



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 29, 2022 – 10:30 AM EDT

PDB ID : 6V99
Title : Agrobacterium tumefaciens ADP-Glucose pyrophosphorylase- S72D in the presence of sulfate
Authors : Zheng, Y.; Alghamdi, M.A.; Ballicora, M.A.; Liu, D.
Deposited on : 2019-12-13
Resolution : 2.29 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

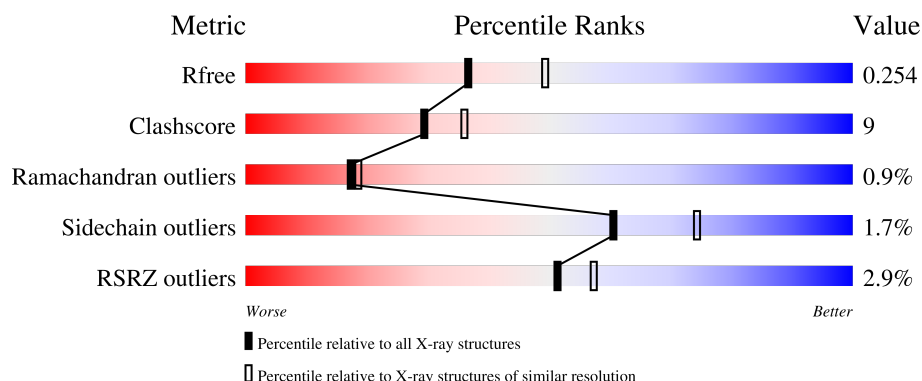
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	 3% 76% 18% 6%
1	B	440	 3% 76% 18% 6%
1	C	440	 2% 75% 19% • 6%
1	D	440	 2% 77% 16% • 6%
1	E	440	 3% 78% 15% • 6%

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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	W	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
2	SO4	B	1201	-	-	-	X
2	SO4	C	509	-	-	X	-
2	SO4	D	501	-	-	X	-
2	SO4	G	507	-	-	-	X
2	SO4	M	501	-	-	X	-
2	SO4	O	506	-	-	X	-
2	SO4	T	503	-	-	X	-
2	SO4	T	508	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 68292 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	A	415	Total	C	N	O	S	0	1	0
			3243	2055	563	612	13			
1	B	415	Total	C	N	O	S	0	1	0
			3242	2055	562	612	13			
1	C	415	Total	C	N	O	S	4	3	0
			3252	2062	564	613	13			
1	D	415	Total	C	N	O	S	4	1	0
			3247	2057	565	612	13			
1	E	415	Total	C	N	O	S	4	3	0
			3257	2063	565	616	13			
1	F	415	Total	C	N	O	S	4	2	0
			3257	2065	564	615	13			
1	G	415	Total	C	N	O	S	4	2	0
			3250	2059	564	614	13			
1	H	415	Total	C	N	O	S	4	3	0
			3257	2063	565	616	13			
1	I	415	Total	C	N	O	S	4	3	0
			3257	2063	565	616	13			
1	J	415	Total	C	N	O	S	4	3	0
			3255	2062	565	615	13			
1	K	415	Total	C	N	O	S	0	3	0
			3254	2062	565	614	13			
1	L	415	Total	C	N	O	S	0	3	0
			3266	2071	566	616	13			
1	M	415	Total	C	N	O	S	0	3	0
			3257	2063	565	616	13			
1	N	415	Total	C	N	O	S	4	1	0
			3232	2050	559	610	13			
1	O	415	Total	C	N	O	S	0	1	0
			3241	2054	562	612	13			
1	P	415	Total	C	N	O	S	4	1	0
			3240	2054	562	611	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	415	Total	C	N	O	S	4	3	0
			3252	2061	564	613	14			
1	R	415	Total	C	N	O	S	4	2	0
			3249	2059	564	613	13			
1	W	415	Total	C	N	O	S	0	2	0
			3250	2059	564	614	13			
1	T	415	Total	C	N	O	S	4	3	0
			3264	2068	569	614	13			

There are 420 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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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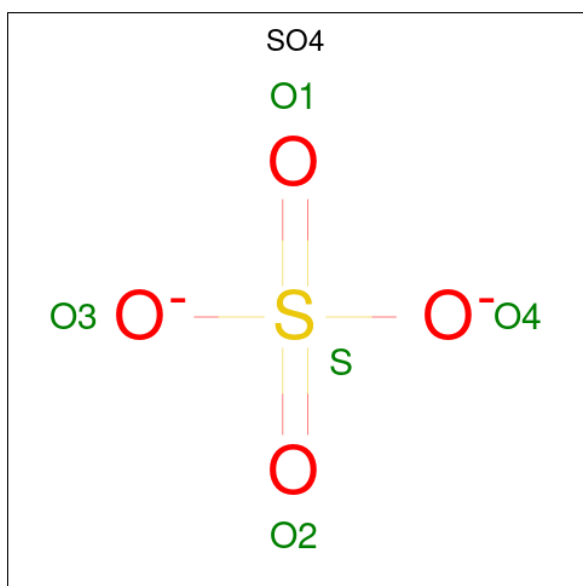
Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	SER	-	expression tag	UNP Q8U8L5
R	-8	SER	-	expression tag	UNP Q8U8L5
R	-7	GLY	-	expression tag	UNP Q8U8L5
R	-6	LEU	-	expression tag	UNP Q8U8L5
R	-5	VAL	-	expression tag	UNP Q8U8L5
R	-4	PRO	-	expression tag	UNP Q8U8L5
R	-3	ARG	-	expression tag	UNP Q8U8L5
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
W	-19	MET	-	expression tag	UNP Q8U8L5
W	-18	GLY	-	expression tag	UNP Q8U8L5
W	-17	SER	-	expression tag	UNP Q8U8L5
W	-16	SER	-	expression tag	UNP Q8U8L5
W	-15	HIS	-	expression tag	UNP Q8U8L5
W	-14	HIS	-	expression tag	UNP Q8U8L5
W	-13	HIS	-	expression tag	UNP Q8U8L5
W	-12	HIS	-	expression tag	UNP Q8U8L5
W	-11	HIS	-	expression tag	UNP Q8U8L5
W	-10	HIS	-	expression tag	UNP Q8U8L5
W	-9	SER	-	expression tag	UNP Q8U8L5
W	-8	SER	-	expression tag	UNP Q8U8L5
W	-7	GLY	-	expression tag	UNP Q8U8L5
W	-6	LEU	-	expression tag	UNP Q8U8L5
W	-5	VAL	-	expression tag	UNP Q8U8L5
W	-4	PRO	-	expression tag	UNP Q8U8L5
W	-3	ARG	-	expression tag	UNP Q8U8L5
W	-2	GLY	-	expression tag	UNP Q8U8L5
W	-1	SER	-	expression tag	UNP Q8U8L5
W	0	HIS	-	expression tag	UNP Q8U8L5
W	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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	W	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	93	Total	O	0	0
			93	93		
3	C	173	Total	O	0	0
			173	173		
3	D	142	Total	O	0	0
			142	142		
3	E	85	Total	O	0	0
			85	85		
3	F	100	Total	O	0	0
			100	100		
3	G	112	Total	O	0	0
			112	112		
3	H	121	Total	O	0	0
			121	121		
3	I	145	Total	O	0	0
			145	145		
3	J	195	Total	O	0	0
			195	195		
3	K	112	Total	O	0	0
			112	112		
3	L	109	Total	O	0	0
			109	109		
3	M	89	Total	O	0	0
			89	89		
3	N	103	Total	O	0	0
			103	103		
3	O	125	Total	O	0	0
			125	125		

