WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 08:08 AM EDT

PDB ID	:	6V9A
Title	:	Agrobacterium tumefaciens ADP-Glucose pyrophosphorylase-S72D
Authors	:	Zheng, Y.; Alghamdi, M.A.; Ballicora, M.A.; Liu, D.
Deposited on	:	2019-12-13
Resolution	:	2.30 Å(reported)

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.30 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 70139 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 Glucose-1-phosphate adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	415	Total 3286	C 2083	N 570	O 620	S 13	0	6	0
1	A	415	Total 3297	C 2089	N 574	O 621	S 13	4	7	0
1	B	415	Total 3286	C 2083	N 570	O 620	S 13	4	6	0
1	C	412	Total 3270	C 2074	N 565	O 617	S 14	4	7	0
1	D	415	Total 3286	C 2083	N 570	O 620	S 13	4	6	0
1	E	415	Total 3286	C 2083	N 570	O 620	S 13	0	6	0
1	F	415	Total 3286	C 2083	N 570	O 620	S 13	4	6	0
1	G	415	Total 3292	C 2086	N 571	O 621	S 14	4	7	0
1	I	415	Total 3303	C 2092	N 575	O 622	S 14	4	8	0
1	J	408	Total 3247	C 2061	N 561	O 611	S 14	4	7	0
1	K	415	Total 3286	C 2083	N 570	O 620	S 13	0	6	0
1	L	415	Total 3294	C 2088	N 571	O 621	S 14	19	7	0
1	M	415	Total 3286	C 2083	N 570	O 620	S 13	0	6	0
1	N	415	Total 3286	C 2083	N 570	O 620	S 13	0	6	0
1	O	415	Total 3304	C 2093	N 573	O 623	S 15	12	8	0
1	P	415	Total 3309	C 2098	N 575	O 623	S 13	4	8	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	415	Total	C	N	O	S	4	7	0
			3298	2092	571	622	13			
1	R	415	Total	C	N	O	S	4	7	0
			3294	2088	571	621	14			
1	V	415	Total	C	N	O	S	4	6	0
			3286	2083	570	620	13			
1	T	415	Total	C	N	O	S	12	7	0
			3294	2088	571	621	14			

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-19	MET	-	expression tag	UNP Q8U8L5
H	-18	GLY	-	expression tag	UNP Q8U8L5
H	-17	SER	-	expression tag	UNP Q8U8L5
H	-16	SER	-	expression tag	UNP Q8U8L5
H	-15	HIS	-	expression tag	UNP Q8U8L5
H	-14	HIS	-	expression tag	UNP Q8U8L5
H	-13	HIS	-	expression tag	UNP Q8U8L5
H	-12	HIS	-	expression tag	UNP Q8U8L5
H	-11	HIS	-	expression tag	UNP Q8U8L5
H	-10	HIS	-	expression tag	UNP Q8U8L5
H	-9	SER	-	expression tag	UNP Q8U8L5
H	-8	SER	-	expression tag	UNP Q8U8L5
H	-7	GLY	-	expression tag	UNP Q8U8L5
H	-6	LEU	-	expression tag	UNP Q8U8L5
H	-5	VAL	-	expression tag	UNP Q8U8L5
H	-4	PRO	-	expression tag	UNP Q8U8L5
H	-3	ARG	-	expression tag	UNP Q8U8L5
H	-2	GLY	-	expression tag	UNP Q8U8L5
H	-1	SER	-	expression tag	UNP Q8U8L5
H	0	HIS	-	expression tag	UNP Q8U8L5
H	72	ASP	SER	engineered mutation	UNP Q8U8L5
A	-19	MET	-	expression tag	UNP Q8U8L5
A	-18	GLY	-	expression tag	UNP Q8U8L5
A	-17	SER	-	expression tag	UNP Q8U8L5
A	-16	SER	-	expression tag	UNP Q8U8L5
A	-15	HIS	-	expression tag	UNP Q8U8L5
A	-14	HIS	-	expression tag	UNP Q8U8L5
A	-13	HIS	-	expression tag	UNP Q8U8L5
A	-12	HIS	-	expression tag	UNP Q8U8L5
A	-11	HIS	-	expression tag	UNP Q8U8L5
A	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	SER	-	expression tag	UNP Q8U8L5
A	-8	SER	-	expression tag	UNP Q8U8L5
A	-7	GLY	-	expression tag	UNP Q8U8L5
A	-6	LEU	-	expression tag	UNP Q8U8L5
A	-5	VAL	-	expression tag	UNP Q8U8L5
A	-4	PRO	-	expression tag	UNP Q8U8L5
A	-3	ARG	-	expression tag	UNP Q8U8L5
A	-2	GLY	-	expression tag	UNP Q8U8L5
A	-1	SER	-	expression tag	UNP Q8U8L5
A	0	HIS	-	expression tag	UNP Q8U8L5
A	72	ASP	SER	engineered mutation	UNP Q8U8L5
B	-19	MET	-	expression tag	UNP Q8U8L5
B	-18	GLY	-	expression tag	UNP Q8U8L5
B	-17	SER	-	expression tag	UNP Q8U8L5
B	-16	SER	-	expression tag	UNP Q8U8L5
B	-15	HIS	-	expression tag	UNP Q8U8L5
B	-14	HIS	-	expression tag	UNP Q8U8L5
B	-13	HIS	-	expression tag	UNP Q8U8L5
B	-12	HIS	-	expression tag	UNP Q8U8L5
B	-11	HIS	-	expression tag	UNP Q8U8L5
B	-10	HIS	-	expression tag	UNP Q8U8L5
B	-9	SER	-	expression tag	UNP Q8U8L5
B	-8	SER	-	expression tag	UNP Q8U8L5
B	-7	GLY	-	expression tag	UNP Q8U8L5
B	-6	LEU	-	expression tag	UNP Q8U8L5
B	-5	VAL	-	expression tag	UNP Q8U8L5
B	-4	PRO	-	expression tag	UNP Q8U8L5
B	-3	ARG	-	expression tag	UNP Q8U8L5
B	-2	GLY	-	expression tag	UNP Q8U8L5
B	-1	SER	-	expression tag	UNP Q8U8L5
B	0	HIS	-	expression tag	UNP Q8U8L5
B	72	ASP	SER	engineered mutation	UNP Q8U8L5
C	-19	MET	-	expression tag	UNP Q8U8L5
C	-18	GLY	-	expression tag	UNP Q8U8L5
C	-17	SER	-	expression tag	UNP Q8U8L5
C	-16	SER	-	expression tag	UNP Q8U8L5
C	-15	HIS	-	expression tag	UNP Q8U8L5
C	-14	HIS	-	expression tag	UNP Q8U8L5
C	-13	HIS	-	expression tag	UNP Q8U8L5
C	-12	HIS	-	expression tag	UNP Q8U8L5
C	-11	HIS	-	expression tag	UNP Q8U8L5
C	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	SER	-	expression tag	UNP Q8U8L5
