



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2022 – 10:23 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)

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 ⓘ 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 ⓘ](#)) 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	:	2.29
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)	:	2.29

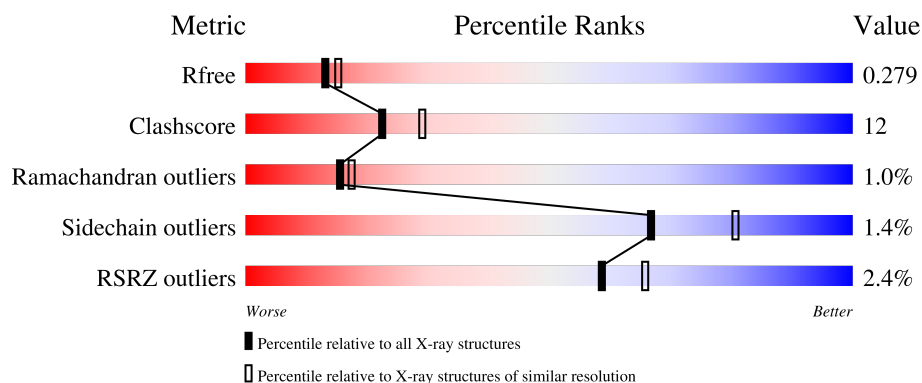
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>6%</div> </div> </div>
1	B	440	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>6%</div> </div> </div>
1	C	440	<div> <div>0%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>6%</div> </div> </div>
1	D	440	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>6%</div> </div> </div>
1	E	440	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	440	
1	G	440	
1	H	440	
1	I	440	
1	J	440	
1	K	440	
1	L	440	
1	M	440	
1	N	440	
1	O	440	
1	P	440	
1	Q	440	
1	R	440	
1	T	440	
1	V	440	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	K	503	-	-	X	-

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

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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

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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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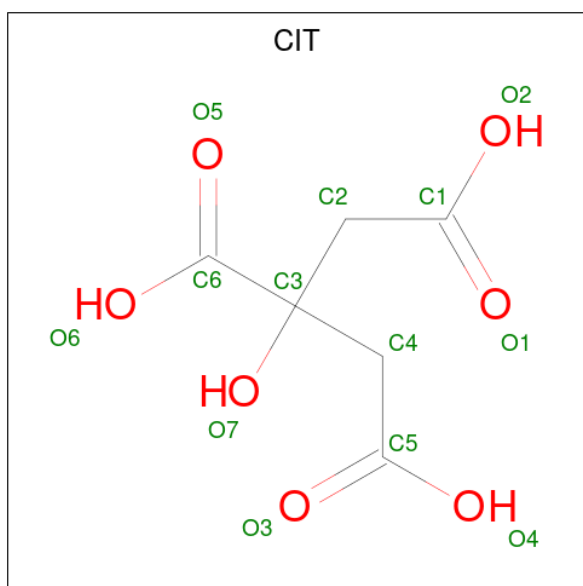
Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	SER	-	expression tag	UNP Q8U8L5
R	-8	SER	-	expression tag	UNP Q8U8L5
R	-7	GLY	-	expression tag	UNP Q8U8L5
R	-6	LEU	-	expression tag	UNP Q8U8L5
R	-5	VAL	-	expression tag	UNP Q8U8L5
R	-4	PRO	-	expression tag	UNP Q8U8L5
R	-3	ARG	-	expression tag	UNP Q8U8L5
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 C O 13 6 7	0	0
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 4 is water.

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

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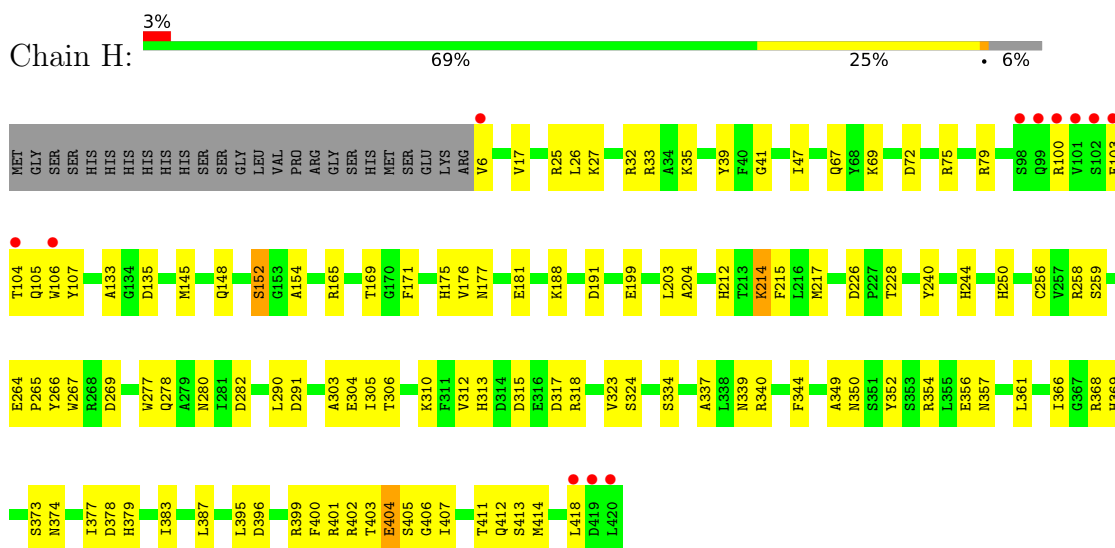
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	173	Total 173	O 173	0	0
4	M	145	Total 145	O 145	0	0
4	N	190	Total 190	O 190	0	0
4	O	178	Total 178	O 178	0	0
4	P	221	Total 221	O 221	0	0
4	Q	274	Total 274	O 274	0	0
4	R	262	Total 262	O 262	0	0
4	V	155	Total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