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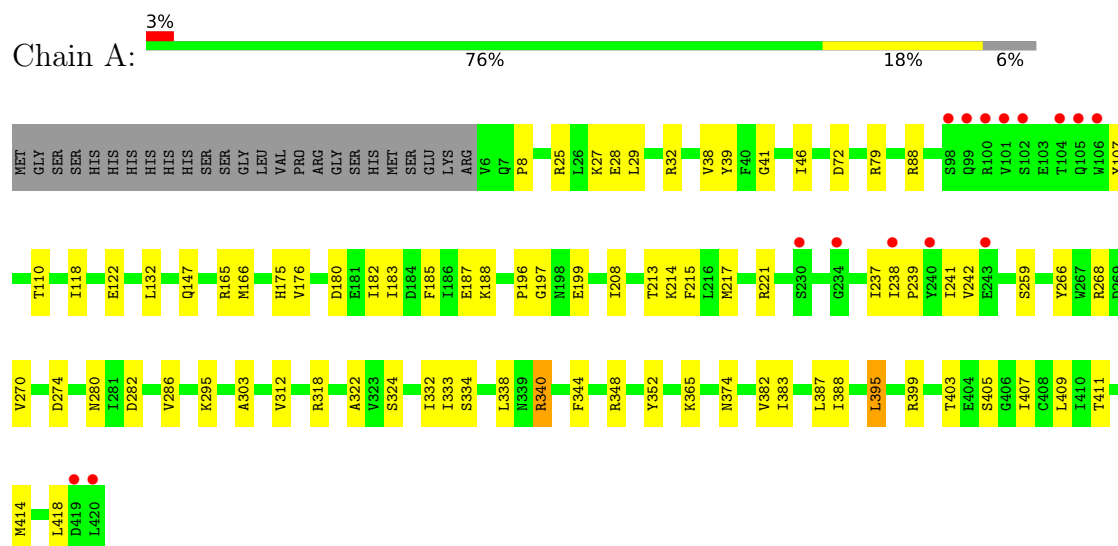
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	137	Total 137	O 137	0	0
3	Q	179	Total 179	O 179	0	0
3	R	192	Total 192	O 192	0	0
3	W	111	Total 111	O 111	0	0
3	T	152	Total 152	O 152	0	0

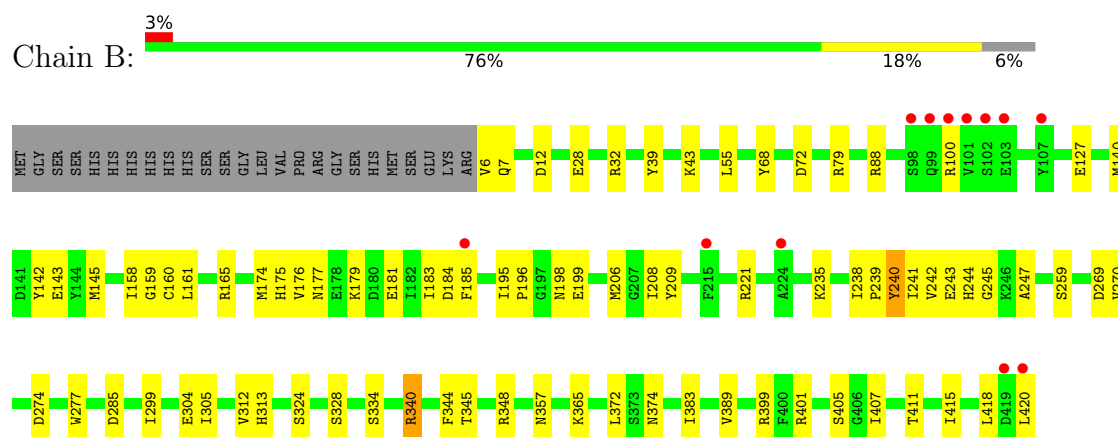
3 Residue-property plots

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.

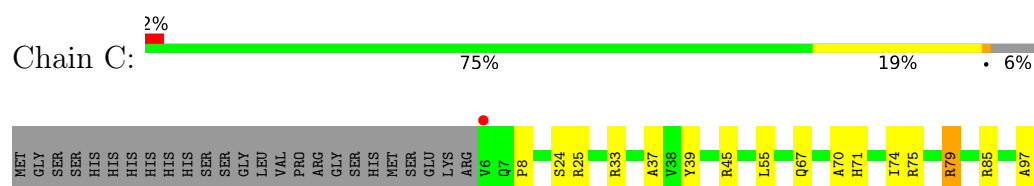
- Molecule 1: Glucose-1-phosphate adenylyltransferase

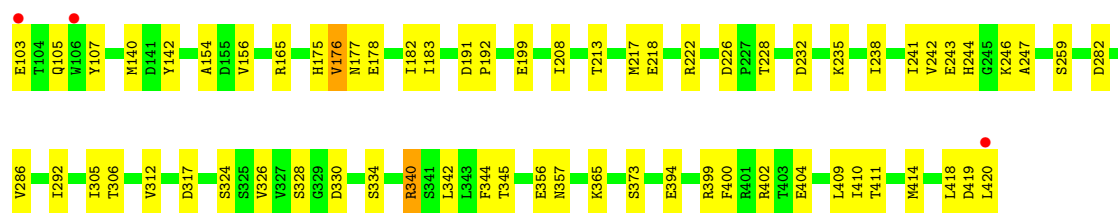


- Molecule 1: Glucose-1-phosphate adenylyltransferase

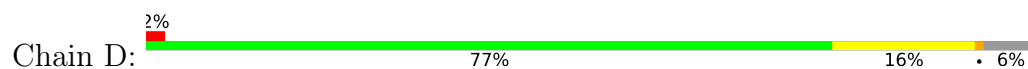


- Molecule 1: Glucose-1-phosphate adenylyltransferase

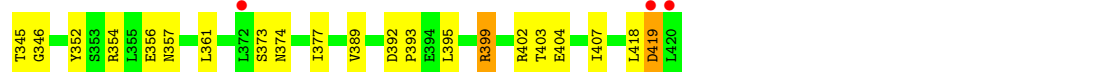
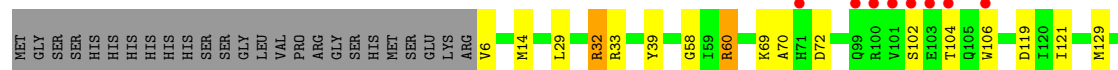
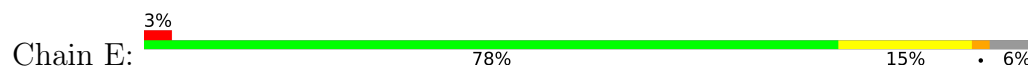




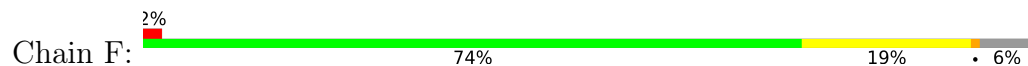
• Molecule 1: Glucose-1-phosphate adenylyltransferase



• Molecule 1: Glucose-1-phosphate adenylyltransferase

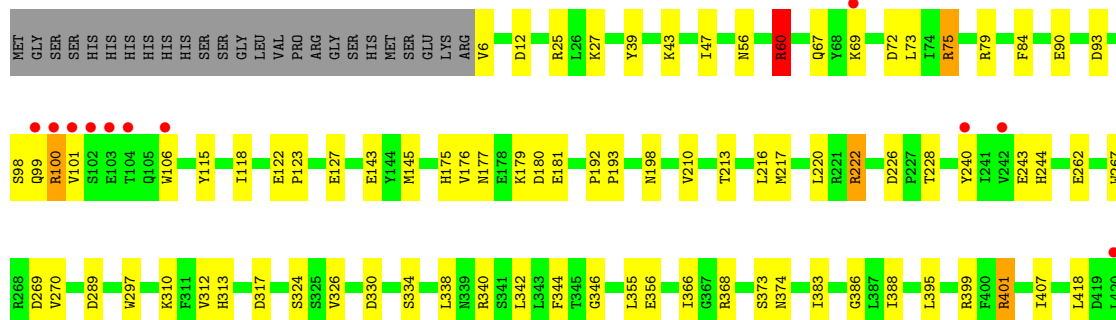
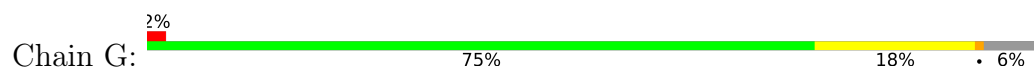


