

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 - 02:10 AM EDT

:	6V96
:	Agrobacterium tumefaciens ADP-Glucose pyrophosphorylase-S72E
:	Zheng, Y.; Hussien, R.; Alghamdi, M.A.; Ballicora, M.A.; Liu, D.
:	2019-12-13
:	1.80 Å(reported)
	: : : :

This is a Full wwPDB X-ray Structure Validation 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:

DB archive December 25th 2019)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 1.80 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 (i)

There are 4 unique types of molecules in this entry. The entry contains 74015 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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	415	Total 3291	C 2086	N 571	O 621	S 13	0	6	0
1	А	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	В	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	С	411	Total 3266	C 2072	N 564	O 616	S 14	0	7	0
1	D	415	Total 3281	C 2081	N 567	O 620	S 13	0	6	0
1	Е	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	F	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	G	415	Total 3293	C 2087	N 571	O 621	S 14	0	7	0
1	Ι	415	Total 3293	C 2087	N 571	O 621	S 14	0	7	0
1	J	408	Total 3248	C 2062	N 561	O 611	S 14	0	7	0
1	K	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	L	415	Total 3295	C 2089	N 571	O 621	$\begin{array}{c} \mathrm{S} \\ 14 \end{array}$	0	7	0
1	М	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	Ν	415	Total 3287	C 2084	N 570	O 620	S 13	0	6	0
1	Ο	415	Total 3301	C 2092	N 572	0 622	S 15	0	8	0
1	Р	415	Total 3310	C 2099	N 575	O 623	S 13	0	8	0

• Molecule 1 is a protein called Glucose-1-phosphate adenylyltransferase.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	0	415	Total	С	Ν	0	\mathbf{S}	0	7	0
1	Q	410	3299	2093	571	622	13	0	1	0
1	D	415	Total	С	Ν	0	S	0	7	0
1	π		3295	2089	571	621	14	0		0
1	V	V 415	Total	С	Ν	0	S	4	6	0
1	v	410	3287	2084	570	620	13	4		0
1	Т	415	Total	С	Ν	0	S	19	7	0
	415	3295	2089	571	621	14	12	4	0	

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There are 420 discrepancies between the modelled and reference sequences:

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



Chain	Residue	Modelled	Actual	Comment	Reference
А	-9	SER	_	expression tag	UNP Q8U8L5
А	-8	SER	_	expression tag	UNP Q8U8L5
А	-7	GLY	-	expression tag	UNP Q8U8L5
А	-6	LEU	-	expression tag	UNP Q8U8L5
А	-5	VAL	-	expression tag	UNP Q8U8L5
А	-4	PRO	-	expression tag	UNP Q8U8L5
А	-3	ARG	-	expression tag	UNP Q8U8L5
А	-2	GLY	-	expression tag	UNP Q8U8L5
А	-1	SER	-	expression tag	UNP Q8U8L5
А	0	HIS	-	expression tag	UNP Q8U8L5
А	72	GLU	SER	engineered mutation	UNP Q8U8L5
В	-19	MET	-	expression tag	UNP Q8U8L5
В	-18	GLY	-	expression tag	UNP Q8U8L5
В	-17	SER	-	expression tag	UNP Q8U8L5
В	-16	SER	-	expression tag	UNP Q8U8L5
В	-15	HIS	-	expression tag	UNP Q8U8L5
В	-14	HIS	-	expression tag	UNP Q8U8L5
В	-13	HIS	-	expression tag	UNP Q8U8L5
В	-12	HIS	-	expression tag	UNP Q8U8L5
В	-11	HIS	-	expression tag	UNP Q8U8L5
В	-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	GLU	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 Q8U8L $\overline{5}$
C	-10	HIS	-	expression tag	UNP Q8U8L5

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



Chain	Residue	Modelled	Actual	Comment	Reference
Е	-9	SER	-	expression tag	UNP Q8U8L5
Е	-8	SER	-	expression tag	UNP Q8U8L5
Е	-7	GLY	_	expression tag	UNP Q8U8L5
Е	-6	LEU	_	expression tag	UNP Q8U8L5
Е	-5	VAL	-	expression tag	UNP Q8U8L5
Е	-4	PRO	-	expression tag	UNP Q8U8L5
Е	-3	ARG	-	expression tag	UNP Q8U8L5
Е	-2	GLY	-	expression tag	UNP Q8U8L5
Е	-1	SER	-	expression tag	UNP Q8U8L5
Е	0	HIS	-	expression tag	UNP Q8U8L5
Е	72	GLU	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
\mathbf{F}	-1	SER	-	expression tag	UNP Q8U8L5
F	0	HIS	-	expression tag	UNP Q8U8L5
F	72	GLU	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

expression tagUNP Q8U8L5Continued on next page...