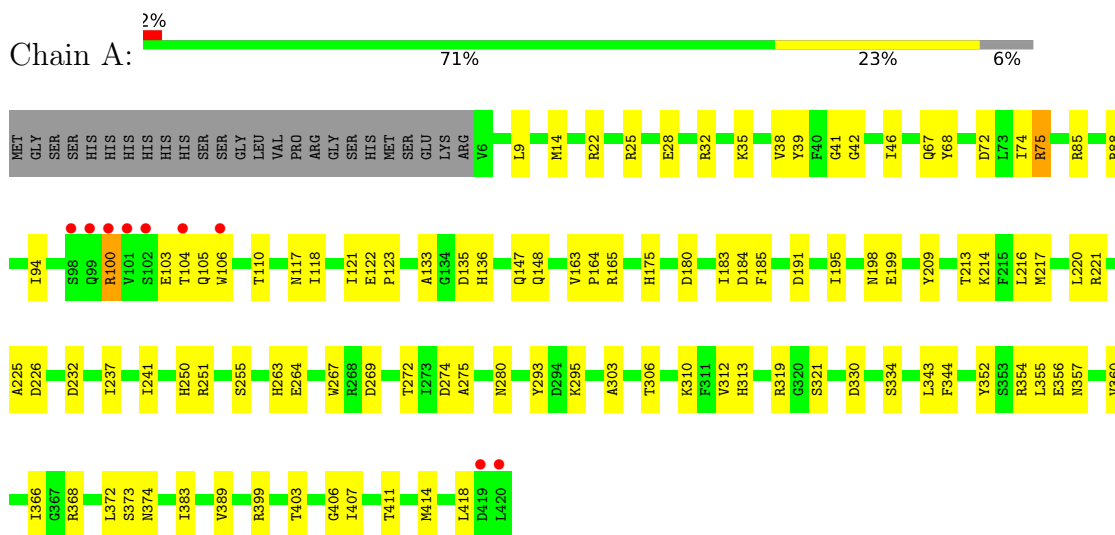
3 Residue-property plots [i](#)

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: Glucose-1-phosphate adenylyltransferase

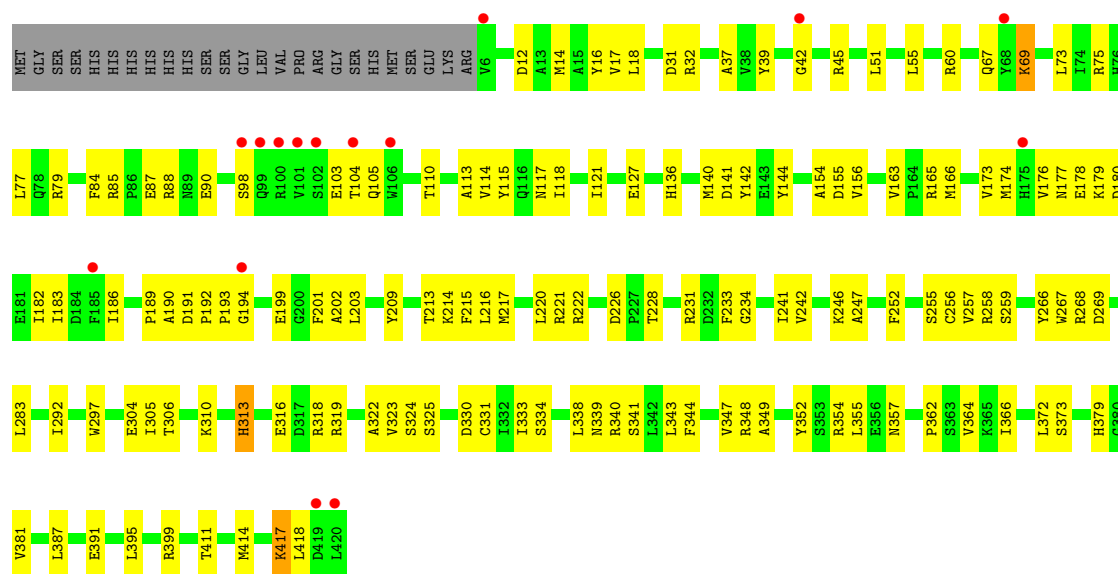


- Molecule 1: Glucose-1-phosphate adenylyltransferase

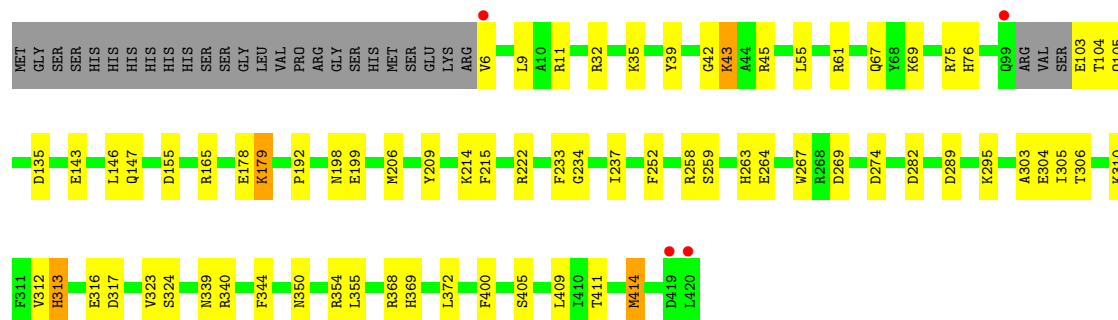
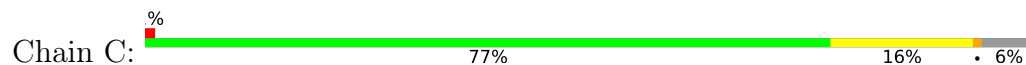