• Molecule 1: Glucose-1-phosphate adenylyltransferase

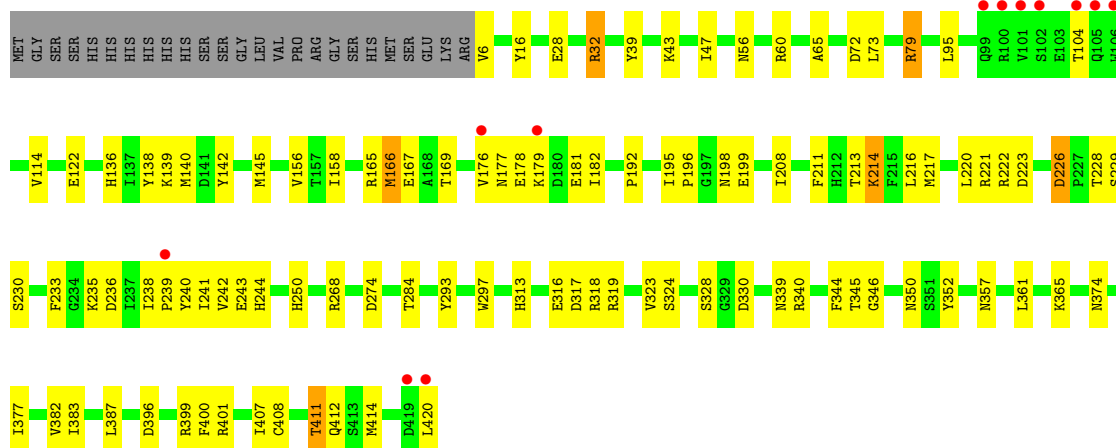




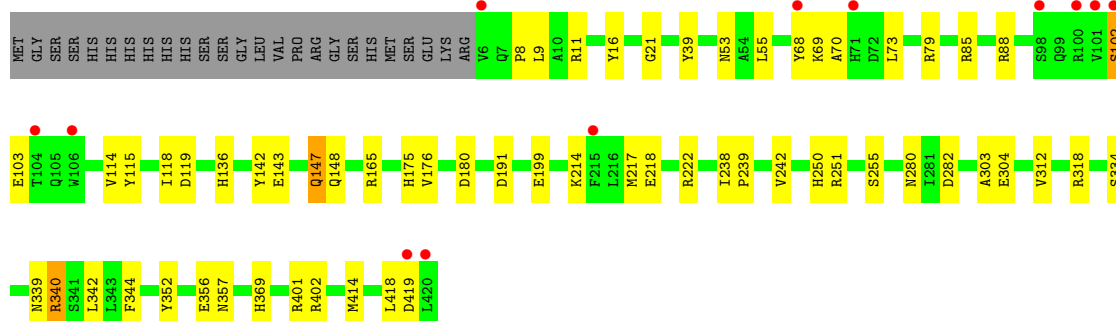
• Molecule 1: Glucose-1-phosphate adenylyltransferase



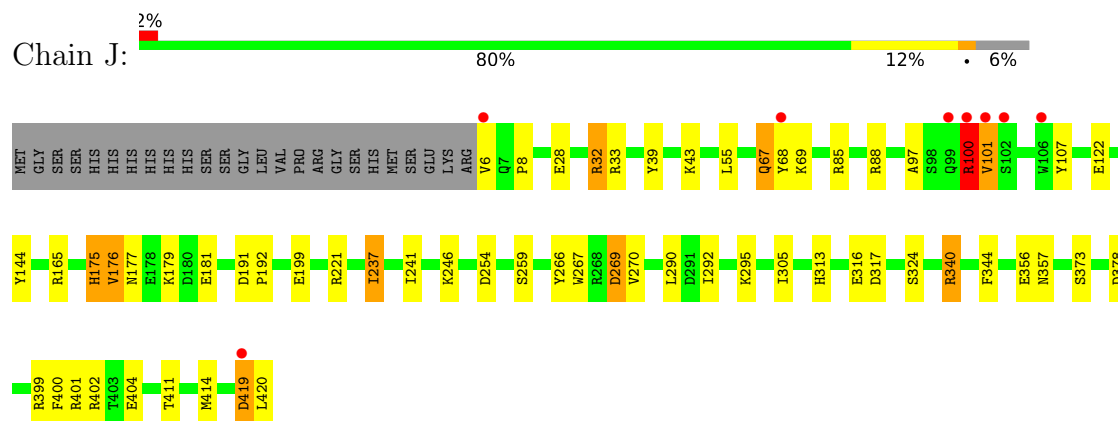
• Molecule 1: Glucose-1-phosphate adenylyltransferase



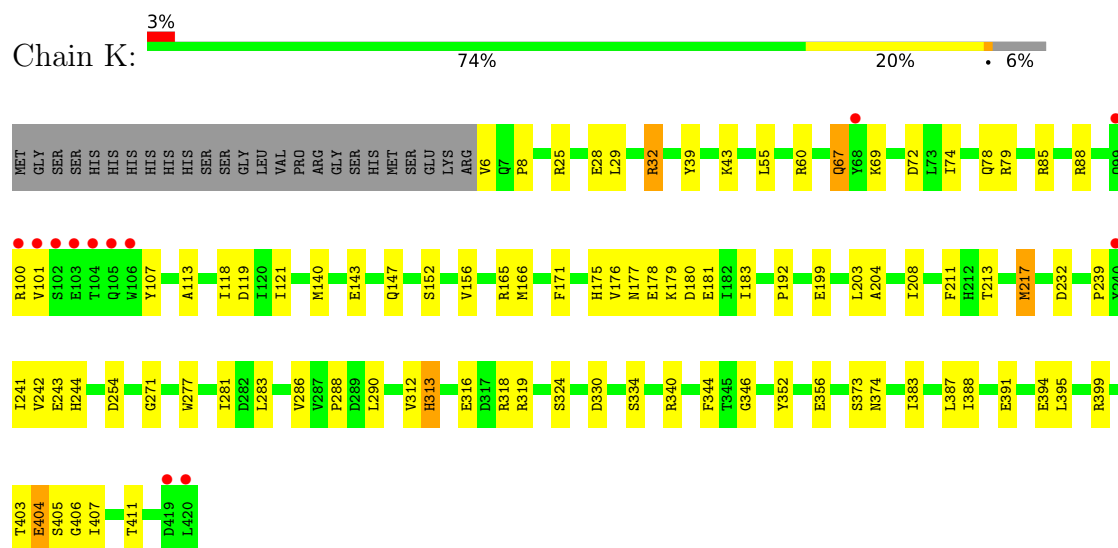
• Molecule 1: Glucose-1-phosphate adenylyltransferase



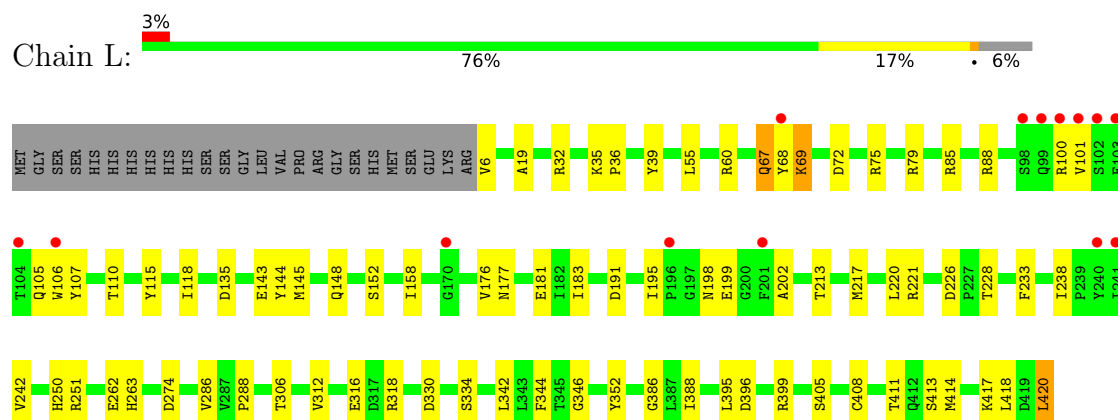
• Molecule 1: Glucose-1-phosphate adenylyltransferase