Comment

Reference

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 Chain
 Residue
 Modelled
 Actual

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	GLU	SER	engineered mutation	UNP Q8U8L5
Ι	-19	MET	-	expression tag	UNP Q8U8L5
Ι	-18	GLY	-	expression tag	UNP Q8U8L5
Ι	-17	SER	-	expression tag	UNP Q8U8L5
Ι	-16	SER	-	expression tag	UNP Q8U8L5
Ι	-15	HIS	-	expression tag	UNP Q8U8L5
Ι	-14	HIS	-	expression tag	UNP Q8U8L5
Ι	-13	HIS	-	expression tag	UNP Q8U8L5
Ι	-12	HIS	-	expression tag	UNP Q8U8L5
Ι	-11	HIS	-	expression tag	UNP Q8U8L5
Ι	-10	HIS	-	expression tag	UNP Q8U8L5
Ι	-9	SER	-	expression tag	UNP Q8U8L5
Ι	-8	SER	-	expression tag	UNP Q8U8L5
Ι	-7	GLY	-	expression tag	UNP Q8U8L5
Ι	-6	LEU	-	expression tag	UNP Q8U8L5
Ι	-5	VAL	-	expression tag	UNP Q8U8L5
Ι	-4	PRO	-	expression tag	UNP Q8U8L5
Ι	-3	ARG	-	expression tag	UNP Q8U8L5
Ι	-2	GLY	-	expression tag	UNP Q8U8L5
Ι	-1	SER	-	expression tag	UNP Q8U8L5
Ι	0	HIS	-	expression tag	UNP Q8U8L5
Ι	72	GLU	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



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	GLU	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	GLU	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



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	GLU	SER	engineered mutation	UNP Q8U8L5
М	-19	MET	-	expression tag	UNP Q8U8L5
М	-18	GLY	-	expression tag	UNP Q8U8L5
М	-17	SER	-	expression tag	UNP Q8U8L5
М	-16	SER	-	expression tag	UNP Q8U8L5
М	-15	HIS	-	expression tag	UNP Q8U8L5
М	-14	HIS	-	expression tag	UNP Q8U8L5
М	-13	HIS	-	expression tag	UNP Q8U8L5
М	-12	HIS	-	expression tag	UNP Q8U8L5
М	-11	HIS	-	expression tag	UNP Q8U8L5
М	-10	HIS	-	expression tag	UNP Q8U8L5
М	-9	SER	-	expression tag	UNP Q8U8L5
М	-8	SER	-	expression tag	UNP Q8U8L5
М	-7	GLY	-	expression tag	UNP Q8U8L5
М	-6	LEU	-	expression tag	UNP Q8U8L5
М	-5	VAL	-	expression tag	UNP Q8U8L5
М	-4	PRO	-	expression tag	UNP Q8U8L5
М	-3	ARG	-	expression tag	UNP Q8U8L5
М	-2	GLY	-	expression tag	UNP Q8U8L5
М	-1	SER	-	expression tag	UNP Q8U8L5
М	0	HIS	-	expression tag	UNP Q8U8L5
М	72	GLU	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
Ν	-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	GLU	SER	engineered mutation	UNP Q8U8L5
0	-19	MET	-	expression tag	UNP Q8U8L5
0	-18	GLY	-	expression tag	UNP Q8U8L5
0	-17	SER	-	expression tag	UNP Q8U8L5
0	-16	SER	-	expression tag	UNP Q8U8L5
0	-15	HIS	-	expression tag	UNP Q8U8L5
0	-14	HIS	-	expression tag	UNP Q8U8L5
0	-13	HIS	-	expression tag	UNP Q8U8L5
0	-12	HIS	-	expression tag	UNP Q8U8L5
0	-11	HIS	-	expression tag	UNP Q8U8L5
0	-10	HIS	-	expression tag	UNP Q8U8L5
0	-9	SER	-	expression tag	UNP Q8U8L5
0	-8	SER	-	expression tag	UNP Q8U8L5
0	-7	GLY	-	expression tag	UNP Q8U8L5
0	-6	LEU	-	expression tag	UNP Q8U8L5
0	-5	VAL	-	expression tag	UNP Q8U8L5
0	-4	PRO	-	expression tag	UNP Q8U8L5
0	-3	ARG	-	expression tag	UNP Q8U8L5
0	-2	GLY	-	expression tag	UNP Q8U8L5
0	-1	SER	-	expression tag	UNP Q8U8L5
0	0	HIS	-	expression tag	UNP Q8U8L5
0	72	GLU	SER	engineered mutation	UNP Q8U8L5
Р	-19	MET	-	expression tag	UNP Q8U8L5
Р	-18	GLY	-	expression tag	UNP Q8U8L5
Р	-17	SER	-	expression tag	UNP Q8U8L5
Р	-16	SER	-	expression tag	UNP Q8U8L5
Р	-15	HIS	-	expression tag	UNP Q8U8L5
Р	-14	HIS	-	expression tag	UNP Q8U8L5
Р	-13	HIS	-	expression tag	UNP Q8U8L5
Р	-12	HIS	-	expression tag	UNP Q8U8L5
Р	-11	HIS	-	expression tag	UNP Q8U8L5
Р	-10	HIS	-	expression tag	UNP Q8U8L5