C	-8	SER	-	expression tag	UNP Q8U8L5
C	-7	GLY	-	expression tag	UNP Q8U8L5
C	-6	LEU	-	expression tag	UNP Q8U8L5
C	-5	VAL	-	expression tag	UNP Q8U8L5
C	-4	PRO	-	expression tag	UNP Q8U8L5
C	-3	ARG	-	expression tag	UNP Q8U8L5
C	-2	GLY	-	expression tag	UNP Q8U8L5
C	-1	SER	-	expression tag	UNP Q8U8L5
C	0	HIS	-	expression tag	UNP Q8U8L5
C	72	ASP	SER	engineered mutation	UNP Q8U8L5
D	-19	MET	-	expression tag	UNP Q8U8L5
D	-18	GLY	-	expression tag	UNP Q8U8L5
D	-17	SER	-	expression tag	UNP Q8U8L5
D	-16	SER	-	expression tag	UNP Q8U8L5
D	-15	HIS	-	expression tag	UNP Q8U8L5
D	-14	HIS	-	expression tag	UNP Q8U8L5
D	-13	HIS	-	expression tag	UNP Q8U8L5
D	-12	HIS	-	expression tag	UNP Q8U8L5
D	-11	HIS	-	expression tag	UNP Q8U8L5
D	-10	HIS	-	expression tag	UNP Q8U8L5
D	-9	SER	-	expression tag	UNP Q8U8L5
D	-8	SER	-	expression tag	UNP Q8U8L5
D	-7	GLY	-	expression tag	UNP Q8U8L5
D	-6	LEU	-	expression tag	UNP Q8U8L5
D	-5	VAL	-	expression tag	UNP Q8U8L5
D	-4	PRO	-	expression tag	UNP Q8U8L5
D	-3	ARG	-	expression tag	UNP Q8U8L5
D	-2	GLY	-	expression tag	UNP Q8U8L5
D	-1	SER	-	expression tag	UNP Q8U8L5
D	0	HIS	-	expression tag	UNP Q8U8L5
D	72	ASP	SER	engineered mutation	UNP Q8U8L5
E	-19	MET	-	expression tag	UNP Q8U8L5
E	-18	GLY	-	expression tag	UNP Q8U8L5
E	-17	SER	-	expression tag	UNP Q8U8L5
E	-16	SER	-	expression tag	UNP Q8U8L5
E	-15	HIS	-	expression tag	UNP Q8U8L5
E	-14	HIS	-	expression tag	UNP Q8U8L5
E	-13	HIS	-	expression tag	UNP Q8U8L5
E	-12	HIS	-	expression tag	UNP Q8U8L5
E	-11	HIS	-	expression tag	UNP Q8U8L5
E	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	SER	-	expression tag	UNP Q8U8L5
E	-8	SER	-	expression tag	UNP Q8U8L5
E	-7	GLY	-	expression tag	UNP Q8U8L5
E	-6	LEU	-	expression tag	UNP Q8U8L5
E	-5	VAL	-	expression tag	UNP Q8U8L5
E	-4	PRO	-	expression tag	UNP Q8U8L5
E	-3	ARG	-	expression tag	UNP Q8U8L5
E	-2	GLY	-	expression tag	UNP Q8U8L5
E	-1	SER	-	expression tag	UNP Q8U8L5
E	0	HIS	-	expression tag	UNP Q8U8L5
E	72	ASP	SER	engineered mutation	UNP Q8U8L5
F	-19	MET	-	expression tag	UNP Q8U8L5
F	-18	GLY	-	expression tag	UNP Q8U8L5
F	-17	SER	-	expression tag	UNP Q8U8L5
F	-16	SER	-	expression tag	UNP Q8U8L5
F	-15	HIS	-	expression tag	UNP Q8U8L5
F	-14	HIS	-	expression tag	UNP Q8U8L5
F	-13	HIS	-	expression tag	UNP Q8U8L5
F	-12	HIS	-	expression tag	UNP Q8U8L5
F	-11	HIS	-	expression tag	UNP Q8U8L5
F	-10	HIS	-	expression tag	UNP Q8U8L5
F	-9	SER	-	expression tag	UNP Q8U8L5
F	-8	SER	-	expression tag	UNP Q8U8L5
F	-7	GLY	-	expression tag	UNP Q8U8L5
F	-6	LEU	-	expression tag	UNP Q8U8L5
F	-5	VAL	-	expression tag	UNP Q8U8L5
F	-4	PRO	-	expression tag	UNP Q8U8L5
F	-3	ARG	-	expression tag	UNP Q8U8L5
F	-2	GLY	-	expression tag	UNP Q8U8L5
F	-1	SER	-	expression tag	UNP Q8U8L5
F	0	HIS	-	expression tag	UNP Q8U8L5
F	72	ASP	SER	engineered mutation	UNP Q8U8L5
G	-19	MET	-	expression tag	UNP Q8U8L5
G	-18	GLY	-	expression tag	UNP Q8U8L5
G	-17	SER	-	expression tag	UNP Q8U8L5
G	-16	SER	-	expression tag	UNP Q8U8L5
G	-15	HIS	-	expression tag	UNP Q8U8L5
G	-14	HIS	-	expression tag	UNP Q8U8L5
G	-13	HIS	-	expression tag	UNP Q8U8L5
G	-12	HIS	-	expression tag	UNP Q8U8L5
G	-11	HIS	-	expression tag	UNP Q8U8L5
G	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-9	SER	-	expression tag	UNP Q8U8L5
G	-8	SER	-	expression tag	UNP Q8U8L5
G	-7	GLY	-	expression tag	UNP Q8U8L5
G	-6	LEU	-	expression tag	UNP Q8U8L5
G	-5	VAL	-	expression tag	UNP Q8U8L5
G	-4	PRO	-	expression tag	UNP Q8U8L5
G	-3	ARG	-	expression tag	UNP Q8U8L5
G	-2	GLY	-	expression tag	UNP Q8U8L5
G	-1	SER	-	expression tag	UNP Q8U8L5
G	0	HIS	-	expression tag	UNP Q8U8L5
G	72	ASP	SER	engineered mutation	UNP Q8U8L5
I	-19	MET	-	expression tag	UNP Q8U8L5
I	-18	GLY	-	expression tag	UNP Q8U8L5
I	-17	SER	-	expression tag	UNP Q8U8L5
I	-16	SER	-	expression tag	UNP Q8U8L5
I	-15	HIS	-	expression tag	UNP Q8U8L5
I	-14	HIS	-	expression tag	UNP Q8U8L5
I	-13	HIS	-	expression tag	UNP Q8U8L5
I	-12	HIS	-	expression tag	UNP Q8U8L5
I	-11	HIS	-	expression tag	UNP Q8U8L5
I	-10	HIS	-	expression tag	UNP Q8U8L5
I	-9	SER	-	expression tag	UNP Q8U8L5
I	-8	SER	-	expression tag	UNP Q8U8L5
I	-7	GLY	-	expression tag	UNP Q8U8L5
I	-6	LEU	-	expression tag	UNP Q8U8L5
I	-5	VAL	-	expression tag	UNP Q8U8L5
I	-4	PRO	-	expression tag	UNP Q8U8L5
I	-3	ARG	-	expression tag	UNP Q8U8L5
I	-2	GLY	-	expression tag	UNP Q8U8L5
I	-1	SER	-	expression tag	UNP Q8U8L5
I	0	HIS	-	expression tag	UNP Q8U8L5
I	72	ASP	SER	engineered mutation	UNP Q8U8L5
J	-19	MET	-	expression tag	UNP Q8U8L5
J	-18	GLY	-	expression tag	UNP Q8U8L5