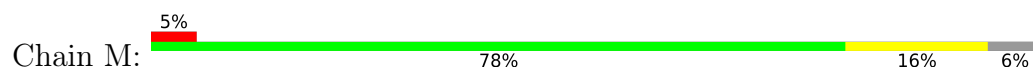
• Molecule 1: Glucose-1-phosphate adenylyltransferase

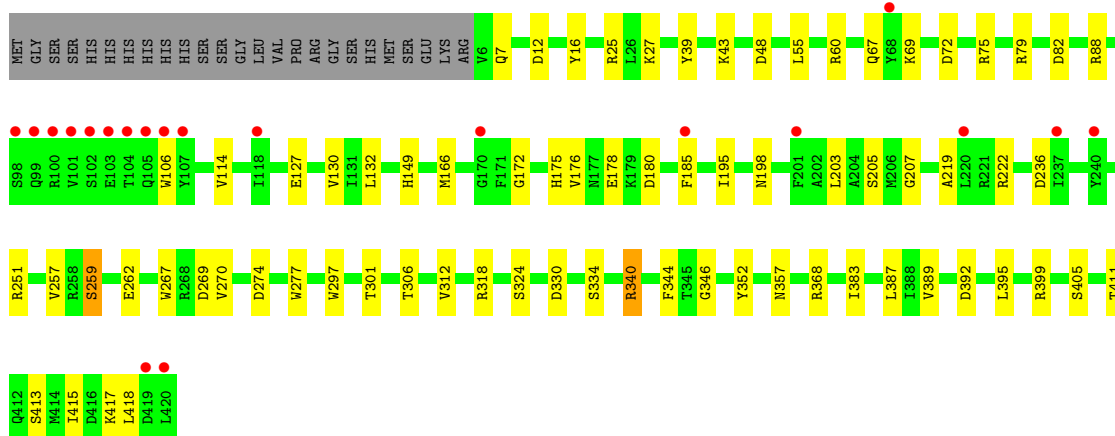


• Molecule 1: Glucose-1-phosphate adenylyltransferase

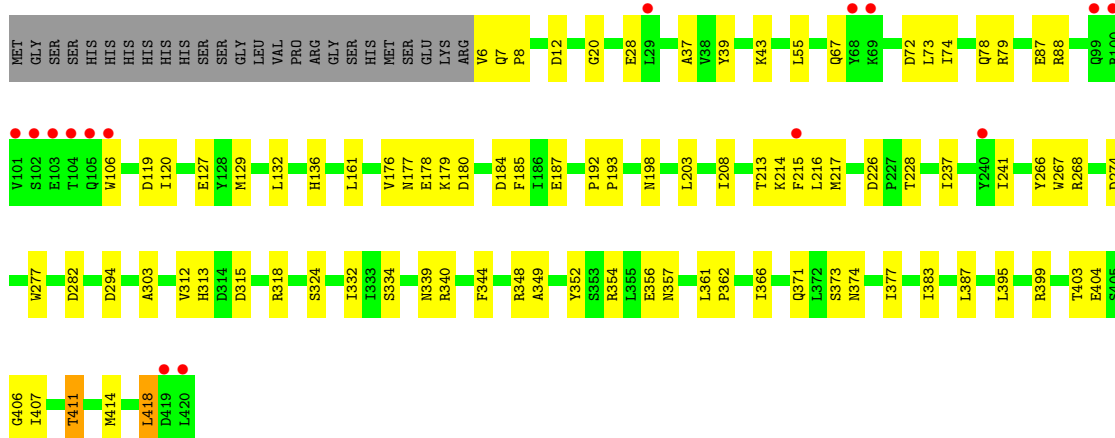
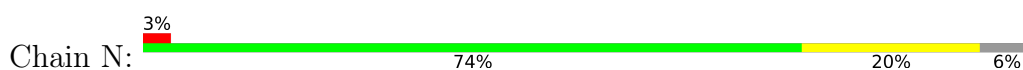


• Molecule 1: Glucose-1-phosphate adenylyltransferase

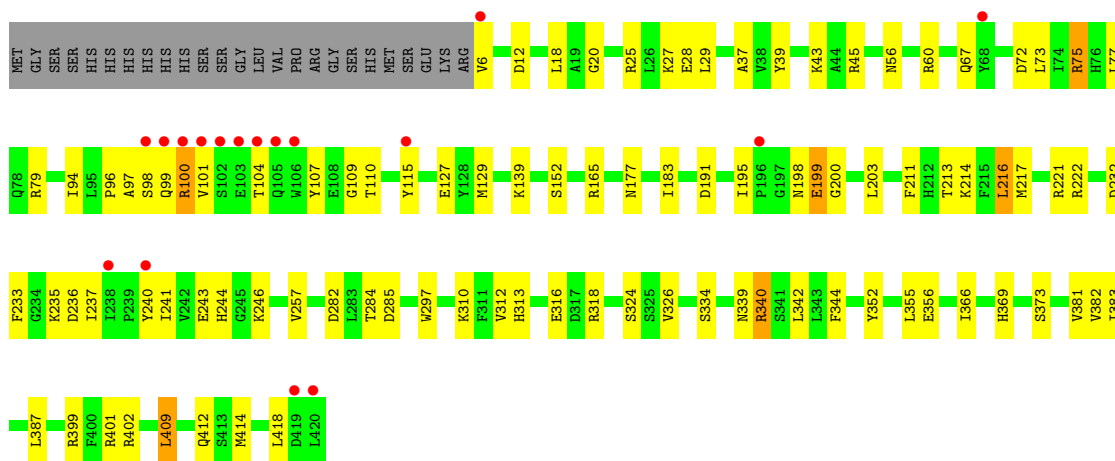





• Molecule 1: Glucose-1-phosphate adenylyltransferase

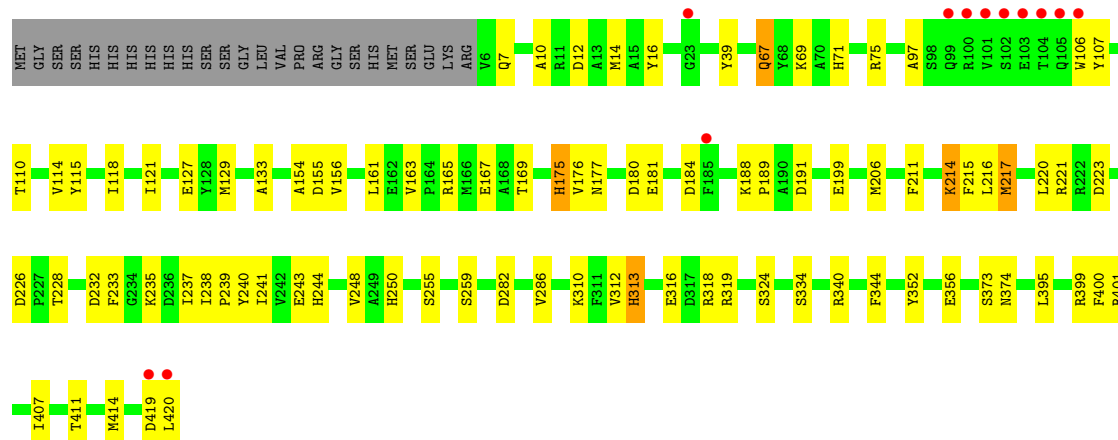


• Molecule 1: Glucose-1-phosphate adenylyltransferase




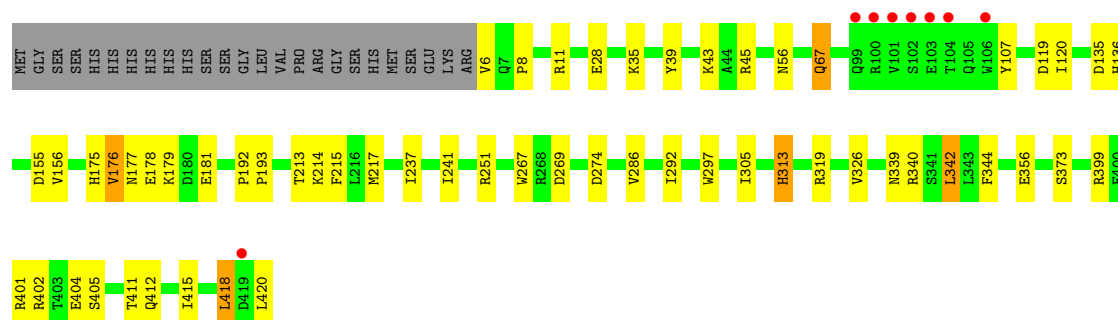
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain P: 