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



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	GLU	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	GLU	SER	engineered mutation	UNP Q8U8L5
Т	-19	MET	-	expression tag	UNP Q8U8L5
Т	-18	GLY	-	expression tag	UNP Q8U8L5
Т	-17	SER	-	expression tag	UNP Q8U8L5
Т	-16	SER	-	expression tag	UNP $Q8\overline{U8L5}$
Т	-15	HIS	-	expression tag	UNP Q8U8L5
Т	-14	HIS	-	expression tag	UNP $Q8U8L5$
Т	-13	HIS	-	expression tag	UNP Q8U8L5
Т	-12	HIS	-	expression tag	UNP Q8U8L5
Т	-11	HIS	-	expression tag	UNP Q8U8L5
Т	-10	HIS	-	expression tag	UNP Q8U8L5



Chain	Residue	Modelled	Actual	Comment	Reference
Т	-9	SER	-	- expression tag	
Т	-8	SER	-	expression tag	UNP Q8U8L5
Т	-7	GLY	-	expression tag	UNP Q8U8L5
Т	-6	LEU	-	expression tag	UNP Q8U8L5
Т	-5	VAL	-	expression tag	UNP Q8U8L5
Т	-4	PRO	-	expression tag	UNP Q8U8L5
Т	-3	ARG	-	expression tag	UNP Q8U8L5
Т	-2	GLY	-	expression tag	UNP Q8U8L5
Т	-1	SER	-	expression tag	UNP Q8U8L5
Т	0	HIS	-	expression tag	UNP Q8U8L5
Т	72	GLU	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	Н	1	Total C O 13 6 7	0	0
2	А	1	Total C O 13 6 7	0	0
2	В	1	Total C O 13 6 7	0	0
2	С	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	Е	1	Total C O 13 6 7	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	Ι	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0
2	K	1	Total C O 13 6 7	0	0
2	L	1	Total C O 13 6 7	0	0
2	М	1	Total C O 13 6 7	0	0
2	Ν	1	Total C O 13 6 7	0	0
2	О	1	Total C O 13 6 7	0	0
2	Р	1	Total C O 13 6 7	0	0
2	Q	1	Total C O 13 6 7	0	0
2	R	1	Total C O 13 6 7	0	0
2	V	1	Total C O 13 6 7	0	0
2	Т	1	Total C O 13 6 7	0	0

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





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	С	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	Ι	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	J	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	К	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	L	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	М	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	Ν	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	О	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	Р	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	Q	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	R	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0
3	V	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	Т	1	$\begin{array}{c cc} Total & C & O \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	394	Total O 394 394	0	0
4	А	364	Total O 364 364	0	0
4	В	346	Total O 346 346	0	0
4	С	434	Total O 434 434	0	0
4	D	393	Total O 393 393	0	0
4	Е	385	Total O 385 385	0	0
4	F	378	Total O 378 378	0	0
4	G	392	Total O 392 392	0	0
4	Ι	412	Total O 412 412	0	0
4	J	412	Total O 412 412	0	0
4	K	404	Total O 404 404	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	372	Total O 372 372	0	0
4	М	361	Total O 361 361	0	0
4	Ν	384	Total O 384 384	0	0
4	О	348	Total O 348 348	0	0
4	Р	400	Total O 400 400	0	0
4	Q	446	Total O 446 446	0	0
4	R	470	Total O 470 470	0	0
4	V	361	Total O 361 361	0	0
4	Т	404	Total O 404 404	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	93.61Å 141.19Å 229.43Å	Depositor
a, b, c, α , β , γ	107.93° 101.72° 89.97°	Depositor
Resolution (Å)	37.39 - 1.80	Depositor
% Data completeness	76 7 (37 30 1 80)	Dopositor
(in resolution range)	10.1 (31.33-1.00)	Depositor
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.92 (at 1.79 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.193 , 0.228	Depositor
Wilson B-factor $(Å^2)$	17.6	Xtriage
Anisotropy	0.044	Xtriage
L-test for twinning ²	$< L >=0.59, < L^2>=0.44$	Xtriage
	0.477 for h,-k,-h-l	
Estimated twinning fraction	0.477 for -h,k,-k-l	Xtriage
	0.477 for -h,-k,h+k+l	
Total number of atoms	74015	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 72.17 % 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 2.3109e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