J	-17	SER	-	expression tag	UNP Q8U8L5
J	-16	SER	-	expression tag	UNP Q8U8L5
J	-15	HIS	-	expression tag	UNP Q8U8L5
J	-14	HIS	-	expression tag	UNP Q8U8L5
J	-13	HIS	-	expression tag	UNP Q8U8L5
J	-12	HIS	-	expression tag	UNP Q8U8L5
J	-11	HIS	-	expression tag	UNP Q8U8L5
J	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-9	SER	-	expression tag	UNP Q8U8L5
J	-8	SER	-	expression tag	UNP Q8U8L5
J	-7	GLY	-	expression tag	UNP Q8U8L5
J	-6	LEU	-	expression tag	UNP Q8U8L5
J	-5	VAL	-	expression tag	UNP Q8U8L5
J	-4	PRO	-	expression tag	UNP Q8U8L5
J	-3	ARG	-	expression tag	UNP Q8U8L5
J	-2	GLY	-	expression tag	UNP Q8U8L5
J	-1	SER	-	expression tag	UNP Q8U8L5
J	0	HIS	-	expression tag	UNP Q8U8L5
J	72	ASP	SER	engineered mutation	UNP Q8U8L5
K	-19	MET	-	expression tag	UNP Q8U8L5
K	-18	GLY	-	expression tag	UNP Q8U8L5
K	-17	SER	-	expression tag	UNP Q8U8L5
K	-16	SER	-	expression tag	UNP Q8U8L5
K	-15	HIS	-	expression tag	UNP Q8U8L5
K	-14	HIS	-	expression tag	UNP Q8U8L5
K	-13	HIS	-	expression tag	UNP Q8U8L5
K	-12	HIS	-	expression tag	UNP Q8U8L5
K	-11	HIS	-	expression tag	UNP Q8U8L5
K	-10	HIS	-	expression tag	UNP Q8U8L5
K	-9	SER	-	expression tag	UNP Q8U8L5
K	-8	SER	-	expression tag	UNP Q8U8L5
K	-7	GLY	-	expression tag	UNP Q8U8L5
K	-6	LEU	-	expression tag	UNP Q8U8L5
K	-5	VAL	-	expression tag	UNP Q8U8L5
K	-4	PRO	-	expression tag	UNP Q8U8L5
K	-3	ARG	-	expression tag	UNP Q8U8L5
K	-2	GLY	-	expression tag	UNP Q8U8L5
K	-1	SER	-	expression tag	UNP Q8U8L5
K	0	HIS	-	expression tag	UNP Q8U8L5
K	72	ASP	SER	engineered mutation	UNP Q8U8L5
L	-19	MET	-	expression tag	UNP Q8U8L5
L	-18	GLY	-	expression tag	UNP Q8U8L5
L	-17	SER	-	expression tag	UNP Q8U8L5
L	-16	SER	-	expression tag	UNP Q8U8L5
L	-15	HIS	-	expression tag	UNP Q8U8L5
L	-14	HIS	-	expression tag	UNP Q8U8L5
L	-13	HIS	-	expression tag	UNP Q8U8L5
L	-12	HIS	-	expression tag	UNP Q8U8L5
L	-11	HIS	-	expression tag	UNP Q8U8L5
L	-10	HIS	-	expression tag	UNP Q8U8L5

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	-9	SER	-	expression tag	UNP Q8U8L5
L	-8	SER	-	expression tag	UNP Q8U8L5
L	-7	GLY	-	expression tag	UNP Q8U8L5
L	-6	LEU	-	expression tag	UNP Q8U8L5
L	-5	VAL	-	expression tag	UNP Q8U8L5
L	-4	PRO	-	expression tag	UNP Q8U8L5
L	-3	ARG	-	expression tag	UNP Q8U8L5
L	-2	GLY	-	expression tag	UNP Q8U8L5
L	-1	SER	-	expression tag	UNP Q8U8L5
L	0	HIS	-	expression tag	UNP Q8U8L5
L	72	ASP	SER	engineered mutation	UNP Q8U8L5
M	-19	MET	-	expression tag	UNP Q8U8L5
M	-18	GLY	-	expression tag	UNP Q8U8L5
M	-17	SER	-	expression tag	UNP Q8U8L5
M	-16	SER	-	expression tag	UNP Q8U8L5
M	-15	HIS	-	expression tag	UNP Q8U8L5
M	-14	HIS	-	expression tag	UNP Q8U8L5
M	-13	HIS	-	expression tag	UNP Q8U8L5
M	-12	HIS	-	expression tag	UNP Q8U8L5
M	-11	HIS	-	expression tag	UNP Q8U8L5
M	-10	HIS	-	expression tag	UNP Q8U8L5
M	-9	SER	-	expression tag	UNP Q8U8L5
M	-8	SER	-	expression tag	UNP Q8U8L5
M	-7	GLY	-	expression tag	UNP Q8U8L5
M	-6	LEU	-	expression tag	UNP Q8U8L5
M	-5	VAL	-	expression tag	UNP Q8U8L5
M	-4	PRO	-	expression tag	UNP Q8U8L5
M	-3	ARG	-	expression tag	UNP Q8U8L5
M	-2	GLY	-	expression tag	UNP Q8U8L5
M	-1	SER	-	expression tag	UNP Q8U8L5
M	0	HIS	-	expression tag	UNP Q8U8L5
M	72	ASP	SER	engineered mutation	UNP Q8U8L5
N	-19	MET	-	expression tag	UNP Q8U8L5
N	-18	GLY	-	expression tag	UNP Q8U8L5
N	-17	SER	-	expression tag	UNP Q8U8L5
N	-16	SER	-	expression tag	UNP Q8U8L5
N	-15	HIS	-	expression tag	UNP Q8U8L5
N	-14	HIS	-	expression tag	UNP Q8U8L5
N	-13	HIS	-	expression tag	UNP Q8U8L5
N	-12	HIS	-	expression tag	UNP Q8U8L5
N	-11	HIS	-	expression tag	UNP Q8U8L5
N	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-9	SER	-	expression tag	UNP Q8U8L5
N	-8	SER	-	expression tag	UNP Q8U8L5
N	-7	GLY	-	expression tag	UNP Q8U8L5
N	-6	LEU	-	expression tag	UNP Q8U8L5
N	-5	VAL	-	expression tag	UNP Q8U8L5
N	-4	PRO	-	expression tag	UNP Q8U8L5
N	-3	ARG	-	expression tag	UNP Q8U8L5
N	-2	GLY	-	expression tag	UNP Q8U8L5
N	-1	SER	-	expression tag	UNP Q8U8L5
N	0	HIS	-	expression tag	UNP Q8U8L5
N	72	ASP	SER	engineered mutation	UNP Q8U8L5
O	-19	MET	-	expression tag	UNP Q8U8L5
O	-18	GLY	-	expression tag	UNP Q8U8L5
O	-17	SER	-	expression tag	UNP Q8U8L5
O	-16	SER	-	expression tag	UNP Q8U8L5
O	-15	HIS	-	expression tag	UNP Q8U8L5
O	-14	HIS	-	expression tag	UNP Q8U8L5
O	-13	HIS	-	expression tag	UNP Q8U8L5
O	-12	HIS	-	expression tag	UNP Q8U8L5
O	-11	HIS	-	expression tag	UNP Q8U8L5
O	-10	HIS	-	expression tag	UNP Q8U8L5
O	-9	SER	-	expression tag	UNP Q8U8L5
O	-8	SER	-	expression tag	UNP Q8U8L5