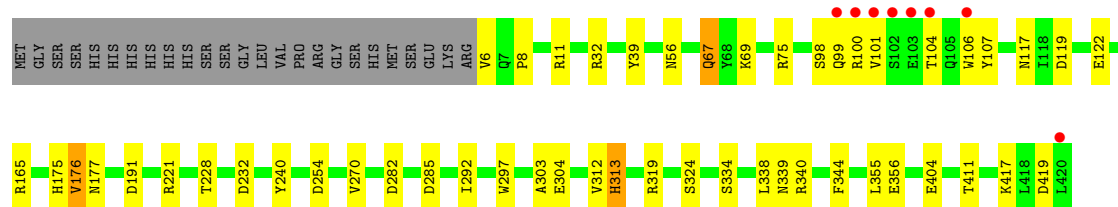
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain Q: 




• Molecule 1: Glucose-1-phosphate adenylyltransferase

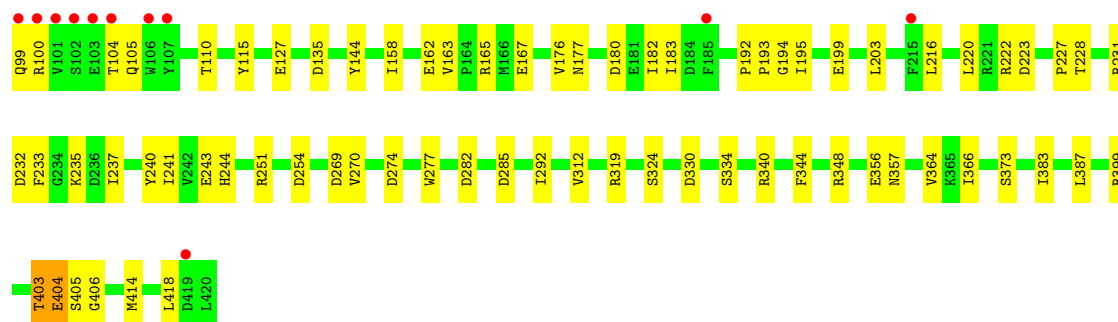
Chain R: 



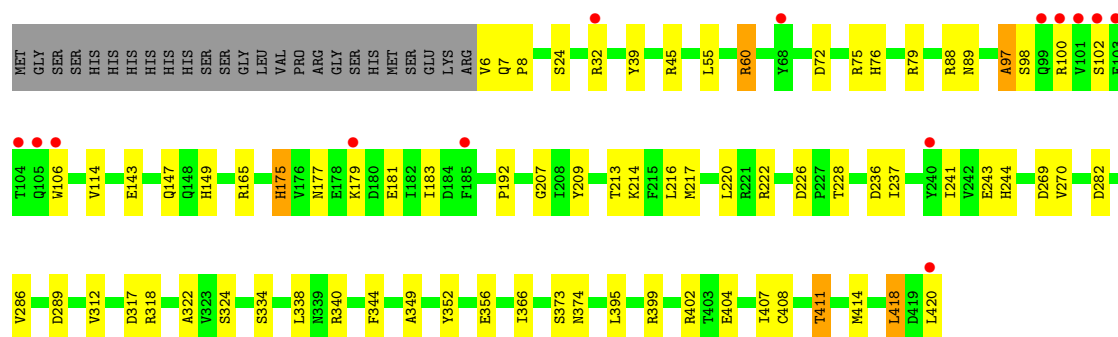
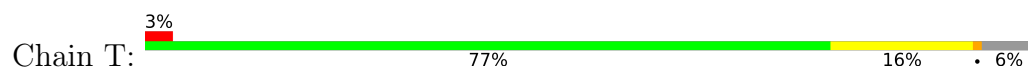
• Molecule 1: Glucose-1-phosphate adenylyltransferase

Chain W: 





● 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	93.42Å 141.58Å 228.32Å 108.07° 101.85° 90.00°	Depositor
Resolution (Å)	72.70 – 2.29 72.74 – 2.29	Depositor EDS
% Data completeness (in resolution range)	97.5 (72.70-2.29) 87.3 (72.74-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.208 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	24319 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-h-l 0.467 for -h,k,-k-l 0.457 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	68292	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 62.75 % 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 1.0735e-05. 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: SO4

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	0.43	1/3322 (0.0%)	0.59	2/4515 (0.0%)
1	B	0.41	0/3321	0.57	0/4515
1	C	0.48	1/3334 (0.0%)	0.77	2/4532 (0.0%)
1	D	0.42	0/3326	0.61	0/4521
1	E	0.38	0/3336	0.55	0/4536
1	F	0.48	2/3337 (0.1%)	0.60	4/4537 (0.1%)
1	G	0.49	4/3329 (0.1%)	0.74	3/4526 (0.1%)
1	H	0.41	0/3336	0.58	1/4536 (0.0%)
1	I	0.41	0/3336	0.59	0/4536
1	J	0.45	0/3334	0.60	0/4533
1	K	0.42	0/3333	0.57	0/4532
1	L	0.43	0/3346	0.56	0/4548
1	M	0.40	0/3336	0.55	0/4536
1	N	0.39	0/3311	0.54	0/4503
1	O	0.40	0/3320	0.60	3/4514 (0.1%)
1	P	0.43	0/3319	0.61	1/4513 (0.0%)
1	Q	0.45	0/3334	0.58	0/4533
1	R	0.46	0/3328	0.59	0/4525
1	T	0.44	0/3343	0.64	2/4543 (0.0%)
1	W	0.42	0/3329	0.58	0/4526
All	All	0.43	8/66610 (0.0%)	0.60	18/90560 (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	C	0	2
1	G	0	1
1	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	1
1	T	0	2
1	W	0	1
All	All	0	8

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	60	ARG	CD-NE	9.54	1.62	1.46
1	F	401	ARG	NE-CZ	8.68	1.44	1.33
1	F	401	ARG	CZ-NH1	7.96	1.43	1.33
1	G	60	ARG	CZ-NH1	6.71	1.41	1.33
1	G	60	ARG	NE-CZ	5.94	1.40	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	ARG	NE-CZ-NH1	24.62	132.61	120.30
1	G	60	ARG	NE-CZ-NH1	-22.14	109.23	120.30
1	C	79	ARG	NE-CZ-NH2	-20.70	109.95	120.30
1	G	60	ARG	NE-CZ-NH2	-16.59	112.00	120.30
1	T	79	ARG	NE-CZ-NH2	-14.42	113.09	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	418	LEU	Peptide
1	C	419	ASP	Peptide
1	G	60	ARG	Sidechain
1	N	418	LEU	Peptide
1	Q	418	LEU	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	3243	0	3143	60	0
1	B	3242	0	3135	69	0
1	C	3252	0	3153	68	0
1	D	3247	0	3150	72	0
1	E	3257	0	3152	55	0
1	F	3257	0	3152	64	0
1	G	3250	0	3144	60	6
1	H	3257	0	3152	78	0
1	I	3257	0	3152	46	0
1	J	3255	0	3147	52	0
1	K	3254	0	3141	84	0
1	L	3266	0	3165	68	0
1	M	3257	0	3152	45	0
1	N	3232	0	3119	69	0
1	O	3241	0	3137	85	0
1	P	3240	0	3135	78	0
1	Q	3252	0	3147	42	0
1	R	3249	0	3142	32	0
1	T	3264	0	3166	51	0
1	W	3250	0	3146	77	0
2	A	30	0	0	3	0
2	B	35	0	0	2	0
2	C	45	0	0	3	0
2	D	30	0	0	2	0
2	E	35	0	0	0	0
2	F	35	0	0	5	0
2	G	35	0	0	0	0
2	H	25	0	0	2	0
2	I	35	0	0	2	0
2	J	40	0	0	2	0
2	K	30	0	0	0	0
2	L	30	0	0	2	0
2	M	20	0	0	2	0
2	N	30	0	0	0	0
2	O	35	0	0	2	6
2	P	50	0	0	3	0
2	Q	40	0	0	4	0
2	R	35	0	0	1	0
2	T	40	0	0	3	0
2	W	25	0	0	0	0
3	A	115	0	0	8	0
3	B	93	0	0	11	0
3	C	173	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	142	0	0	12	0
3	E	85	0	0	10	1
3	F	100	0	0	11	1
3	G	112	0	0	9	0
3	H	121	0	0	13	1
3	I	145	0	0	10	0
3	J	195	0	0	15	0
3	K	112	0	0	12	0
3	L	109	0	0	16	0
3	M	89	0	0	11	0
3	N	103	0	0	8	0
3	O	125	0	0	8	0
3	P	137	0	0	14	1
3	Q	179	0	0	9	0
3	R	192	0	0	12	2
3	T	152	0	0	12	0
3	W	111	0	0	11	0
All	All	68292	0	62930	1217	9

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 9.