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



					Bond longths			Bond angles			
Mol	Type	Chain	Res	Link	Counts	BMSZ	# Z > 2	Counts	BMSZ	# Z > 2	
2	CIT	V	501	_	12.12.12	1.16	0	17.17.17	1.82	$\frac{1}{4}(23\%)$	
2	CIT	J	501	_	12,12,12	1.14	1 (8%)	17,17,17	2.08	5 (29%)	
3	GOL	А	502	-	5,5,5	0.27	0	5,5,5	1.28	1 (20%)	
2	CIT	K	501	-	12,12,12	0.94	0	17,17,17	1.88	2 (11%)	
2	CIT	N	501	-	12,12,12	0.98	0	17,17,17	1.75	3 (17%)	
2	CIT	Н	501	-	12,12,12	0.98	0	17,17,17	1.89	7 (41%)	
2	CIT	R	501	-	12,12,12	1.14	0	17,17,17	1.97	7 (41%)	
2	CIT	А	501	-	12,12,12	1.00	0	17,17,17	1.97	5 (29%)	
3	GOL	R	502	_	5,5,5	0.32	0	5,5,5	0.87	0	
2	CIT	Q	501	_	12,12,12	0.99	0	17,17,17	1.92	6 (35%)	
3	GOL	K	502	-	5,5,5	0.39	0	$5,\!5,\!5$	0.98	0	
3	GOL	Q	502	-	5,5,5	0.36	0	5,5,5	0.71	0	
3	GOL	Т	502	-	5,5,5	0.40	0	5,5,5	0.77	0	
3	GOL	N	502	-	5,5,5	0.19	0	5, 5, 5	1.02	0	
2	CIT	Р	501	-	12,12,12	1.13	0	17,17,17	2.09	6 (35%)	
2	CIT	F	501	-	12,12,12	1.10	0	17,17,17	1.81	5 (29%)	
2	CIT	Т	501	-	12,12,12	1.01	0	17,17,17	1.93	5 (29%)	
2	CIT	М	501	-	12,12,12	1.17	1 (8%)	17,17,17	1.94	5 (29%)	
3	GOL	Р	502	-	5,5,5	0.38	0	$5,\!5,\!5$	0.30	0	
3	GOL	K	503	-	5,5,5	0.45	0	5, 5, 5	0.48	0	
3	GOL	В	502	-	5,5,5	0.26	0	$5,\!5,\!5$	0.63	0	
3	GOL	J	502	-	$5,\!5,\!5$	0.34	0	$5,\!5,\!5$	0.28	0	
2	CIT	С	501	-	12,12,12	1.20	1 (8%)	17,17,17	1.94	5 (29%)	
2	CIT	В	501	-	12,12,12	1.14	1 (8%)	17,17,17	1.81	5 (29%)	
2	CIT	L	501	-	12,12,12	1.12	0	17,17,17	2.01	5 (29%)	
3	GOL	С	502	-	$5,\!5,\!5$	0.50	0	$5,\!5,\!5$	0.56	0	
2	CIT	D	501	-	12,12,12	0.99	0	17,17,17	1.95	4 (23%)	
2	CIT	G	501	-	12,12,12	1.19	1 (8%)	17,17,17	1.73	4 (23%)	
3	GOL	Н	502	-	5,5,5	0.41	0	$5,\!5,\!5$	0.26	0	
3	GOL	V	502	-	5,5,5	0.22	0	$5,\!5,\!5$	0.85	0	
3	GOL	М	502	-	5,5,5	0.36	0	$5,\!5,\!5$	0.55	0	
3	GOL	D	502	-	5,5,5	0.44	0	$5,\!5,\!5$	0.78	0	
2	CIT	Ι	501	-	12,12,12	1.08	0	17,17,17	1.80	3 (17%)	
2	CIT	Е	501	-	12,12,12	1.02	0	17,17,17	1.77	4 (23%)	
3	GOL	F	502	-	5,5,5	0.37	0	$5,\!5,\!5$	0.64	0	

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).



Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
INIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	L	502	-	$5,\!5,\!5$	0.46	0	$5,\!5,\!5$	0.47	0
3	GOL	Ε	502	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.34	0
3	GOL	J	503	-	$5,\!5,\!5$	0.51	0	$5,\!5,\!5$	1.70	2(40%)
2	CIT	0	501	-	12,12,12	1.03	0	17,17,17	1.90	5 (29%)
3	GOL	G	502	-	$5,\!5,\!5$	0.58	0	$5,\!5,\!5$	0.87	0
3	GOL	0	502	-	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.62	0
3	GOL	Ι	502	-	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.55	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	CIT	V	501	-	-	$\frac{5/16/16/16}{}$	-
2	CIT	J	501	-	-	5/16/16/16	-
3	GOL	А	502	-	-	4/4/4/4	-
2	CIT	К	501	-	-	5/16/16/16	-
2	CIT	Ν	501	-	-	5/16/16/16	-
2	CIT	Н	501	-	-	5/16/16/16	-
2	CIT	R	501	-	-	5/16/16/16	-
2	CIT	А	501	-	-	5/16/16/16	-
3	GOL	R	502	-	-	2/4/4/4	-
2	CIT	Q	501	-	-	5/16/16/16	-
3	GOL	К	502	-	-	2/4/4/4	-
3	GOL	Q	502	-	-	1/4/4/4	-
3	GOL	Т	502	-	-	2/4/4/4	-
3	GOL	Ν	502	-	-	2/4/4/4	-
2	CIT	Р	501	-	-	5/16/16/16	-
2	CIT	F	501	-	-	5/16/16/16	-
2	CIT	Т	501	-	-	5/16/16/16	-
2	CIT	М	501	-	-	6/16/16/16	-
3	GOL	Р	502	-	-	0/4/4/4	-
3	GOL	К	503	-	-	2/4/4/4	-
3	GOL	В	502	-	-	0/4/4/4	-
3	GOL	J	502	-	-	0/4/4/4	-
2	CIT	С	501	-	-	8/16/16/16	-
2	CIT	В	501	-	-	6/16/16/16	-



Mol	Type	Chain	\mathbf{Res}	Link	Chirals	Torsions	Rings
2	CIT	L	501	-	-	5/16/16/16	-
3	GOL	С	502	-	-	0/4/4/4	-
2	CIT	D	501	-	-	5/16/16/16	-
2	CIT	G	501	-	-	5/16/16/16	-
3	GOL	Н	502	-	-	0/4/4/4	-
3	GOL	V	502	-	-	0/4/4/4	-
3	GOL	М	502	-	-	0/4/4/4	-
3	GOL	D	502	-	-	1/4/4/4	-
2	CIT	Ι	501	-	-	5/16/16/16	-
2	CIT	Е	501	-	-	5/16/16/16	-
3	GOL	F	502	-	-	0/4/4/4	-
3	GOL	L	502	-	-	0/4/4/4	-
3	GOL	Е	502	-	-	3/4/4/4	-
3	GOL	J	503	-	-	3/4/4/4	-
2	CIT	Ο	501	-	-	5/16/16/16	-
3	GOL	G	502	-	-	3/4/4/4	-
3	GOL	0	502	-	-	0/4/4/4	-
3	GOL	Ι	502	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	М	501	CIT	C3-C6	-2.40	1.50	1.53
2	С	501	CIT	C3-C6	-2.38	1.50	1.53
2	J	501	CIT	C3-C6	-2.19	1.51	1.53
2	G	501	CIT	C3-C6	-2.12	1.51	1.53
2	В	501	CIT	C3-C6	-2.06	1.51	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Р	501	CIT	C3-C2-C1	-5.11	101.44	113.81
2	Т	501	CIT	C3-C2-C1	-4.89	101.97	113.81
2	Κ	501	CIT	O6-C6-C3	4.57	120.99	113.05
2	Ν	501	CIT	O6-C6-C3	4.44	120.77	113.05
2	J	501	CIT	O6-C6-C3	4.39	120.67	113.05
2	R	501	CIT	O6-C6-C3	4.32	120.56	113.05
2	А	501	CIT	O6-C6-C3	4.31	120.53	113.05
2	С	501	CIT	C3-C2-C1	-4.28	103.45	113.81
2	Ē	501	CIT	O6-C6-C3	4.24	120.41	113.05



Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(°)
2	М	501	CIT	C3-C2-C1	-4.22	103.61	113.81
2	А	501	CIT	C3-C2-C1	-4.18	103.70	113.81
2	L	501	CIT	C3-C2-C1	-4.07	103.95	113.81
2	Н	501	CIT	O6-C6-C3	4.07	120.11	113.05
2	K	501	CIT	C3-C2-C1	-3.98	104.19	113.81
2	J	501	CIT	C3-C2-C1	-3.95	104.25	113.81
2	0	501	CIT	O6-C6-C3	3.92	119.85	113.05
2	Q	501	CIT	O6-C6-C3	3.90	119.83	113.05
2	Ι	501	CIT	O6-C6-C3	3.86	119.75	113.05
2	D	501	CIT	C3-C2-C1	-3.80	104.62	113.81
2	F	501	CIT	O6-C6-C3	3.80	119.64	113.05
2	Р	501	CIT	O6-C6-C3	3.79	119.64	113.05
2	В	501	CIT	O6-C6-C3	3.78	119.61	113.05
2	G	501	CIT	O7-C3-C6	-3.77	103.57	108.86
2	L	501	CIT	O6-C6-C3	3.70	119.48	113.05
2	F	501	CIT	C3-C2-C1	-3.64	105.01	113.81
2	V	501	CIT	O6-C6-C3	3.62	119.33	113.05
2	Ι	501	CIT	C3-C2-C1	-3.61	105.08	113.81
2	V	501	CIT	O7-C3-C6	-3.60	103.81	108.86
2	Н	501	CIT	C3-C2-C1	-3.59	105.12	113.81
2	D	501	CIT	O6-C6-C3	3.57	119.25	113.05
2	В	501	CIT	O7-C3-C6	-3.52	103.92	108.86
2	М	501	CIT	O6-C6-C3	3.48	119.10	113.05
2	Q	501	CIT	C3-C2-C1	-3.39	105.61	113.81
2	V	501	CIT	C3-C2-C1	-3.36	105.67	113.81
2	0	501	CIT	C3-C2-C1	-3.35	105.70	113.81
2	R	501	CIT	O7-C3-C6	-3.34	104.17	108.86
2	Т	501	CIT	O6-C6-C3	3.25	118.69	113.05
2	J	501	CIT	O5-C6-C3	-3.07	117.90	122.25
2	L	501	CIT	02-C1-C2	3.06	124.17	114.35
2	N	501	CIT	C3-C2-C1	-3.02	106.50	113.81
2	C	501	CIT	07-C3-C6	-2.98	104.69	108.86
2	G	501	CIT	06-C6-C3	2.96	118.19	113.05
2	E	501	CIT	C3-C2-C1	-2.96	106.65	113.81
2	C	501	CIT	06-C6-C3	2.92	118.11	113.05
		501	CIT	O4-C5-C4	2.90	123.67	114.35
2	K R	501	CIT	<u>C3-C2-C1</u>	-2.83	106.97	113.81
2		501	CIT	O4-C5-C4	2.77	123.25	114.35
	В	501		$\frac{\text{U3-U2-U1}}{\text{O4-U2-U1}}$	-2.73	107.19	113.81
2	J	501	CIT	04-C5-O3	-2.70	110.58	123.30
2	J	501	CIT	04-C5-C4	2.67	122.94	114.35
2	U	501	CIT	02-C1-C2	2.63	122.78	114.35