- Molecule 1: Glucose-1-phosphate adenylyltransferase

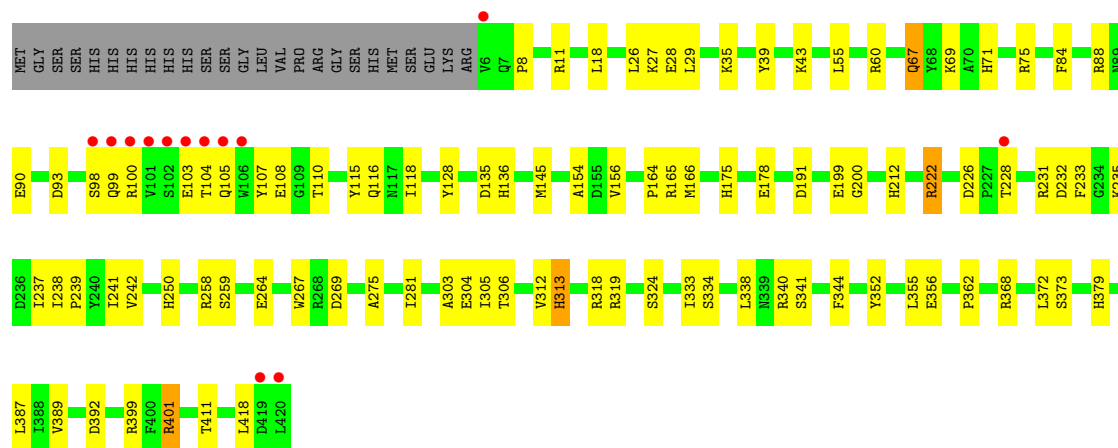




- Molecule 1: Glucose-1-phosphate adenylyltransferase

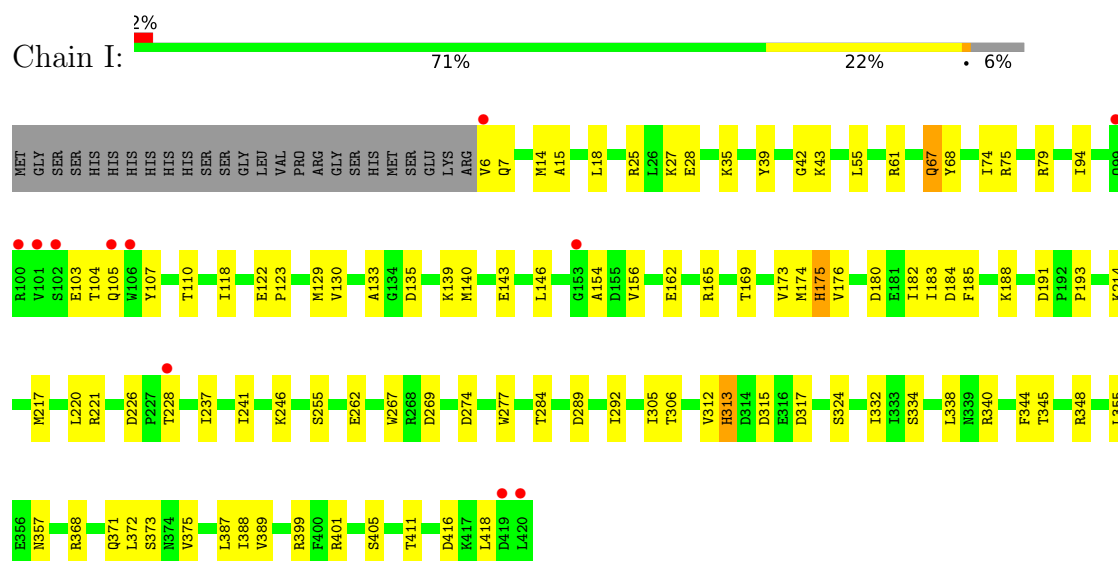


- Molecule 1: Glucose-1-phosphate adenylyltransferase

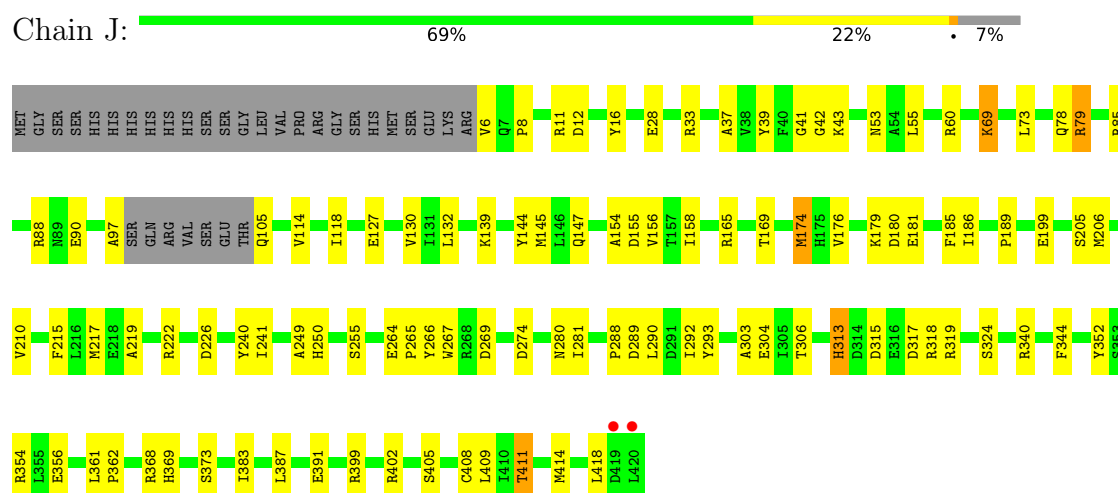


- Molecule 1: Glucose-1-phosphate adenylyltransferase

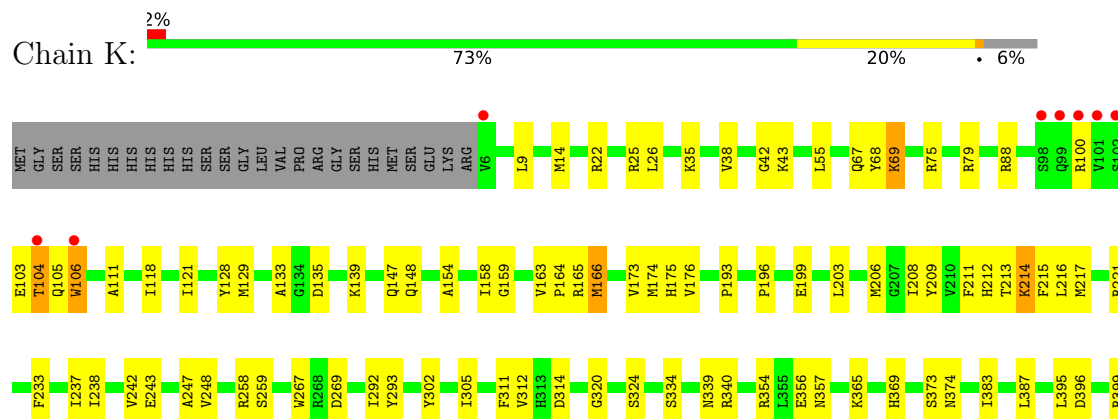
- Molecule 1: Glucose-1-phosphate adenylyltransferase