The worst 5 of 1217 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:P:400:PHE:HA	1:P:414:MET:HE2	1.24	1.16
1:D:22:ARG:CZ	1:D:24:SER:H	1.62	1.12
1:P:216:LEU:HD23	1:P:220:LEU:HD13	1.24	1.08
1:O:6:VAL:N	3:O:601:HOH:O	1.89	1.04
1:G:6:VAL:N	3:G:601:HOH:O	1.92	1.01

The worst 5 of 9 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)
1:G:60:ARG:NH2	2:O:506:SO4:O2[1_565]	0.66	1.54
1:G:60:ARG:CZ	2:O:506:SO4:S[1_565]	1.23	0.97
1:G:60:ARG:CZ	2:O:506:SO4:O2[1_565]	1.41	0.79
1:G:60:ARG:NH1	2:O:506:SO4:S[1_565]	1.65	0.55
1:G:60:ARG:NH2	2:O:506:SO4:S[1_565]	1.84	0.36

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	414/440 (94%)	393 (95%)	21 (5%)	0	100	100
1	B	414/440 (94%)	393 (95%)	18 (4%)	3 (1%)	22	25
1	C	416/440 (94%)	396 (95%)	16 (4%)	4 (1%)	15	16
1	D	414/440 (94%)	388 (94%)	20 (5%)	6 (1%)	11	10
1	E	416/440 (94%)	392 (94%)	20 (5%)	4 (1%)	15	16
1	F	415/440 (94%)	390 (94%)	20 (5%)	5 (1%)	13	12
1	G	415/440 (94%)	388 (94%)	21 (5%)	6 (1%)	11	10
1	H	416/440 (94%)	391 (94%)	22 (5%)	3 (1%)	22	25
1	I	416/440 (94%)	394 (95%)	19 (5%)	3 (1%)	22	25
1	J	416/440 (94%)	397 (95%)	12 (3%)	7 (2%)	9	7
1	K	416/440 (94%)	394 (95%)	19 (5%)	3 (1%)	22	25
1	L	416/440 (94%)	395 (95%)	18 (4%)	3 (1%)	22	25
1	M	416/440 (94%)	392 (94%)	22 (5%)	2 (0%)	29	34
1	N	414/440 (94%)	396 (96%)	17 (4%)	1 (0%)	47	57
1	O	414/440 (94%)	389 (94%)	21 (5%)	4 (1%)	15	16
1	P	414/440 (94%)	393 (95%)	19 (5%)	2 (0%)	29	34
1	Q	416/440 (94%)	399 (96%)	15 (4%)	2 (0%)	29	34
1	R	415/440 (94%)	394 (95%)	13 (3%)	8 (2%)	8	6
1	T	416/440 (94%)	397 (95%)	17 (4%)	2 (0%)	29	34
1	W	415/440 (94%)	391 (94%)	20 (5%)	4 (1%)	15	16
All	All	8304/8800 (94%)	7862 (95%)	370 (4%)	72 (1%)	17	18

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	TYR

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Mol	Chain	Res	Type
1	C	100	ARG
1	D	103	GLU
1	E	419	ASP
1	G	99	GLN

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	340/369 (92%)	332 (98%)	8 (2%)	49	63
1	B	339/369 (92%)	330 (97%)	9 (3%)	44	59
1	C	341/369 (92%)	336 (98%)	5 (2%)	65	77
1	D	341/369 (92%)	337 (99%)	4 (1%)	71	82
1	E	342/369 (93%)	335 (98%)	7 (2%)	55	70
1	F	342/369 (93%)	334 (98%)	8 (2%)	50	65
1	G	341/369 (92%)	335 (98%)	6 (2%)	59	72
1	H	342/369 (93%)	333 (97%)	9 (3%)	46	60
1	I	342/369 (93%)	337 (98%)	5 (2%)	65	77
1	J	341/369 (92%)	334 (98%)	7 (2%)	53	68
1	K	340/369 (92%)	332 (98%)	8 (2%)	49	63
1	L	343/369 (93%)	337 (98%)	6 (2%)	60	74
1	M	342/369 (93%)	335 (98%)	7 (2%)	55	70
1	N	337/369 (91%)	333 (99%)	4 (1%)	71	82
1	O	340/369 (92%)	334 (98%)	6 (2%)	59	72
1	P	339/369 (92%)	332 (98%)	7 (2%)	53	68
1	Q	341/369 (92%)	336 (98%)	5 (2%)	65	77
1	R	340/369 (92%)	334 (98%)	6 (2%)	59	72
1	T	342/369 (93%)	332 (97%)	10 (3%)	42	56
1	W	341/369 (92%)	340 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	6816/7380 (92%)	6688 (98%)	128 (2%)	60 71

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	411[A]	THR
1	T	60	ARG
1	H	60	ARG
1	H	32	ARG
1	T	75[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	78	GLN
1	Q	369	HIS
1	K	175	HIS
1	W	117	ASN
1	O	412	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