O	-7	GLY	-	expression tag	UNP Q8U8L5
O	-6	LEU	-	expression tag	UNP Q8U8L5
O	-5	VAL	-	expression tag	UNP Q8U8L5
O	-4	PRO	-	expression tag	UNP Q8U8L5
O	-3	ARG	-	expression tag	UNP Q8U8L5
O	-2	GLY	-	expression tag	UNP Q8U8L5
O	-1	SER	-	expression tag	UNP Q8U8L5
O	0	HIS	-	expression tag	UNP Q8U8L5
O	72	ASP	SER	engineered mutation	UNP Q8U8L5
P	-19	MET	-	expression tag	UNP Q8U8L5
P	-18	GLY	-	expression tag	UNP Q8U8L5
P	-17	SER	-	expression tag	UNP Q8U8L5
P	-16	SER	-	expression tag	UNP Q8U8L5
P	-15	HIS	-	expression tag	UNP Q8U8L5
P	-14	HIS	-	expression tag	UNP Q8U8L5
P	-13	HIS	-	expression tag	UNP Q8U8L5
P	-12	HIS	-	expression tag	UNP Q8U8L5
P	-11	HIS	-	expression tag	UNP Q8U8L5
P	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-9	SER	-	expression tag	UNP Q8U8L5
P	-8	SER	-	expression tag	UNP Q8U8L5
P	-7	GLY	-	expression tag	UNP Q8U8L5
P	-6	LEU	-	expression tag	UNP Q8U8L5
P	-5	VAL	-	expression tag	UNP Q8U8L5
P	-4	PRO	-	expression tag	UNP Q8U8L5
P	-3	ARG	-	expression tag	UNP Q8U8L5
P	-2	GLY	-	expression tag	UNP Q8U8L5
P	-1	SER	-	expression tag	UNP Q8U8L5
P	0	HIS	-	expression tag	UNP Q8U8L5
P	72	ASP	SER	engineered mutation	UNP Q8U8L5
Q	-19	MET	-	expression tag	UNP Q8U8L5
Q	-18	GLY	-	expression tag	UNP Q8U8L5
Q	-17	SER	-	expression tag	UNP Q8U8L5
Q	-16	SER	-	expression tag	UNP Q8U8L5
Q	-15	HIS	-	expression tag	UNP Q8U8L5
Q	-14	HIS	-	expression tag	UNP Q8U8L5
Q	-13	HIS	-	expression tag	UNP Q8U8L5
Q	-12	HIS	-	expression tag	UNP Q8U8L5
Q	-11	HIS	-	expression tag	UNP Q8U8L5
Q	-10	HIS	-	expression tag	UNP Q8U8L5
Q	-9	SER	-	expression tag	UNP Q8U8L5
Q	-8	SER	-	expression tag	UNP Q8U8L5
Q	-7	GLY	-	expression tag	UNP Q8U8L5
Q	-6	LEU	-	expression tag	UNP Q8U8L5
Q	-5	VAL	-	expression tag	UNP Q8U8L5
Q	-4	PRO	-	expression tag	UNP Q8U8L5
Q	-3	ARG	-	expression tag	UNP Q8U8L5
Q	-2	GLY	-	expression tag	UNP Q8U8L5
Q	-1	SER	-	expression tag	UNP Q8U8L5
Q	0	HIS	-	expression tag	UNP Q8U8L5
Q	72	ASP	SER	engineered mutation	UNP Q8U8L5
R	-19	MET	-	expression tag	UNP Q8U8L5
R	-18	GLY	-	expression tag	UNP Q8U8L5
R	-17	SER	-	expression tag	UNP Q8U8L5
R	-16	SER	-	expression tag	UNP Q8U8L5
R	-15	HIS	-	expression tag	UNP Q8U8L5
R	-14	HIS	-	expression tag	UNP Q8U8L5
R	-13	HIS	-	expression tag	UNP Q8U8L5
R	-12	HIS	-	expression tag	UNP Q8U8L5
R	-11	HIS	-	expression tag	UNP Q8U8L5
R	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	SER	-	expression tag	UNP Q8U8L5
R	-8	SER	-	expression tag	UNP Q8U8L5
R	-7	GLY	-	expression tag	UNP Q8U8L5
R	-6	LEU	-	expression tag	UNP Q8U8L5
R	-5	VAL	-	expression tag	UNP Q8U8L5
R	-4	PRO	-	expression tag	UNP Q8U8L5
R	-3	ARG	-	expression tag	UNP Q8U8L5
R	-2	GLY	-	expression tag	UNP Q8U8L5
R	-1	SER	-	expression tag	UNP Q8U8L5
R	0	HIS	-	expression tag	UNP Q8U8L5
R	72	ASP	SER	engineered mutation	UNP Q8U8L5
V	-19	MET	-	expression tag	UNP Q8U8L5
V	-18	GLY	-	expression tag	UNP Q8U8L5
V	-17	SER	-	expression tag	UNP Q8U8L5
V	-16	SER	-	expression tag	UNP Q8U8L5
V	-15	HIS	-	expression tag	UNP Q8U8L5
V	-14	HIS	-	expression tag	UNP Q8U8L5
V	-13	HIS	-	expression tag	UNP Q8U8L5
V	-12	HIS	-	expression tag	UNP Q8U8L5
V	-11	HIS	-	expression tag	UNP Q8U8L5
V	-10	HIS	-	expression tag	UNP Q8U8L5
V	-9	SER	-	expression tag	UNP Q8U8L5
V	-8	SER	-	expression tag	UNP Q8U8L5
V	-7	GLY	-	expression tag	UNP Q8U8L5
V	-6	LEU	-	expression tag	UNP Q8U8L5
V	-5	VAL	-	expression tag	UNP Q8U8L5
V	-4	PRO	-	expression tag	UNP Q8U8L5
V	-3	ARG	-	expression tag	UNP Q8U8L5
V	-2	GLY	-	expression tag	UNP Q8U8L5
V	-1	SER	-	expression tag	UNP Q8U8L5
V	0	HIS	-	expression tag	UNP Q8U8L5
V	72	ASP	SER	engineered mutation	UNP Q8U8L5
T	-19	MET	-	expression tag	UNP Q8U8L5
T	-18	GLY	-	expression tag	UNP Q8U8L5
T	-17	SER	-	expression tag	UNP Q8U8L5
T	-16	SER	-	expression tag	UNP Q8U8L5
T	-15	HIS	-	expression tag	UNP Q8U8L5
T	-14	HIS	-	expression tag	UNP Q8U8L5
T	-13	HIS	-	expression tag	UNP Q8U8L5
T	-12	HIS	-	expression tag	UNP Q8U8L5
T	-11	HIS	-	expression tag	UNP Q8U8L5
T	-10	HIS	-	expression tag	UNP Q8U8L5

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-9	SER	-	expression tag	UNP Q8U8L5
T	-8	SER	-	expression tag	UNP Q8U8L5
T	-7	GLY	-	expression tag	UNP Q8U8L5
T	-6	LEU	-	expression tag	UNP Q8U8L5
T	-5	VAL	-	expression tag	UNP Q8U8L5
T	-4	PRO	-	expression tag	UNP Q8U8L5
T	-3	ARG	-	expression tag	UNP Q8U8L5
T	-2	GLY	-	expression tag	UNP Q8U8L5
T	-1	SER	-	expression tag	UNP Q8U8L5
T	0	HIS	-	expression tag	UNP Q8U8L5
T	72	ASP	SER	engineered mutation	UNP Q8U8L5

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).