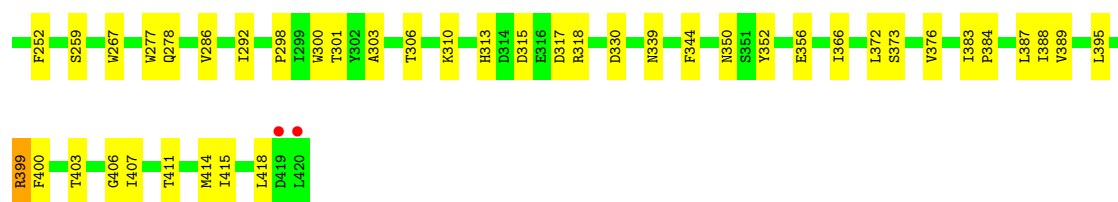


- Molecule 1: Glucose-1-phosphate adenylyltransferase

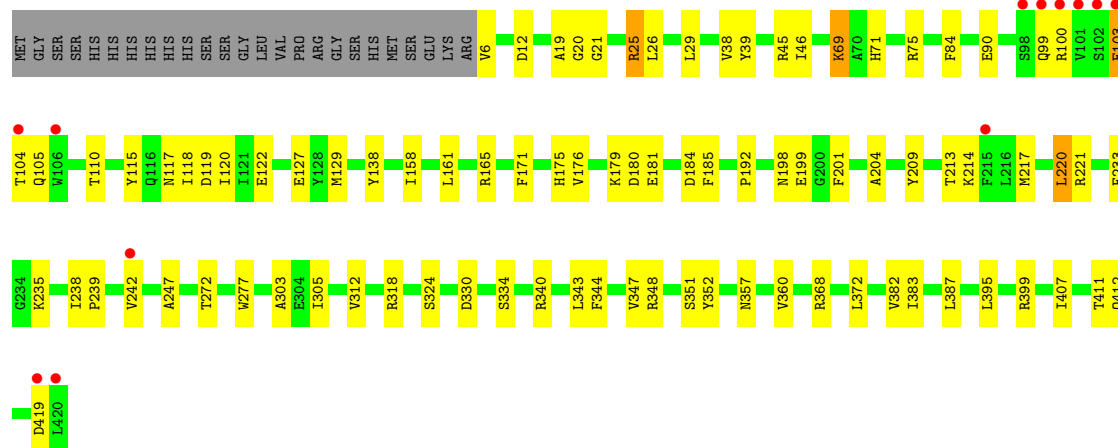
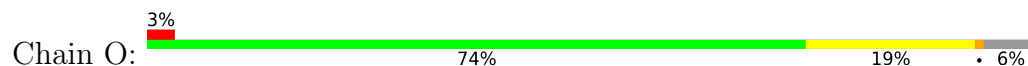


- Molecule 1: Glucose-1-phosphate adenylyltransferase

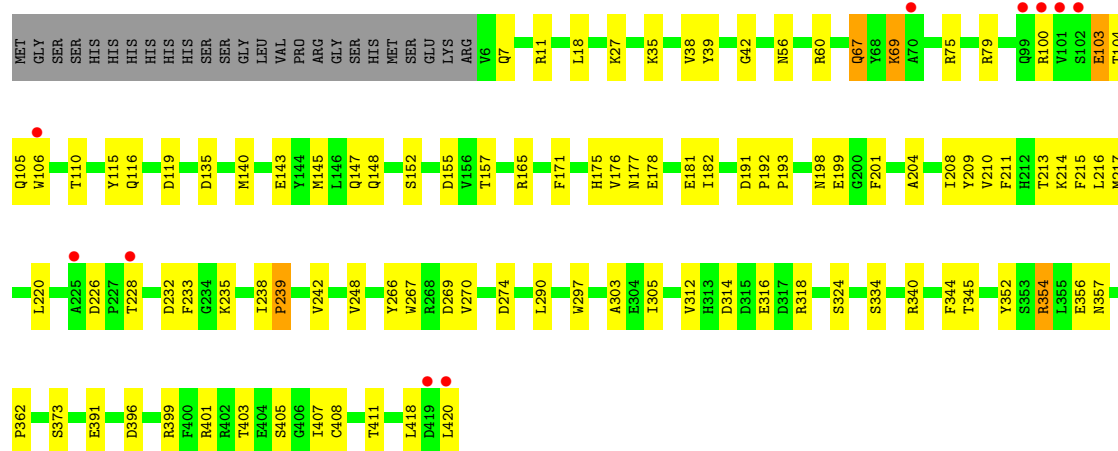




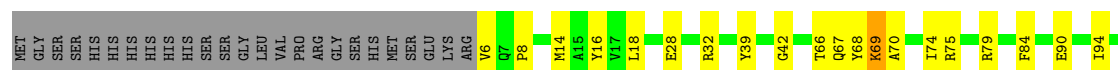
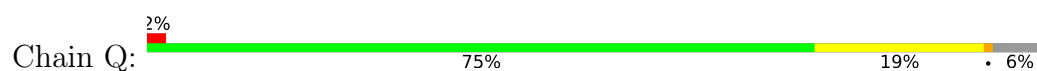
• Molecule 1: Glucose-1-phosphate adenylyltransferase

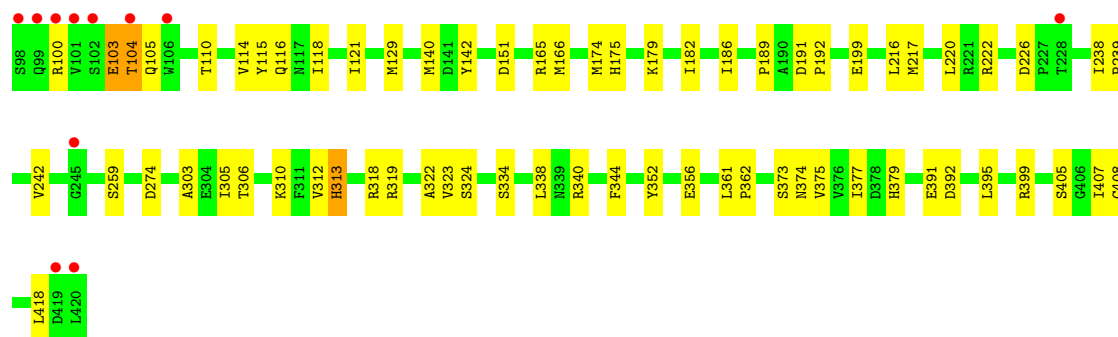


• Molecule 1: Glucose-1-phosphate adenylyltransferase

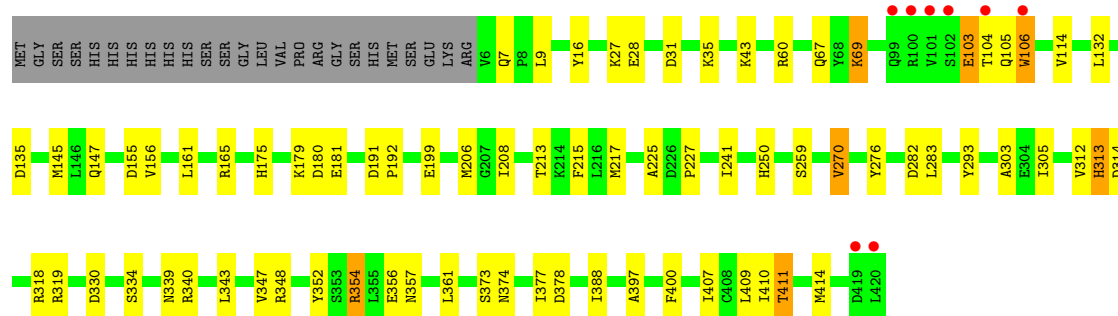
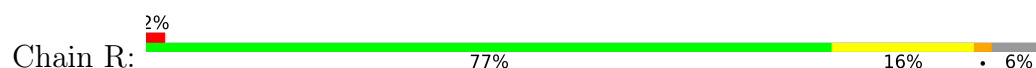