136 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	SO4	O	507	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	R	503	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	C	501	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	M	502	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	P	1107	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	J	504	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	O	502	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.45	0
2	SO4	D	506	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	R	507	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	T	505	-	4,4,4	0.15	0	6,6,6	0.35	0
2	SO4	G	502	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	Q	505	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	P	1104	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	I	503	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	Q	503	-	4,4,4	0.15	0	6,6,6	0.15	0
2	SO4	B	1202	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	E	505	-	4,4,4	0.14	0	6,6,6	0.28	0
2	SO4	T	508	-	4,4,4	0.58	0	6,6,6	0.50	0
2	SO4	E	503	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	G	506	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	C	505	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	P	1101	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	W	503	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	I	504	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	N	502	-	4,4,4	0.37	0	6,6,6	0.24	0
2	SO4	P	1105	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	C	507	-	4,4,4	0.08	0	6,6,6	0.26	0
2	SO4	E	502	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	H	502	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	J	505	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	W	504	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	N	506	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	O	503	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	H	504	-	4,4,4	0.10	0	6,6,6	0.28	0
2	SO4	N	503	-	4,4,4	0.13	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	P	1108	-	4,4,4	0.17	0	6,6,6	0.44	0
2	SO4	F	507	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	K	502	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	K	503	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	L	506	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	R	502	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	I	506	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	F	503	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	Q	507	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	W	501	-	4,4,4	0.19	0	6,6,6	0.40	0
2	SO4	Q	506	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	I	507	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	O	505	-	4,4,4	0.14	0	6,6,6	0.25	0
2	SO4	T	507	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	D	503	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	L	501	-	4,4,4	0.17	0	6,6,6	0.45	0
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	G	503	-	4,4,4	0.11	0	6,6,6	0.13	0
2	SO4	J	502	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	T	502	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	F	502	-	4,4,4	0.74	0	6,6,6	2.13	3 (50%)
2	SO4	K	505	-	4,4,4	0.39	0	6,6,6	0.58	0
2	SO4	B	1207	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	N	501	-	4,4,4	0.11	0	6,6,6	0.32	0
2	SO4	P	1110	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	J	503	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	E	504	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	G	504	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	M	503	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	G	501	-	4,4,4	0.19	0	6,6,6	0.40	0
2	SO4	L	505	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	H	503	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	C	509	-	4,4,4	0.67	0	6,6,6	1.26	0
2	SO4	O	504	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	B	1206	-	4,4,4	0.10	0	6,6,6	0.17	0
2	SO4	Q	502	-	4,4,4	0.15	0	6,6,6	0.34	0
2	SO4	Q	504	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	P	1106	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	I	501	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	N	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	W	505	-	4,4,4	0.13	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	E	501	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	K	501	-	4,4,4	0.21	0	6,6,6	0.44	0
2	SO4	O	506	-	4,4,4	0.86	0	6,6,6	5.92	3 (50%)
2	SO4	T	501	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	P	1102	-	4,4,4	0.17	0	6,6,6	0.49	0
2	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	F	504	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	R	506	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	N	505	-	4,4,4	0.10	0	6,6,6	0.22	0
2	SO4	K	506	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	J	508	-	4,4,4	0.19	0	6,6,6	0.30	0
2	SO4	O	501	-	4,4,4	0.13	0	6,6,6	0.35	0
2	SO4	M	504	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	I	502	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	H	505	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.41	0
2	SO4	E	507	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	Q	508	-	4,4,4	0.43	0	6,6,6	0.17	0
2	SO4	R	504	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	R	501	-	4,4,4	0.27	0	6,6,6	0.59	0
2	SO4	B	1205	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	F	506	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	L	503	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	W	502	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	P	1103	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	T	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	P	1109	-	4,4,4	0.25	0	6,6,6	0.31	0
2	SO4	C	502	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	C	504	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	Q	501	-	4,4,4	0.20	0	6,6,6	0.47	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.43	0
2	SO4	A	505	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	E	506	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	T	506	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	J	506	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	T	503	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	B	1201	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	C	506	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	J	501	-	4,4,4	0.28	0	6,6,6	0.48	0
2	SO4	B	1203	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	G	507	-	4,4,4	0.33	0	6,6,6	0.22	0
2	SO4	C	508	-	4,4,4	0.17	0	6,6,6	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	R	505	-	4,4,4	0.10	0	6,6,6	0.22	0
2	SO4	H	501	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	I	505	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	G	505	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	K	504	-	4,4,4	0.65	0	6,6,6	0.30	0
2	SO4	F	505	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	L	502	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	J	507	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	M	501	-	4,4,4	0.18	0	6,6,6	0.20	0
2	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	B	1204	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	L	504	-	4,4,4	0.15	0	6,6,6	0.09	0

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	506	SO4	O4-S-O3	-12.28	56.62	109.06
2	O	506	SO4	O4-S-O2	-6.39	75.93	109.31
2	O	506	SO4	O3-S-O2	4.08	130.58	109.31
2	F	502	SO4	O4-S-O1	-3.16	92.84	109.31
2	F	502	SO4	O3-S-O2	2.19	120.71	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

35 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	SO4	2	0
2	Q	505	SO4	1	0
2	P	1104	SO4	1	0
2	I	503	SO4	1	0
2	I	504	SO4	1	0
2	O	503	SO4	1	0
2	H	504	SO4	1	0
2	P	1108	SO4	1	0
2	F	507	SO4	1	0
2	L	506	SO4	1	0
2	F	503	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	507	SO4	1	0
2	Q	506	SO4	1	0
2	F	502	SO4	1	0
2	P	1110	SO4	1	0
2	C	509	SO4	2	0
2	O	504	SO4	1	0
2	B	1206	SO4	1	0
2	A	504	SO4	1	0
2	O	506	SO4	0	6
2	J	508	SO4	1	0
2	Q	508	SO4	1	0
2	F	506	SO4	1	0
2	F	501	SO4	1	0
2	A	505	SO4	1	0
2	T	506	SO4	1	0
2	T	503	SO4	2	0
2	B	1203	SO4	1	0
2	C	508	SO4	1	0
2	R	505	SO4	1	0
2	H	501	SO4	1	0
2	J	507	SO4	1	0
2	M	501	SO4	2	0
2	A	502	SO4	1	0
2	L	504	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.08	15 (3%) 42 48	32, 57, 93, 163	0
1	B	415/440 (94%)	0.11	12 (2%) 51 57	32, 58, 95, 147	0
1	C	415/440 (94%)	-0.04	8 (1%) 66 72	27, 45, 78, 136	0
1	D	415/440 (94%)	0.08	11 (2%) 54 60	28, 53, 96, 160	0
1	E	415/440 (94%)	0.15	12 (2%) 51 57	36, 61, 88, 154	0
1	F	415/440 (94%)	0.08	8 (1%) 66 72	36, 60, 89, 151	0
1	G	415/440 (94%)	0.06	11 (2%) 54 60	31, 54, 94, 141	0
1	H	415/440 (94%)	0.07	12 (2%) 51 57	30, 55, 95, 156	0
1	I	415/440 (94%)	0.01	12 (2%) 51 57	28, 50, 86, 150	0
1	J	415/440 (94%)	-0.02	8 (1%) 66 72	27, 43, 74, 127	0
1	K	415/440 (94%)	0.07	12 (2%) 51 57	31, 56, 99, 156	0
1	L	415/440 (94%)	0.11	14 (3%) 45 50	31, 55, 95, 155	0
1	M	415/440 (94%)	0.16	20 (4%) 30 36	33, 59, 96, 144	0
1	N	415/440 (94%)	0.06	15 (3%) 42 48	33, 58, 90, 160	0
1	O	415/440 (94%)	0.16	17 (4%) 37 42	30, 55, 97, 173	0
1	P	415/440 (94%)	0.09	12 (2%) 51 57	28, 53, 95, 170	0
1	Q	415/440 (94%)	-0.06	8 (1%) 66 72	26, 41, 69, 131	0
1	R	415/440 (94%)	-0.03	8 (1%) 66 72	27, 41, 71, 136	0
1	T	415/440 (94%)	0.10	14 (3%) 45 50	27, 51, 90, 170	0
1	W	415/440 (94%)	0.15	14 (3%) 45 50	29, 57, 101, 153	0
All	All	8300/8800 (94%)	0.07	243 (2%) 51 57	26, 53, 93, 173	0

The worst 5 of 243 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	101	VAL	16.5
1	T	101	VAL	15.3
1	P	99	GLN	14.9
1	L	101	VAL	14.1
1	G	101	VAL	13.7