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	501	CIT	O4-C5-O3	-2.61	116.80	123.30
2	Q	501	CIT	O4-C5-C4	2.60	122.70	114.35
2	D	501	CIT	O2-C1-C2	2.58	122.63	114.35
2	G	501	CIT	C3-C2-C1	-2.55	107.65	113.81
3	А	502	GOL	C3-C2-C1	-2.51	101.93	111.70
2	Т	501	CIT	O2-C1-C2	2.50	122.39	114.35
2	Q	501	CIT	O2-C1-C2	2.47	122.28	114.35
3	J	503	GOL	O2-C2-C1	2.46	119.96	109.12
2	Р	501	CIT	O7-C3-C6	-2.45	105.42	108.86
2	R	501	CIT	O4-C5-O3	-2.44	117.22	123.30
2	М	501	CIT	O2-C1-C2	2.44	122.18	114.35
2	F	501	CIT	O4-C5-C4	2.38	122.00	114.35
2	0	501	CIT	O4-C5-C4	2.38	122.00	114.35
3	J	503	GOL	O1-C1-C2	2.37	121.55	110.20
2	L	501	CIT	O2-C1-O1	-2.35	117.45	123.30
2	Е	501	CIT	O4-C5-C4	2.35	121.89	114.35
2	R	501	CIT	O5-C6-C3	-2.34	118.94	122.25
2	Н	501	CIT	O2-C1-C2	2.31	121.76	114.35
2	А	501	CIT	O4-C5-C4	2.31	121.75	114.35
2	Q	501	CIT	O4-C5-O3	-2.30	117.57	123.30
2	F	501	CIT	O4-C5-O3	-2.28	117.61	123.30
2	М	501	CIT	O4-C5-C4	2.28	121.67	114.35
2	Н	501	CIT	O4-C5-C4	2.27	121.64	114.35
2	М	501	CIT	O5-C6-C3	-2.27	119.04	122.25
2	V	501	CIT	O4-C5-O3	-2.26	117.66	123.30
2	Т	501	CIT	O4-C5-O3	-2.26	117.68	123.30
2	N	501	CIT	O4-C5-O3	-2.22	117.77	123.30
2	F	501	CIT	O2-C1-C2	2.21	121.44	114.35
2	Ι	501	CIT	O5-C6-C3	-2.20	119.14	122.25
2	Н	501	CIT	O2-C1-O1	-2.19	117.83	123.30
2	В	501	CIT	O4-C5-O3	-2.19	117.84	123.30
2	G	501	CIT	O2-C1-O1	-2.17	117.89	123.30
2	В	501	CIT	O5-C6-C3	-2.16	119.20	122.25
2	Р	501	CIT	C4-C3-C6	2.14	114.70	110.11
2	Т	501	CIT	C3-C4-C5	-2.10	108.72	113.81
2	С	501	CIT	O4-C5-O3	-2.10	118.06	123.30
2	Ο	501	CIT	O4-C5-O3	-2.09	118.09	123.30
2	L	501	CIT	O7-C3-C6	-2.09	105.93	108.86
2	Р	501	CIT	O4-C5-C4	2.08	121.03	114.35
2	Н	501	CIT	C3-C4-C5	-2.08	108.78	113.81
2	А	501	CIT	O4-C5-O3	-2.08	118.12	123.30
2	А	501	CIT	O2-C1-C2	2.03	120.88	114.35



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Q	501	CIT	O5-C6-C3	-2.03	119.37	122.25
2	R	501	CIT	O4-C5-C4	2.03	120.86	114.35
2	Н	501	CIT	O4-C5-O3	-2.02	118.27	123.30
2	Р	501	CIT	O4-C5-O3	-2.01	118.28	123.30
2	R	501	CIT	O2-C1-O1	-2.01	118.30	123.30

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There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	Н	501	CIT	C2-C3-C6-O5
2	Н	501	CIT	C2-C3-C6-O6
2	Н	501	CIT	O7-C3-C6-O5
2	Н	501	CIT	O7-C3-C6-O6
2	А	501	CIT	C2-C3-C6-O5
2	А	501	CIT	C2-C3-C6-O6
2	А	501	CIT	O7-C3-C6-O5
2	А	501	CIT	O7-C3-C6-O6
2	В	501	CIT	C2-C3-C6-O5
2	В	501	CIT	C2-C3-C6-O6
2	В	501	CIT	O7-C3-C6-O5
2	В	501	CIT	O7-C3-C6-O6
2	С	501	CIT	C2-C3-C6-O5
2	С	501	CIT	C2-C3-C6-O6
2	С	501	CIT	O7-C3-C6-O5
2	С	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	Е	501	CIT	C2-C3-C6-O5
2	Е	501	CIT	C2-C3-C6-O6
2	Е	501	CIT	O7-C3-C6-O5
2	Е	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
2	G	501	CIT	C2-C3-C6-O6
2	G	501	CIT	O7-C3-C6-O5
2	G	501	CIT	O7-C3-C6-O6