• Molecule 1: Glucose-1-phosphate adenylyltransferase

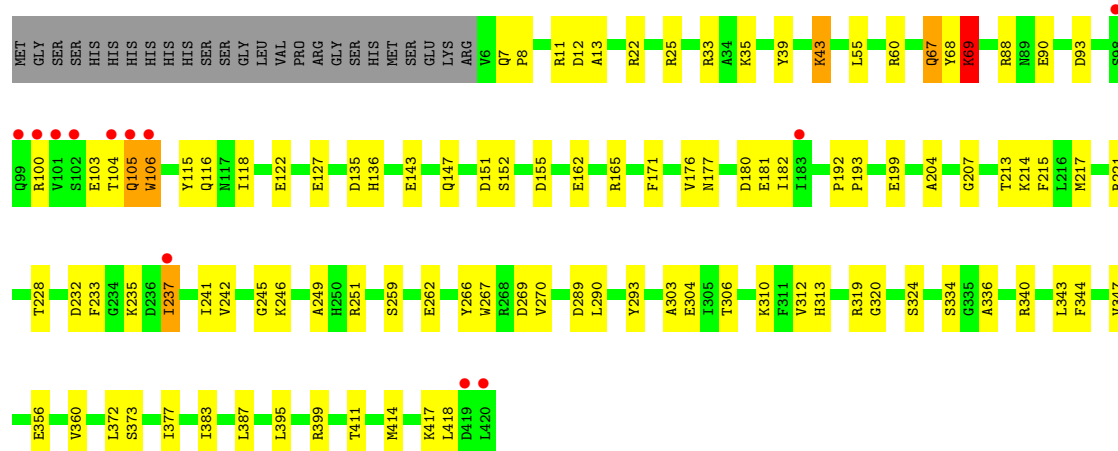




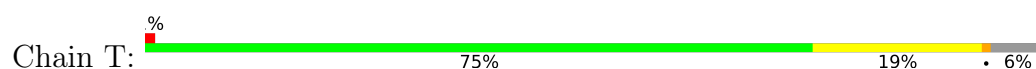
• Molecule 1: Glucose-1-phosphate adenylyltransferase

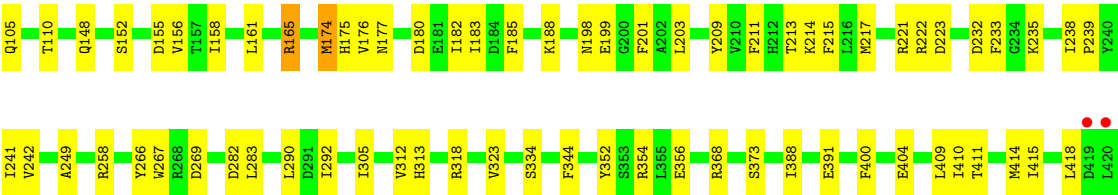


• Molecule 1: Glucose-1-phosphate adenylyltransferase



• Molecule 1: Glucose-1-phosphate adenylyltransferase





4 Data and refinement statistics

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 77.26 – 2.04	Depositor EDS
% Data completeness (in resolution range)	97.6 (62.50-2.30) 83.3 (77.26-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.234 , 0.279 0.234 , 0.279	Depositor DCC
R_{free} test set	23600 reflections (3.52%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.58$, $\langle L^2 \rangle = 0.42$	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
F_o, F_c correlation	0.94	EDS
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.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

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

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	0.34	1/3377 (0.0%)	0.52	0/4588
1	B	0.33	0/3366	0.54	1/4574 (0.0%)
1	C	0.31	0/3349	0.50	0/4549
1	D	0.30	0/3366	0.51	1/4574 (0.0%)
1	E	0.43	2/3366 (0.1%)	0.55	1/4574 (0.0%)
1	F	0.32	1/3366 (0.0%)	0.51	0/4574
1	G	0.30	0/3372	0.51	0/4582
1	H	0.30	0/3366	0.52	1/4574 (0.0%)
1	I	0.33	0/3383	0.53	0/4596
1	J	0.31	0/3326	0.51	1/4517 (0.0%)
1	K	0.29	0/3366	0.50	0/4574
1	L	0.31	0/3374	0.55	4/4584 (0.1%)
1	M	0.31	0/3366	0.52	1/4574 (0.0%)
1	N	0.31	0/3366	0.52	0/4574
1	O	0.30	0/3384	0.51	1/4597 (0.0%)
1	P	0.47	1/3390 (0.0%)	0.54	1/4606 (0.0%)
1	Q	0.30	0/3379	0.50	0/4592
1	R	0.35	2/3374 (0.1%)	0.54	1/4584 (0.0%)
1	T	0.31	0/3374	0.50	0/4584
1	V	0.30	0/3366	0.55	2/4574 (0.0%)
All	All	0.33	7/67376 (0.0%)	0.52	15/91545 (0.0%)