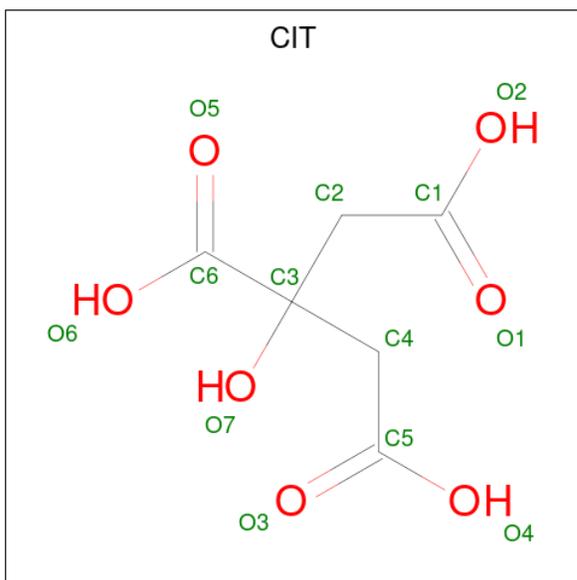
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total 13	C 6	O 7	0	0
2	A	1	Total 13	C 6	O 7	0	0
2	B	1	Total 13	C 6	O 7	0	0
2	C	1	Total 13	C 6	O 7	0	0
2	D	1	Total 13	C 6	O 7	0	0
2	E	1	Total 13	C 6	O 7	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 13	C 6	O 7	0	0
2	G	1	Total 13	C 6	O 7	0	0
2	I	1	Total 13	C 6	O 7	0	0
2	J	1	Total 13	C 6	O 7	0	0
2	K	1	Total 13	C 6	O 7	0	0
2	L	1	Total 13	C 6	O 7	0	0
2	M	1	Total 13	C 6	O 7	0	0
2	N	1	Total 13	C 6	O 7	0	0
2	O	1	Total 13	C 6	O 7	0	0
2	P	1	Total 13	C 6	O 7	0	0
2	Q	1	Total 13	C 6	O 7	0	0
2	R	1	Total 13	C 6	O 7	0	0
2	V	1	Total 13	C 6	O 7	0	0
2	T	1	Total 13	C 6	O 7	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
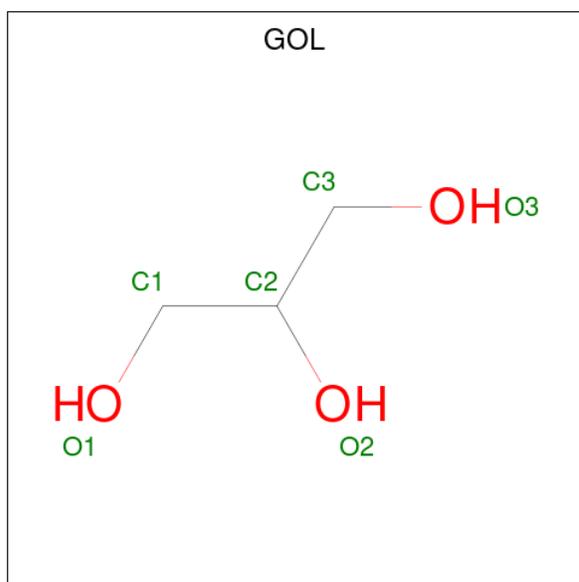
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	A	1	Total 6	C 3	O 3	0	0
3	C	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	E	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0
3	G	1	Total 6	C 3	O 3	0	0
3	I	1	Total 6	C 3	O 3	0	0
3	J	1	Total 6	C 3	O 3	0	0
3	J	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0
3	K	1	Total 6	C 3	O 3	0	0
3	L	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	M	1	Total 6	C 3	O 3	0	0
3	N	1	Total 6	C 3	O 3	0	0
3	O	1	Total 6	C 3	O 3	0	0
3	P	1	Total 6	C 3	O 3	0	0
3	Q	1	Total 6	C 3	O 3	0	0
3	R	1	Total 6	C 3	O 3	0	0
3	V	1	Total 6	C 3	O 3	0	0
3	T	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	172	Total 172	O 172	0	0
4	A	181	Total 181	O 181	0	0
4	B	179	Total 179	O 179	0	0
4	C	243	Total 243	O 243	0	0
4	D	209	Total 209	O 209	0	0
4	E	185	Total 185	O 185	0	0
4	F	160	Total 160	O 160	0	0
4	G	175	Total 175	O 175	0	0
4	I	214	Total 214	O 214	0	0
4	J	274	Total 274	O 274	0	0
4	K	177	Total 177	O 177	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	173	Total 173	O 173	0	0
4	M	145	Total 145	O 145	0	0
4	N	190	Total 190	O 190	0	0
4	O	178	Total 178	O 178	0	0
4	P	221	Total 221	O 221	0	0
4	Q	274	Total 274	O 274	0	0
4	R	262	Total 262	O 262	0	0
4	V	155	Total 155	O 155	0	0
4	T	204	Total 204	O 204	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics ⓘ

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.23Å 141.40Å 228.65Å 108.00° 101.63° 90.02°	Depositor
Resolution (Å)	62.50 – 2.30	Depositor
% Data completeness (in resolution range)	97.6 (62.50-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	0.47 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.234 , 0.279	Depositor
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.730	Xtriage
L-test for twinning[2]	$<|L|> = 0.58$, $<L^2> = 0.42$	Xtriage
Estimated twinning fraction	0.388 for h,-k,-h-l 0.407 for -h,k,-k-l 0.397 for -h,-k,h+k+l	Xtriage
Total number of atoms	70139	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7352e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

42 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	$\#\|Z\| > 2$
3	GOL	A	503	-	5,5,5	0.37	0	5,5,5	0.29	0
2	CIT	L	501	-	12,12,12	1.02	0	17,17,17	1.64	6 (35%)
3	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.53	0