All (130) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
2	Ι	501	CIT	C2-C3-C6-O5
2	Ι	501	CIT	C2-C3-C6-O6
2	Ι	501	CIT	O7-C3-C6-O5
2	Ι	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	Κ	501	CIT	C2-C3-C6-O5
2	Κ	501	CIT	C2-C3-C6-O6
2	Κ	501	CIT	O7-C3-C6-O5
2	Κ	501	CIT	O7-C3-C6-O6
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	М	501	CIT	C2-C3-C6-O5
2	М	501	CIT	C2-C3-C6-O6
2	М	501	CIT	O7-C3-C6-O5
2	М	501	CIT	O7-C3-C6-O6
2	Ν	501	CIT	C2-C3-C6-O5
2	Ν	501	CIT	C2-C3-C6-O6
2	Ν	501	CIT	O7-C3-C6-O5
2	Ν	501	CIT	O7-C3-C6-O6
2	0	501	CIT	C2-C3-C6-O5
2	0	501	CIT	C2-C3-C6-O6
2	0	501	CIT	O7-C3-C6-O5
2	0	501	CIT	O7-C3-C6-O6
2	Р	501	CIT	C2-C3-C6-O5
2	Р	501	CIT	C2-C3-C6-O6
2	Р	501	CIT	O7-C3-C6-O5
2	Р	501	CIT	O7-C3-C6-O6
2	Q	501	CIT	C2-C3-C6-O5
2	Q	501	CIT	C2-C3-C6-O6
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

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Mol	Chain	Res	Type	Atoms
2	V	501	CIT	O7-C3-C6-O5
2	V	501	CIT	O7-C3-C6-O6
2	Т	501	CIT	C2-C3-C6-O5
2	Т	501	CIT	C2-C3-C6-O6
2	Т	501	CIT	O7-C3-C6-O5
2	Т	501	CIT	O7-C3-C6-O6
3	G	502	GOL	O1-C1-C2-C3
3	G	502	GOL	C1-C2-C3-O3
3	J	503	GOL	O1-C1-C2-C3
3	Κ	503	GOL	C1-C2-C3-O3
3	N	502	GOL	C1-C2-C3-O3
3	Т	502	GOL	01-C1-C2-C3
3	N	502	GOL	O2-C2-C3-O3
3	А	502	GOL	01-C1-C2-C3
3	А	502	GOL	C1-C2-C3-O3
3	Е	502	GOL	C1-C2-C3-O3
3	А	502	GOL	O2-C2-C3-O3
3	Е	502	GOL	O2-C2-C3-O3
3	G	502	GOL	O1-C1-C2-O2
3	J	503	GOL	O1-C1-C2-O2
3	Κ	503	GOL	O2-C2-C3-O3
3	R	502	GOL	O1-C1-C2-C3
3	J	503	GOL	O2-C2-C3-O3
3	K	502	GOL	O1-C1-C2-O2
3	Т	502	GOL	O1-C1-C2-O2
2	D	501	CIT	O7-C3-C4-C5
2	Ι	501	CIT	O7-C3-C4-C5
2	0	501	CIT	O7-C3-C4-C5
2	R	501	CIT	O7-C3-C4-C5
2	V	501	CIT	O7-C3-C4-C5
2	Н	501	CIT	07-C3-C4-C5
2	A	501	CIT	07-C3-C4-C5
2	G	501	CIT	07-C3-C4-C5
2	J	501	CIT	07-C3-C4-C5
2	K	501	CIT	O7-C3-C4-C5
2	N	501	CIT	07-C3-C4-C5
2	Т	501	CIT	07-C3-C4-C5
2	М	501	CIT	07-C3-C4-C5
2	Р	501	CIT	O7-C3-C4-C5
3	A	502	GOL	01-C1-C2-O2
3	R	502	GOL	01-C1-C2-O2
2	B	501	CIT	07-C3-C4-C5

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6	V	9	6	
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Mol	Chain	Res	Type	Atoms
2	С	501	CIT	O7-C3-C4-C5
2	Е	501	CIT	O7-C3-C4-C5
2	F	501	CIT	O7-C3-C4-C5
2	L	501	CIT	O7-C3-C4-C5
2	Q	501	CIT	O7-C3-C4-C5
2	С	501	CIT	C4-C3-C6-O6
2	М	501	CIT	C2-C3-C4-C5
3	Κ	502	GOL	O1-C1-C2-C3
2	С	501	CIT	C3-C4-C5-O4
2	С	501	CIT	C3-C4-C5-O3
3	D	502	GOL	O1-C1-C2-O2
3	Е	502	GOL	O1-C1-C2-C3
2	В	501	CIT	C2-C3-C4-C5
3	Q	502	GOL	O1-C1-C2-O2

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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.