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	R	0	1
1	T	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	239	PRO	N-CD	-20.50	1.19	1.47
1	E	75	ARG	NE-CZ	13.80	1.50	1.33
1	E	199	GLU	CB-CG	7.41	1.66	1.52
1	A	75	ARG	NE-CZ	7.25	1.42	1.33
1	R	354	ARG	NE-CZ	-6.49	1.24	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	25	ARG	NE-CZ-NH1	-11.83	114.39	120.30
1	P	354	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	E	75	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	L	220	LEU	CB-CG-CD2	-8.66	96.29	111.00
1	R	354	ARG	NE-CZ-NH1	-8.33	116.14	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	354	ARG	Sidechain
1	T	211	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3297	0	3202	88	0
1	B	3286	0	3190	115	0
1	C	3270	0	3170	53	0
1	D	3286	0	3190	74	0
1	E	3286	0	3190	82	0
1	F	3286	0	3190	81	0
1	G	3292	0	3194	75	0
1	H	3286	0	3190	85	1
1	I	3303	0	3206	85	0
1	J	3247	0	3154	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	3286	0	3190	80	0
1	L	3294	0	3198	94	0
1	M	3286	0	3190	86	0
1	N	3286	0	3190	70	0
1	O	3304	0	3208	78	0
1	P	3309	0	3210	81	0
1	Q	3298	0	3198	66	0
1	R	3294	0	3198	56	0
1	T	3294	0	3198	66	0
1	V	3286	0	3190	76	0
2	A	13	0	5	2	0
2	B	13	0	5	3	0
2	C	13	0	5	4	0
2	D	13	0	5	2	0
2	E	13	0	5	2	0
2	F	13	0	5	4	0
2	G	13	0	5	4	0
2	H	13	0	5	5	0
2	I	13	0	5	3	0
2	J	13	0	5	2	0
2	K	13	0	5	0	0
2	L	13	0	5	4	0
2	M	13	0	5	1	0
2	N	13	0	5	2	0
2	O	13	0	5	3	0
2	P	13	0	5	0	0
2	Q	13	0	5	1	0
2	R	13	0	5	2	0
2	T	13	0	5	3	0
2	V	13	0	5	1	0
3	A	12	0	16	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	J	12	0	16	0	0
3	K	12	0	16	5	0
3	L	6	0	8	0	0
3	M	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	6	0	8	1	0
3	O	6	0	8	0	0
3	P	6	0	8	0	0
3	Q	6	0	8	0	0
3	R	6	0	8	0	0
3	T	6	0	8	0	0
3	V	6	0	8	3	0
4	A	181	0	0	16	1
4	B	179	0	0	28	0
4	C	243	0	0	13	0
4	D	209	0	0	17	0
4	E	185	0	0	18	2
4	F	160	0	0	16	0
4	G	175	0	0	21	1
4	H	172	0	0	16	0
4	I	214	0	0	20	1
4	J	274	0	0	28	1
4	K	177	0	0	17	0
4	L	173	0	0	21	0
4	M	145	0	0	17	0
4	N	190	0	0	14	0
4	O	178	0	0	15	0
4	P	221	0	0	17	1
4	Q	274	0	0	16	2
4	R	262	0	0	12	1
4	T	204	0	0	15	1
4	V	155	0	0	12	0
All	All	70139	0	64122	1515	6

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 12.

The worst 5 of 1515 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:A:118:ILE:HG12	1:A:217:MET:HE1	1.12	1.11
1:J:6:VAL:N	4:J:601:HOH:O	1.83	1.07
1:M:75:ARG:NH2	4:M:601:HOH:O	1.89	1.03
1:G:319:ARG:NH1	4:G:601:HOH:O	1.93	1.01
1:B:231:ARG:NH1	4:B:601:HOH:O	1.81	1.01

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:737:HOH:O	4:Q:732:HOH:O[1_565]	1.90	0.30
1:H:6:VAL:O	4:P:602:HOH:O[1_565]	2.00	0.20
4:I:637:HOH:O	4:T:654:HOH:O[1_556]	2.02	0.18
4:A:760:HOH:O	4:G:765:HOH:O[1_455]	2.13	0.07
4:J:854:HOH:O	4:R:628:HOH:O[1_455]	2.13	0.07

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	420/440 (96%)	396 (94%)	22 (5%)	2 (0%)	29	35
1	B	419/440 (95%)	392 (94%)	24 (6%)	3 (1%)	22	26
1	C	415/440 (94%)	399 (96%)	9 (2%)	7 (2%)	9	8
1	D	419/440 (95%)	398 (95%)	15 (4%)	6 (1%)	11	11
1	E	419/440 (95%)	397 (95%)	17 (4%)	5 (1%)	13	14
1	F	419/440 (95%)	397 (95%)	20 (5%)	2 (0%)	29	35
1	G	420/440 (96%)	399 (95%)	16 (4%)	5 (1%)	13	14
1	H	419/440 (95%)	394 (94%)	23 (6%)	2 (0%)	29	35
1	I	421/440 (96%)	400 (95%)	16 (4%)	5 (1%)	13	14
1	J	411/440 (93%)	393 (96%)	16 (4%)	2 (0%)	29	35
1	K	419/440 (95%)	399 (95%)	18 (4%)	2 (0%)	29	35
1	L	420/440 (96%)	394 (94%)	19 (4%)	7 (2%)	9	8
1	M	419/440 (95%)	392 (94%)	23 (6%)	4 (1%)	15	17
1	N	419/440 (95%)	398 (95%)	19 (4%)	2 (0%)	29	35
1	O	421/440 (96%)	397 (94%)	21 (5%)	3 (1%)	22	26
1	P	421/440 (96%)	401 (95%)	15 (4%)	5 (1%)	13	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	420/440 (96%)	392 (93%)	23 (6%)	5 (1%)	13	14
1	R	420/440 (96%)	397 (94%)	18 (4%)	5 (1%)	13	14
1	T	420/440 (96%)	396 (94%)	19 (4%)	5 (1%)	13	14
1	V	419/440 (95%)	398 (95%)	12 (3%)	9 (2%)	7	5
All	All	8380/8800 (95%)	7929 (95%)	365 (4%)	86 (1%)	15	17

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	104	THR
1	A	104	THR
1	B	104	THR
1	C	104	THR
1	D	104	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/369 (94%)	343 (99%)	3 (1%)	78	89
1	B	345/369 (94%)	338 (98%)	7 (2%)	55	72
1	C	343/369 (93%)	336 (98%)	7 (2%)	55	72
1	D	345/369 (94%)	339 (98%)	6 (2%)	60	76
1	E	345/369 (94%)	339 (98%)	6 (2%)	60	76
1	F	345/369 (94%)	340 (99%)	5 (1%)	67	81
1	G	346/369 (94%)	342 (99%)	4 (1%)	71	84
1	H	345/369 (94%)	335 (97%)	10 (3%)	42	58
1	I	347/369 (94%)	342 (99%)	5 (1%)	67	81
1	J	341/369 (92%)	337 (99%)	4 (1%)	71	84
1	K	345/369 (94%)	338 (98%)	7 (2%)	55	72
1	L	346/369 (94%)	339 (98%)	7 (2%)	55	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	345/369 (94%)	340 (99%)	5 (1%)	67	81
1	N	345/369 (94%)	338 (98%)	7 (2%)	55	72
1	O	348/369 (94%)	344 (99%)	4 (1%)	73	86
1	P	347/369 (94%)	343 (99%)	4 (1%)	71	84
1	Q	346/369 (94%)	344 (99%)	2 (1%)	86	94
1	R	346/369 (94%)	341 (99%)	5 (1%)	67	81
1	T	346/369 (94%)	339 (98%)	7 (2%)	55	72
1	V	345/369 (94%)	338 (98%)	7 (2%)	55	72
All	All	6907/7380 (94%)	6795 (98%)	112 (2%)	67	78