3	GOL	O	502	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	V	502	-	5,5,5	0.36	0	5,5,5	0.33	0
2	CIT	M	501	-	12,12,12	1.01	0	17,17,17	1.61	3 (17%)
2	CIT	C	501	-	12,12,12	1.06	0	17,17,17	1.81	4 (23%)
3	GOL	L	502	-	5,5,5	0.35	0	5,5,5	0.31	0
3	GOL	R	502	-	5,5,5	0.36	0	5,5,5	0.34	0
2	CIT	F	501	-	12,12,12	1.10	0	17,17,17	1.89	3 (17%)
2	CIT	D	501	-	12,12,12	1.02	0	17,17,17	1.67	3 (17%)
3	GOL	H	502	-	5,5,5	0.34	0	5,5,5	0.37	0
2	CIT	E	501	-	12,12,12	1.02	0	17,17,17	1.54	2 (11%)
2	CIT	V	501	-	12,12,12	1.06	0	17,17,17	1.62	2 (11%)
3	GOL	K	502	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	Q	502	-	5,5,5	0.37	0	5,5,5	0.39	0
2	CIT	K	501	-	12,12,12	1.04	0	17,17,17	1.62	1 (5%)
3	GOL	P	502	-	5,5,5	0.35	0	5,5,5	0.23	0
3	GOL	C	502	-	5,5,5	0.37	0	5,5,5	0.30	0
2	CIT	T	501	-	12,12,12	1.05	0	17,17,17	1.57	2 (11%)
3	GOL	J	502	-	5,5,5	0.35	0	5,5,5	0.33	0
3	GOL	M	502	-	5,5,5	0.36	0	5,5,5	0.24	0
2	CIT	G	501	-	12,12,12	1.06	0	17,17,17	1.70	3 (17%)
2	CIT	I	501	-	12,12,12	1.07	0	17,17,17	1.63	2 (11%)
3	GOL	K	503	-	5,5,5	0.38	0	5,5,5	0.47	0
2	CIT	P	501	-	12,12,12	1.06	0	17,17,17	1.71	3 (17%)
2	CIT	Q	501	-	12,12,12	1.00	0	17,17,17	1.74	3 (17%)
2	CIT	J	501	-	12,12,12	1.05	0	17,17,17	1.72	2 (11%)
3	GOL	F	502	-	5,5,5	0.39	0	5,5,5	0.31	0
3	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	E	502	-	5,5,5	0.38	0	5,5,5	0.28	0
2	CIT	O	501	-	12,12,12	1.08	0	17,17,17	1.65	4 (23%)
3	GOL	N	502	-	5,5,5	0.37	0	5,5,5	0.32	0
3	GOL	T	502	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	G	502	-	5,5,5	0.36	0	5,5,5	0.32	0
2	CIT	A	501	-	12,12,12	0.92	0	17,17,17	1.92	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	CIT	N	501	-	12,12,12	1.03	0	17,17,17	1.65	2 (11%)
2	CIT	H	501	-	12,12,12	0.95	0	17,17,17	1.88	6 (35%)
2	CIT	R	501	-	12,12,12	1.10	0	17,17,17	1.68	3 (17%)
3	GOL	I	502	-	5,5,5	0.39	0	5,5,5	0.34	0
3	GOL	J	503	-	5,5,5	0.38	0	5,5,5	0.29	0
2	CIT	B	501	-	12,12,12	1.18	0	17,17,17	2.02	6 (35%)

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
3	GOL	A	503	-	-	0/4/4/4	-
2	CIT	L	501	-	-	9/16/16/16	-
3	GOL	A	502	-	-	0/4/4/4	-
3	GOL	O	502	-	-	0/4/4/4	-
3	GOL	V	502	-	-	2/4/4/4	-
2	CIT	M	501	-	-	10/16/16/16	-
2	CIT	C	501	-	-	9/16/16/16	-
3	GOL	L	502	-	-	2/4/4/4	-
3	GOL	R	502	-	-	0/4/4/4	-
2	CIT	F	501	-	-	6/16/16/16	-
2	CIT	D	501	-	-	6/16/16/16	-
3	GOL	H	502	-	-	0/4/4/4	-
2	CIT	E	501	-	-	7/16/16/16	-
2	CIT	V	501	-	-	7/16/16/16	-
3	GOL	K	502	-	-	2/4/4/4	-
3	GOL	Q	502	-	-	0/4/4/4	-
2	CIT	K	501	-	-	7/16/16/16	-
3	GOL	P	502	-	-	2/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-
2	CIT	T	501	-	-	5/16/16/16	-
3	GOL	J	502	-	-	4/4/4/4	-
3	GOL	M	502	-	-	0/4/4/4	-
2	CIT	G	501	-	-	10/16/16/16	-
2	CIT	I	501	-	-	8/16/16/16	-
3	GOL	K	503	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	P	501	-	-	5/16/16/16	-
2	CIT	Q	501	-	-	5/16/16/16	-
2	CIT	J	501	-	-	5/16/16/16	-
3	GOL	F	502	-	-	0/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	E	502	-	-	2/4/4/4	-
2	CIT	O	501	-	-	9/16/16/16	-
3	GOL	N	502	-	-	2/4/4/4	-
3	GOL	T	502	-	-	2/4/4/4	-
3	GOL	G	502	-	-	2/4/4/4	-
2	CIT	A	501	-	-	5/16/16/16	-
2	CIT	N	501	-	-	8/16/16/16	-
