (10%)	7 10
1	J	296/339 (87%)	275 (93%)	21 (7%)	14 22
All	All	2889/3390 (85%)	2666 (92%)	223 (8%)	13 19

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

Mol	Chain	Res	Type
1	F	251	THR
1	J	378	GLU
1	G	285	GLN
1	J	339	THR
1	I	343	THR

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

Mol	Chain	Res	Type
1	H	92	ASN

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Mol	Chain	Res	Type
1	I	293	GLN
1	H	172	HIS
1	I	92	ASN
1	J	92	ASN

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

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	J	406	-	5,5,5	0.35	0	5,5,5	0.35	0
2	GOL	B	410	-	5,5,5	0.27	0	5,5,5	0.40	0
2	GOL	C	401	-	5,5,5	0.40	0	5,5,5	0.36	0
2	GOL	E	402	-	5,5,5	0.36	0	5,5,5	0.16	0
2	GOL	H	404	-	5,5,5	0.31	0	5,5,5	0.32	0
2	GOL	E	408	-	5,5,5	0.34	0	5,5,5	0.31	0
2	GOL	F	411	-	5,5,5	0.35	0	5,5,5	0.64	0
2	GOL	G	403	-	5,5,5	0.42	0	5,5,5	0.43	0
2	GOL	I	405	-	5,5,5	0.38	0	5,5,5	0.62	0
2	GOL	F	407	-	5,5,5	0.34	0	5,5,5	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	409	-	5,5,5	0.36	0	5,5,5	0.19	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	J	406	-	-	3/4/4/4	-
2	GOL	B	410	-	-	2/4/4/4	-
2	GOL	C	401	-	-	4/4/4/4	-
2	GOL	E	402	-	-	2/4/4/4	-
2	GOL	H	404	-	-	0/4/4/4	-
2	GOL	E	408	-	-	4/4/4/4	-
2	GOL	F	411	-	-	4/4/4/4	-
2	GOL	G	403	-	-	2/4/4/4	-
2	GOL	I	405	-	-	0/4/4/4	-
2	GOL	F	407	-	-	0/4/4/4	-
2	GOL	A	409	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	409	GOL	O1-C1-C2-C3
2	B	410	GOL	O1-C1-C2-C3
2	E	402	GOL	O1-C1-C2-O2
2	E	402	GOL	O1-C1-C2-C3
2	E	408	GOL	C1-C2-C3-O3

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	H	404	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	408	GOL	1	0
2	I	405	GOL	2	0

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

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^{th} 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%)	-0.28	5 (1%)	75	73	22, 36, 53, 63	1 (0%)
1	B	364/404 (90%)	-0.21	1 (0%)	94	93	23, 36, 63, 70	1 (0%)
1	C	360/404 (89%)	0.10	19 (5%)	26	24	27, 47, 72, 77	1 (0%)
1	D	358/404 (88%)	0.11	17 (4%)	31	29	25, 46, 74, 84	1 (0%)
1	E	364/404 (90%)	-0.34	2 (0%)	91	89	24, 37, 58, 68	1 (0%)
1	F	364/404 (90%)	-0.18	8 (2%)	62	59	24, 39, 57, 66	1 (0%)
1	G	364/404 (90%)	-0.06	8 (2%)	62	59	23, 37, 66, 75	2 (0%)
1	H	362/404 (89%)	-0.31	3 (0%)	86	84	24, 36, 54, 63	1 (0%)
1	I	362/404 (89%)	-0.24	5 (1%)	75	73	23, 37, 57, 64	1 (0%)
1	J	362/404 (89%)	0.01	18 (4%)	28	26	23, 39, 70, 80	1 (0%)
All	All	3624/4040 (89%)	-0.14	86 (2%)	59	56	22, 39, 66, 84	11 (0%)

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ILE	8.1
1	G	370	PRO	7.2
1	E	370	PRO	4.9
1	J	255	ALA	4.7
1	D	267	GLU	4.6

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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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, 95^{th} 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	GOL	B	410	6/6	0.77	0.26	57,59,60,60	0
2	GOL	C	401	6/6	0.78	0.23	64,66,67,68	0
2	GOL	F	411	6/6	0.79	0.20	53,55,56,56	0
2	GOL	I	405	6/6	0.82	0.19	53,56,57,57	0
2	GOL	H	404	6/6	0.83	0.19	49,49,50,52	0
2	GOL	E	402	6/6	0.83	0.20	59,61,62,62	0
2	GOL	F	407	6/6	0.84	0.20	63,64,64,64	0
2	GOL	G	403	6/6	0.84	0.24	56,58,60,60	0
2	GOL	J	406	6/6	0.87	0.20	61,61,62,63	0
2	GOL	E	408	6/6	0.90	0.18	65,66,66,67	0
2	GOL	A	409	6/6	0.91	0.17	54,55,55,56	0

6.5 Other polymers (i)

There are no such residues in this entry.