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	106	TRP
1	T	411[A]	THR
1	M	174	MET
1	T	404	GLU
1	V	43[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	371	GLN
1	P	117	ASN
1	M	78	GLN
1	N	371	GLN
1	P	371	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 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 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	CIT	F	501	-	12,12,12	1.10	0	17,17,17	1.89	3 (17%)
2	CIT	B	501	-	12,12,12	1.18	0	17,17,17	2.02	6 (35%)
3	GOL	O	502	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	T	502	-	5,5,5	0.38	0	5,5,5	0.30	0
3	GOL	F	502	-	5,5,5	0.39	0	5,5,5	0.31	0
3	GOL	V	502	-	5,5,5	0.36	0	5,5,5	0.33	0
3	GOL	E	502	-	5,5,5	0.38	0	5,5,5	0.28	0
3	GOL	J	502	-	5,5,5	0.35	0	5,5,5	0.33	0
2	CIT	P	501	-	12,12,12	1.06	0	17,17,17	1.71	3 (17%)
3	GOL	M	502	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	H	502	-	5,5,5	0.34	0	5,5,5	0.37	0
2	CIT	T	501	-	12,12,12	1.05	0	17,17,17	1.57	2 (11%)
3	GOL	Q	502	-	5,5,5	0.37	0	5,5,5	0.39	0
3	GOL	K	502	-	5,5,5	0.37	0	5,5,5	0.30	0
3	GOL	K	503	-	5,5,5	0.38	0	5,5,5	0.47	0
2	CIT	V	501	-	12,12,12	1.06	0	17,17,17	1.62	2 (11%)
2	CIT	H	501	-	12,12,12	0.95	0	17,17,17	1.88	6 (35%)
3	GOL	D	502	-	5,5,5	0.37	0	5,5,5	0.29	0
3	GOL	R	502	-	5,5,5	0.36	0	5,5,5	0.34	0
2	CIT	N	501	-	12,12,12	1.03	0	17,17,17	1.65	2 (11%)
3	GOL	J	503	-	5,5,5	0.38	0	5,5,5	0.29	0
2	CIT	C	501	-	12,12,12	1.06	0	17,17,17	1.81	4 (23%)
3	GOL	G	502	-	5,5,5	0.36	0	5,5,5	0.32	0
2	CIT	O	501	-	12,12,12	1.08	0	17,17,17	1.65	4 (23%)
3	GOL	I	502	-	5,5,5	0.39	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	G	501	-	12,12,12	1.06	0	17,17,17	1.70	3 (17%)
2	CIT	J	501	-	12,12,12	1.05	0	17,17,17	1.72	2 (11%)
2	CIT	Q	501	-	12,12,12	1.00	0	17,17,17	1.74	3 (17%)
3	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.53	0
2	CIT	M	501	-	12,12,12	1.01	0	17,17,17	1.61	3 (17%)
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%)
2	CIT	A	501	-	12,12,12	0.92	0	17,17,17	1.92	7 (41%)
3	GOL	L	502	-	5,5,5	0.35	0	5,5,5	0.31	0
2	CIT	E	501	-	12,12,12	1.02	0	17,17,17	1.54	2 (11%)
2	CIT	K	501	-	12,12,12	1.04	0	17,17,17	1.62	1 (5%)
2	CIT	I	501	-	12,12,12	1.07	0	17,17,17	1.63	2 (11%)
2	CIT	D	501	-	12,12,12	1.02	0	17,17,17	1.67	3 (17%)
2	CIT	R	501	-	12,12,12	1.10	0	17,17,17	1.68	3 (17%)
3	GOL	N	502	-	5,5,5	0.37	0	5,5,5	0.32	0
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

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	F	501	-	-	6/16/16/16	-
2	CIT	B	501	-	-	10/16/16/16	-
3	GOL	O	502	-	-	0/4/4/4	-
3	GOL	T	502	-	-	2/4/4/4	-
3	GOL	F	502	-	-	0/4/4/4	-
3	GOL	V	502	-	-	2/4/4/4	-
3	GOL	E	502	-	-	2/4/4/4	-
3	GOL	J	502	-	-	4/4/4/4	-
2	CIT	P	501	-	-	5/16/16/16	-
3	GOL	M	502	-	-	0/4/4/4	-
3	GOL	H	502	-	-	0/4/4/4	-
2	CIT	T	501	-	-	5/16/16/16	-
3	GOL	Q	502	-	-	0/4/4/4	-
3	GOL	K	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	K	503	-	-	3/4/4/4	-
2	CIT	V	501	-	-	7/16/16/16	-
2	CIT	H	501	-	-	5/16/16/16	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	R	502	-	-	0/4/4/4	-
2	CIT	N	501	-	-	8/16/16/16	-
3	GOL	J	503	-	-	1/4/4/4	-
2	CIT	C	501	-	-	9/16/16/16	-
3	GOL	G	502	-	-	2/4/4/4	-
2	CIT	O	501	-	-	9/16/16/16	-
3	GOL	I	502	-	-	1/4/4/4	-
2	CIT	G	501	-	-	10/16/16/16	-
2	CIT	J	501	-	-	5/16/16/16	-
2	CIT	Q	501	-	-	5/16/16/16	-
3	GOL	A	502	-	-	0/4/4/4	-
2	CIT	M	501	-	-	10/16/16/16	-
3	GOL	A	503	-	-	0/4/4/4	-
2	CIT	L	501	-	-	9/16/16/16	-
2	CIT	A	501	-	-	5/16/16/16	-
3	GOL	L	502	-	-	2/4/4/4	-
2	CIT	E	501	-	-	7/16/16/16	-
2	CIT	K	501	-	-	7/16/16/16	-
2	CIT	I	501	-	-	8/16/16/16	-
2	CIT	D	501	-	-	6/16/16/16	-
2	CIT	R	501	-	-	5/16/16/16	-
3	GOL	N	502	-	-	2/4/4/4	-
3	GOL	P	502	-	-	2/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-

There are no bond length outliers.