2	CIT	H	501	-	-	5/16/16/16	-
2	CIT	R	501	-	-	5/16/16/16	-
3	GOL	I	502	-	-	1/4/4/4	-
3	GOL	J	503	-	-	1/4/4/4	-
2	CIT	B	501	-	-	10/16/16/16	-

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	CIT	O6-C6-C3	4.70	121.21	113.05
2	F	501	CIT	O6-C6-C3	4.44	120.76	113.05
2	P	501	CIT	O6-C6-C3	4.36	120.63	113.05
2	K	501	CIT	O6-C6-C3	4.35	120.61	113.05
2	N	501	CIT	O6-C6-C3	4.32	120.56	113.05
2	Q	501	CIT	O6-C6-C3	4.31	120.53	113.05
2	G	501	CIT	O6-C6-C3	4.26	120.45	113.05
2	J	501	CIT	O6-C6-C3	4.25	120.44	113.05
2	V	501	CIT	O6-C6-C3	4.23	120.40	113.05
2	D	501	CIT	O6-C6-C3	4.18	120.30	113.05
2	F	501	CIT	C3-C2-C1	-4.15	103.76	113.81
2	I	501	CIT	O6-C6-C3	4.13	120.22	113.05
2	A	501	CIT	O6-C6-C3	4.07	120.12	113.05
2	T	501	CIT	O6-C6-C3	3.99	119.98	113.05
2	R	501	CIT	O6-C6-C3	3.98	119.96	113.05
2	C	501	CIT	O6-C6-C3	3.95	119.90	113.05
2	H	501	CIT	O6-C6-C3	3.93	119.87	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	CIT	O6-C6-C3	3.82	119.67	113.05
2	M	501	CIT	O6-C6-C3	3.62	119.34	113.05
2	L	501	CIT	O6-C6-C3	3.49	119.11	113.05
2	O	501	CIT	C4-C3-C6	-3.33	102.95	110.11
2	C	501	CIT	C3-C2-C1	-3.30	105.83	113.81
2	O	501	CIT	O6-C6-C3	3.29	118.76	113.05
2	B	501	CIT	C4-C3-C6	-3.20	103.24	110.11
2	P	501	CIT	C3-C2-C1	-2.92	106.75	113.81
2	R	501	CIT	C3-C2-C1	-2.82	106.98	113.81
2	C	501	CIT	O4-C5-C4	2.79	123.30	114.35
2	J	501	CIT	C3-C2-C1	-2.66	107.37	113.81
2	G	501	CIT	C3-C2-C1	-2.63	107.44	113.81
2	A	501	CIT	O2-C1-C2	2.56	122.58	114.35
2	B	501	CIT	C3-C4-C5	-2.54	107.67	113.81
2	O	501	CIT	C4-C3-C2	2.53	115.76	109.16
2	A	501	CIT	O4-C5-C4	2.53	122.47	114.35
2	L	501	CIT	C4-C3-C6	-2.53	104.67	110.11
2	H	501	CIT	O4-C5-C4	2.51	122.42	114.35
2	H	501	CIT	C4-C3-C2	2.46	115.58	109.16
2	A	501	CIT	C3-C4-C5	-2.42	107.95	113.81
2	B	501	CIT	O5-C6-C3	-2.42	118.83	122.25
2	T	501	CIT	C3-C2-C1	-2.40	107.99	113.81
2	N	501	CIT	C3-C2-C1	-2.39	108.02	113.81
2	B	501	CIT	C4-C3-C2	2.33	115.23	109.16
2	Q	501	CIT	C3-C2-C1	-2.31	108.21	113.81
2	M	501	CIT	O2-C1-C2	2.26	121.61	114.35
2	B	501	CIT	O2-C1-O1	-2.25	117.69	123.30
2	M	501	CIT	C3-C2-C1	-2.25	108.36	113.81
2	F	501	CIT	O2-C1-C2	2.25	121.58	114.35
2	C	501	CIT	O4-C5-O3	-2.22	117.75	123.30
2	V	501	CIT	C3-C2-C1	-2.22	108.45	113.81
2	L	501	CIT	O2-C1-C2	2.20	121.41	114.35
2	H	501	CIT	O2-C1-C2	2.20	121.40	114.35
2	L	501	CIT	O4-C5-C4	2.19	121.37	114.35
2	A	501	CIT	C4-C3-C2	2.18	114.83	109.16
2	Q	501	CIT	O2-C1-C2	2.15	121.26	114.35
2	P	501	CIT	O4-C5-C4	2.13	121.19	114.35
2	L	501	CIT	O2-C1-O1	-2.10	118.07	123.30
2	A	501	CIT	C3-C2-C1	-2.10	108.74	113.81
2	H	501	CIT	C4-C3-C6	-2.09	105.61	110.11
2	L	501	CIT	C4-C3-C2	2.08	114.58	109.16
2	D	501	CIT	O2-C1-C2	2.07	120.99	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	CIT	O4-C5-C4	2.06	120.96	114.35
2	H	501	CIT	C3-C4-C5	-2.05	108.86	113.81
2	I	501	CIT	O2-C1-C2	2.04	120.91	114.35
2	E	501	CIT	O4-C5-C4	2.02	120.83	114.35
2	A	501	CIT	O2-C1-O1	-2.01	118.28	123.30
2	R	501	CIT	C3-C4-C5	-2.01	108.94	113.81
2	O	501	CIT	O2-C1-O1	-2.01	118.29	123.30
2	G	501	CIT	O4-C5-C4	2.00	120.78	114.35

There are no chirality outliers.