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	501	CIT	O6-C6-C3	4.32	120.56	113.05

There are no chirality outliers.

5 of 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

There are no ring outliers.

21 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	CIT	4	0
2	B	501	CIT	3	0
3	V	502	GOL	3	0
2	T	501	CIT	3	0
3	K	503	GOL	5	0
2	V	501	CIT	1	0
2	H	501	CIT	5	0
2	N	501	CIT	2	0
2	C	501	CIT	4	0
2	O	501	CIT	3	0
2	G	501	CIT	4	0
2	J	501	CIT	2	0
2	Q	501	CIT	1	0
2	M	501	CIT	1	0
2	L	501	CIT	4	0
2	A	501	CIT	2	0
2	E	501	CIT	2	0
2	I	501	CIT	3	0
2	D	501	CIT	2	0
2	R	501	CIT	2	0
3	N	502	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/440 (94%)	-0.15	9 (2%) 62 69	22, 40, 64, 114	0
1	B	415/440 (94%)	0.05	15 (3%) 42 49	27, 42, 76, 106	0
1	C	412/440 (93%)	-0.29	4 (0%) 82 86	19, 34, 58, 91	0
1	D	415/440 (94%)	-0.13	13 (3%) 49 56	19, 39, 66, 104	0
1	E	415/440 (94%)	-0.09	8 (1%) 66 73	24, 41, 64, 109	0
1	F	415/440 (94%)	-0.12	9 (2%) 62 69	23, 41, 64, 114	0
1	G	415/440 (94%)	-0.08	12 (2%) 51 58	20, 41, 68, 100	0
1	H	415/440 (94%)	-0.21	12 (2%) 51 58	23, 40, 64, 108	0
1	I	415/440 (94%)	-0.19	11 (2%) 54 62	20, 39, 68, 97	0
1	J	408/440 (92%)	-0.31	2 (0%) 91 94	18, 33, 53, 93	0
1	K	415/440 (94%)	-0.24	10 (2%) 59 66	21, 40, 64, 108	0
1	L	415/440 (94%)	0.00	14 (3%) 45 52	21, 42, 71, 114	0
1	M	415/440 (94%)	-0.06	12 (2%) 51 58	23, 43, 75, 108	0
1	N	415/440 (94%)	-0.16	8 (1%) 66 73	24, 41, 67, 116	0
1	O	415/440 (94%)	-0.12	12 (2%) 51 58	24, 40, 70, 108	0
1	P	415/440 (94%)	-0.19	10 (2%) 59 66	20, 37, 65, 106	0
1	Q	415/440 (94%)	-0.23	11 (2%) 54 62	20, 32, 55, 106	0
1	R	415/440 (94%)	-0.28	8 (1%) 66 73	19, 32, 54, 94	0
1	T	415/440 (94%)	-0.21	6 (1%) 75 80	21, 37, 66, 112	0
1	V	415/440 (94%)	-0.15	12 (2%) 51 58	23, 41, 72, 115	0
All	All	8290/8800 (94%)	-0.16	198 (2%) 59 66	18, 39, 67, 116	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	LEU	20.4
1	E	420	LEU	16.5
1	O	420	LEU	15.5
1	P	420	LEU	15.2
1	Q	420	LEU	14.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CIT	J	501	13/13	0.81	0.21	29,55,75,79	0
3	GOL	K	503	6/6	0.81	0.44	81,88,90,91	0
2	CIT	F	501	13/13	0.82	0.17	57,76,85,86	0
2	CIT	Q	501	13/13	0.83	0.19	44,72,79,80	0
2	CIT	I	501	13/13	0.84	0.19	49,67,76,83	0
2	CIT	L	501	13/13	0.85	0.15	33,61,72,72	0
2	CIT	E	501	13/13	0.85	0.17	56,81,92,93	0
3	GOL	G	502	6/6	0.85	0.23	43,57,60,66	0
2	CIT	D	501	13/13	0.85	0.17	32,60,75,80	0
2	CIT	N	501	13/13	0.87	0.16	52,77,84,84	0
2	CIT	A	501	13/13	0.87	0.16	49,69,71,72	0
2	CIT	K	501	13/13	0.87	0.17	49,61,74,79	0
2	CIT	B	501	13/13	0.87	0.19	41,61,71,71	0
2	CIT	O	501	13/13	0.88	0.16	44,68,74,77	0
2	CIT	H	501	13/13	0.88	0.16	39,56,66,72	0
2	CIT	G	501	13/13	0.89	0.18	26,61,82,82	0
3	GOL	J	503	6/6	0.89	0.14	38,61,63,64	0
2	CIT	V	501	13/13	0.89	0.14	37,70,82,85	0
3	GOL	O	502	6/6	0.89	0.14	34,44,47,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	P	502	6/6	0.89	0.17	38,44,48,48	0
3	GOL	V	502	6/6	0.89	0.12	36,40,43,48	0
2	CIT	R	501	13/13	0.90	0.15	39,61,75,77	0
3	GOL	A	503	6/6	0.91	0.14	39,56,59,64	0
3	GOL	L	502	6/6	0.91	0.13	50,57,63,64	0
3	GOL	M	502	6/6	0.91	0.17	48,58,59,60	0
3	GOL	A	502	6/6	0.92	0.15	39,52,60,64	0
3	GOL	J	502	6/6	0.92	0.16	46,52,54,55	0
2	CIT	P	501	13/13	0.92	0.17	35,50,75,77	0
2	CIT	T	501	13/13	0.93	0.12	37,57,72,73	0
2	CIT	C	501	13/13	0.93	0.14	26,52,62,67	0
3	GOL	Q	502	6/6	0.93	0.13	24,43,45,51	0
3	GOL	R	502	6/6	0.93	0.13	25,43,46,49	0
2	CIT	M	501	13/13	0.93	0.13	34,64,76,77	0
3	GOL	K	502	6/6	0.94	0.12	35,37,49,56	0
3	GOL	T	502	6/6	0.94	0.10	43,44,47,48	0
3	GOL	D	502	6/6	0.95	0.12	22,37,39,40	0
3	GOL	F	502	6/6	0.95	0.14	35,40,47,49	0
3	GOL	C	502	6/6	0.95	0.14	32,41,46,48	0
3	GOL	I	502	6/6	0.95	0.14	30,40,44,48	0
3	GOL	E	502	6/6	0.96	0.14	34,39,47,48	0
3	GOL	N	502	6/6	0.96	0.14	32,44,47,53	0
3	GOL	H	502	6/6	0.97	0.12	31,37,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.