All (168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	501	CIT	C2-C3-C6-O5
2	H	501	CIT	C2-C3-C6-O6
2	H	501	CIT	O7-C3-C6-O5
2	H	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C2-C3-C6-O5
2	A	501	CIT	C2-C3-C6-O6
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6
2	B	501	CIT	C2-C3-C6-O5
2	B	501	CIT	C2-C3-C6-O6
2	B	501	CIT	O7-C3-C6-O5
2	B	501	CIT	O7-C3-C6-O6
2	C	501	CIT	C2-C3-C6-O5
2	C	501	CIT	C2-C3-C6-O6
2	C	501	CIT	O7-C3-C6-O5
2	C	501	CIT	O7-C3-C6-O6
2	D	501	CIT	C2-C3-C6-O5
2	D	501	CIT	C2-C3-C6-O6
2	D	501	CIT	O7-C3-C6-O5
2	D	501	CIT	O7-C3-C6-O6
2	E	501	CIT	C2-C3-C6-O5
2	E	501	CIT	C2-C3-C6-O6
2	E	501	CIT	O7-C3-C6-O5
2	E	501	CIT	O7-C3-C6-O6
2	F	501	CIT	C2-C3-C6-O5
2	F	501	CIT	C2-C3-C6-O6
2	F	501	CIT	O7-C3-C6-O5
2	F	501	CIT	O7-C3-C6-O6
2	G	501	CIT	C2-C3-C6-O5

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Mol	Chain	Res	Type	Atoms
2	G	501	CIT	C2-C3-C6-O6
2	G	501	CIT	O7-C3-C6-O5
2	G	501	CIT	O7-C3-C6-O6
2	I	501	CIT	C2-C3-C6-O6
2	I	501	CIT	O7-C3-C6-O5
2	I	501	CIT	O7-C3-C6-O6
2	J	501	CIT	C2-C3-C6-O5
2	J	501	CIT	C2-C3-C6-O6
2	J	501	CIT	O7-C3-C6-O5
2	J	501	CIT	O7-C3-C6-O6
2	K	501	CIT	C2-C3-C6-O5
2	K	501	CIT	C2-C3-C6-O6
2	K	501	CIT	O7-C3-C6-O5
2	K	501	CIT	O7-C3-C6-O6
2	L	501	CIT	C2-C3-C4-C5
2	L	501	CIT	O7-C3-C4-C5
2	L	501	CIT	C2-C3-C6-O5
2	L	501	CIT	C2-C3-C6-O6
2	L	501	CIT	O7-C3-C6-O5
2	L	501	CIT	O7-C3-C6-O6
2	M	501	CIT	C2-C3-C4-C5
2	M	501	CIT	O7-C3-C4-C5
2	M	501	CIT	C2-C3-C6-O5
2	M	501	CIT	C2-C3-C6-O6
2	M	501	CIT	O7-C3-C6-O5
2	M	501	CIT	O7-C3-C6-O6
2	N	501	CIT	C2-C3-C6-O5
2	N	501	CIT	C2-C3-C6-O6
2	N	501	CIT	O7-C3-C6-O5
2	N	501	CIT	O7-C3-C6-O6
2	O	501	CIT	C2-C3-C4-C5
2	O	501	CIT	O7-C3-C4-C5
2	O	501	CIT	C2-C3-C6-O5
2	O	501	CIT	C2-C3-C6-O6
2	O	501	CIT	O7-C3-C6-O5
2	O	501	CIT	O7-C3-C6-O6
2	P	501	CIT	C2-C3-C6-O5
2	P	501	CIT	C2-C3-C6-O6
2	P	501	CIT	O7-C3-C6-O5
2	P	501	CIT	O7-C3-C6-O6
2	Q	501	CIT	C2-C3-C6-O5
2	Q	501	CIT	C2-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	Q	501	CIT	O7-C3-C6-O5
2	Q	501	CIT	O7-C3-C6-O6
2	R	501	CIT	C2-C3-C6-O5
2	R	501	CIT	C2-C3-C6-O6
2	R	501	CIT	O7-C3-C6-O5
2	R	501	CIT	O7-C3-C6-O6
2	V	501	CIT	C2-C3-C6-O5
2	V	501	CIT	C2-C3-C6-O6
2	V	501	CIT	O7-C3-C6-O5
2	V	501	CIT	O7-C3-C6-O6
2	T	501	CIT	C2-C3-C6-O5
2	T	501	CIT	C2-C3-C6-O6
2	T	501	CIT	O7-C3-C6-O5
2	T	501	CIT	O7-C3-C6-O6
3	K	502	GOL	O1-C1-C2-C3
3	N	502	GOL	C1-C2-C3-O3
3	V	502	GOL	O1-C1-C2-C3
3	T	502	GOL	O1-C1-C2-C3
2	M	501	CIT	C1-C2-C3-C4
2	M	501	CIT	C1-C2-C3-C6
3	G	502	GOL	O1-C1-C2-O2
3	V	502	GOL	O1-C1-C2-O2
2	E	501	CIT	C2-C3-C4-C5
2	E	501	CIT	O7-C3-C4-C5
2	L	501	CIT	C6-C3-C4-C5
2	M	501	CIT	C6-C3-C4-C5
2	O	501	CIT	C6-C3-C4-C5
3	D	502	GOL	O1-C1-C2-C3
3	E	502	GOL	C1-C2-C3-O3
3	G	502	GOL	O1-C1-C2-C3
3	J	502	GOL	O1-C1-C2-C3
3	J	502	GOL	C1-C2-C3-O3
3	P	502	GOL	O1-C1-C2-C3
2	I	501	CIT	C4-C3-C6-O5
2	O	501	CIT	C4-C3-C6-O6
3	E	502	GOL	O2-C2-C3-O3
3	K	502	GOL	O1-C1-C2-O2
3	N	502	GOL	O2-C2-C3-O3
3	T	502	GOL	O1-C1-C2-O2
2	B	501	CIT	C2-C3-C4-C5
2	B	501	CIT	O7-C3-C4-C5
2	F	501	CIT	O7-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	G	501	CIT	O7-C3-C4-C5
2	I	501	CIT	C2-C3-C4-C5
2	I	501	CIT	O7-C3-C4-C5
2	N	501	CIT	O7-C3-C4-C5
2	M	501	CIT	C1-C2-C3-O7
3	I	502	GOL	O1-C1-C2-C3
3	L	502	GOL	O1-C1-C2-C3
2	B	501	CIT	C4-C3-C6-O5
2	B	501	CIT	C4-C3-C6-O6
2	C	501	CIT	C4-C3-C6-O5
2	C	501	CIT	C4-C3-C6-O6
2	G	501	CIT	C4-C3-C6-O5
2	G	501	CIT	C4-C3-C6-O6
2	I	501	CIT	C2-C3-C6-O5
2	I	501	CIT	C4-C3-C6-O6
2	K	501	CIT	C4-C3-C6-O5
2	K	501	CIT	C4-C3-C6-O6
2	N	501	CIT	C4-C3-C6-O5
2	N	501	CIT	C4-C3-C6-O6
2	V	501	CIT	C4-C3-C6-O5
2	V	501	CIT	C4-C3-C6-O6
3	K	503	GOL	O1-C1-C2-O2
2	E	501	CIT	C6-C3-C4-C5
2	G	501	CIT	C2-C3-C4-C5
2	C	501	CIT	O7-C3-C4-C5
2	D	501	CIT	O7-C3-C4-C5
3	J	502	GOL	O2-C2-C3-O3
2	H	501	CIT	O7-C3-C4-C5
2	G	501	CIT	C1-C2-C3-C6
2	K	501	CIT	O7-C3-C4-C5
2	R	501	CIT	O7-C3-C4-C5
2	V	501	CIT	O7-C3-C4-C5
2	T	501	CIT	O7-C3-C4-C5
2	L	501	CIT	C4-C3-C6-O6
3	J	502	GOL	O1-C1-C2-O2
3	K	503	GOL	O2-C2-C3-O3
2	G	501	CIT	C1-C2-C3-C4
2	J	501	CIT	O7-C3-C4-C5
2	P	501	CIT	O7-C3-C4-C5
2	Q	501	CIT	O7-C3-C4-C5
3	D	502	GOL	O1-C1-C2-O2
3	J	503	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	P	502	GOL	O1-C1-C2-O2
2	A	501	CIT	O7-C3-C4-C5
2	B	501	CIT	C1-C2-C3-C4
2	O	501	CIT	C4-C3-C6-O5
2	F	501	CIT	C2-C3-C4-C5
2	C	501	CIT	C3-C4-C5-O3
2	C	501	CIT	C3-C4-C5-O4
2	L	501	CIT	C1-C2-C3-C4
2	N	501	CIT	C2-C3-C4-C5
2	D	501	CIT	C4-C3-C6-O6
3	L	502	GOL	O1-C1-C2-O2
3	K	503	GOL	O1-C1-C2-C3
2	B	501	CIT	C6-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.