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	SO4	T	508	5/5	0.71	0.56	92,103,112,115	0
2	SO4	B	1201	5/5	0.73	0.46	149,152,153,155	0
2	SO4	K	505	5/5	0.74	0.26	113,122,122,124	0
2	SO4	F	502	5/5	0.75	0.31	114,121,124,127	0
2	SO4	P	1101	5/5	0.76	0.34	161,163,163,164	0
2	SO4	O	506	5/5	0.76	0.39	126,129,131,131	0
2	SO4	N	502	5/5	0.78	0.16	85,88,91,92	0
2	SO4	G	507	5/5	0.79	0.60	123,138,139,140	0
2	SO4	K	504	5/5	0.82	0.20	76,77,86,92	0
2	SO4	N	506	5/5	0.83	0.20	121,123,123,125	0
2	SO4	A	503	5/5	0.84	0.14	119,120,121,122	0
2	SO4	I	507	5/5	0.85	0.20	95,97,98,101	0
2	SO4	P	1108	5/5	0.85	0.24	81,86,91,96	0
2	SO4	Q	503	5/5	0.85	0.16	81,83,88,90	0
2	SO4	C	509	5/5	0.85	0.37	102,118,120,123	0
2	SO4	Q	507	5/5	0.86	0.18	121,122,123,123	0
2	SO4	T	502	5/5	0.86	0.18	99,104,106,107	0
2	SO4	C	504	5/5	0.86	0.17	82,88,92,93	0
2	SO4	E	507	5/5	0.87	0.17	122,123,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	O	507	5/5	0.87	0.15	102,107,108,108	0
2	SO4	H	504	5/5	0.88	0.16	104,106,107,109	0
2	SO4	L	502	5/5	0.88	0.15	103,103,106,109	0
2	SO4	R	507	5/5	0.88	0.13	119,121,121,123	0
2	SO4	G	506	5/5	0.88	0.22	100,107,108,109	0
2	SO4	E	503	5/5	0.88	0.18	129,133,134,136	0
2	SO4	E	502	5/5	0.89	0.23	118,119,122,122	0
2	SO4	M	504	5/5	0.89	0.13	92,102,103,104	0
2	SO4	Q	508	5/5	0.89	0.37	74,89,91,92	0
2	SO4	A	502	5/5	0.90	0.20	118,120,123,124	0
2	SO4	K	506	5/5	0.90	0.14	86,92,95,97	0
2	SO4	E	505	5/5	0.90	0.46	149,150,151,153	0
2	SO4	A	504	5/5	0.90	0.17	94,96,98,102	0
2	SO4	M	503	5/5	0.91	0.15	107,109,110,110	0
2	SO4	G	503	5/5	0.91	0.17	113,115,115,118	0
2	SO4	J	503	5/5	0.91	0.14	89,92,95,95	0
2	SO4	B	1205	5/5	0.91	0.12	93,97,98,102	0
2	SO4	R	504	5/5	0.91	0.15	92,94,94,97	0
2	SO4	C	503	5/5	0.91	0.12	88,90,97,97	0
2	SO4	W	502	5/5	0.91	0.12	104,104,106,107	0
2	SO4	H	503	5/5	0.91	0.22	117,117,118,119	0
2	SO4	A	506	5/5	0.91	0.14	108,109,110,110	0
2	SO4	P	1110	5/5	0.92	0.22	123,127,127,128	0
2	SO4	N	504	5/5	0.92	0.13	115,117,119,119	0
2	SO4	N	505	5/5	0.92	0.14	84,89,92,94	0
2	SO4	D	506	5/5	0.92	0.14	97,98,99,103	0
2	SO4	O	504	5/5	0.92	0.33	107,107,108,112	0
2	SO4	L	506	5/5	0.92	0.12	113,115,115,118	0
2	SO4	I	503	5/5	0.92	0.18	105,106,107,108	0
2	SO4	W	503	5/5	0.92	0.14	85,85,88,89	0
2	SO4	I	506	5/5	0.92	0.13	99,102,103,105	0
2	SO4	F	504	5/5	0.92	0.21	125,126,127,128	0
2	SO4	Q	504	5/5	0.93	0.11	92,92,94,97	0
2	SO4	K	503	5/5	0.93	0.12	99,102,104,108	0
2	SO4	G	502	5/5	0.93	0.14	94,102,104,106	0
2	SO4	E	506	5/5	0.93	0.14	116,117,119,120	0
2	SO4	D	505	5/5	0.93	0.15	100,100,103,103	0
2	SO4	P	1107	5/5	0.93	0.18	94,95,96,98	0
2	SO4	F	506	5/5	0.93	0.15	120,122,124,124	0
2	SO4	F	507	5/5	0.93	0.26	123,123,125,125	0
2	SO4	T	504	5/5	0.93	0.19	130,131,131,132	0
2	SO4	O	503	5/5	0.93	0.11	108,110,111,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	507	5/5	0.94	0.16	77,83,84,91	0
2	SO4	H	502	5/5	0.94	0.12	105,107,108,109	0
2	SO4	J	504	5/5	0.94	0.11	81,82,89,91	0
2	SO4	J	507	5/5	0.94	0.15	71,73,80,80	0
2	SO4	K	502	5/5	0.94	0.11	91,91,94,96	0
2	SO4	F	501	5/5	0.94	0.15	65,67,74,77	0
2	SO4	R	502	5/5	0.94	0.16	75,76,79,86	0
2	SO4	B	1207	5/5	0.94	0.08	95,102,102,104	0
2	SO4	H	505	5/5	0.94	0.14	100,102,103,107	0
2	SO4	I	502	5/5	0.94	0.12	106,106,107,109	0
2	SO4	F	503	5/5	0.94	0.13	76,93,95,95	0
2	SO4	L	505	5/5	0.94	0.11	101,103,105,106	0
2	SO4	P	1103	5/5	0.94	0.10	98,98,99,100	0
2	SO4	T	506	5/5	0.94	0.12	88,90,90,93	0
2	SO4	D	502	5/5	0.94	0.17	124,124,124,125	0
2	SO4	J	508	5/5	0.95	0.25	61,84,87,89	0
2	SO4	B	1206	5/5	0.95	0.16	104,106,107,108	0
2	SO4	E	504	5/5	0.95	0.12	81,87,87,90	0
2	SO4	D	504	5/5	0.95	0.13	81,86,88,92	0
2	SO4	Q	506	5/5	0.95	0.13	79,80,81,83	0
2	SO4	F	505	5/5	0.95	0.12	90,93,95,97	0
2	SO4	O	502	5/5	0.95	0.14	90,94,96,97	0
2	SO4	J	502	5/5	0.95	0.13	72,74,75,86	0
2	SO4	R	503	5/5	0.95	0.12	85,90,90,93	0
2	SO4	B	1203	5/5	0.95	0.14	111,112,115,117	0
2	SO4	L	504	5/5	0.95	0.15	103,104,105,107	0
2	SO4	C	508	5/5	0.95	0.12	95,96,99,101	0
2	SO4	J	505	5/5	0.95	0.13	109,110,112,113	0
2	SO4	M	502	5/5	0.95	0.15	91,93,94,98	0
2	SO4	T	503	5/5	0.95	0.14	69,80,87,92	0
2	SO4	P	1104	5/5	0.95	0.11	96,102,104,105	0
2	SO4	P	1105	5/5	0.95	0.18	104,107,110,110	0
2	SO4	T	507	5/5	0.95	0.12	89,91,92,96	0
2	SO4	A	505	5/5	0.95	0.14	100,102,103,104	0
2	SO4	C	505	5/5	0.96	0.09	108,110,111,111	0
2	SO4	P	1106	5/5	0.96	0.15	89,89,91,97	0
2	SO4	C	506	5/5	0.96	0.19	84,88,90,93	0
2	SO4	R	505	5/5	0.96	0.12	70,73,76,86	0
2	SO4	R	506	5/5	0.96	0.19	78,84,87,92	0
2	SO4	B	1204	5/5	0.96	0.12	93,95,98,99	0
2	SO4	P	1109	5/5	0.96	0.19	69,89,91,94	0
2	SO4	I	505	5/5	0.96	0.16	76,78,85,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	W	505	5/5	0.96	0.14	106,106,111,113	0
2	SO4	Q	502	5/5	0.96	0.16	69,70,73,81	0
2	SO4	J	506	5/5	0.96	0.16	82,83,84,88	0
2	SO4	C	502	5/5	0.96	0.12	70,73,74,81	0
2	SO4	T	505	5/5	0.96	0.13	72,73,78,88	0
2	SO4	N	503	5/5	0.96	0.11	100,103,104,105	0
2	SO4	L	503	5/5	0.96	0.13	90,90,94,95	0
2	SO4	G	504	5/5	0.96	0.14	95,96,97,99	0
2	SO4	E	501	5/5	0.97	0.10	70,71,73,82	0
2	SO4	Q	505	5/5	0.97	0.16	87,90,92,93	0
2	SO4	G	505	5/5	0.97	0.09	94,95,97,99	0
2	SO4	W	504	5/5	0.97	0.13	91,93,94,98	0
2	SO4	O	505	5/5	0.97	0.15	91,92,92,95	0
2	SO4	D	503	5/5	0.97	0.10	78,78,79,82	0
2	SO4	N	501	5/5	0.98	0.11	57,62,67,70	0
2	SO4	I	504	5/5	0.98	0.09	67,71,74,79	0
2	SO4	G	501	5/5	0.98	0.12	47,50,52,54	0
2	SO4	C	501	5/5	0.99	0.14	34,35,41,42	0
2	SO4	B	1202	5/5	0.99	0.10	56,58,61,63	0
2	SO4	Q	501	5/5	0.99	0.14	40,41,44,50	0
2	SO4	L	501	5/5	0.99	0.12	49,52,55,59	0
2	SO4	I	501	5/5	0.99	0.13	45,46,50,53	0
2	SO4	J	501	5/5	0.99	0.15	40,41,45,47	0
2	SO4	P	1102	5/5	0.99	0.12	42,43,46,48	0
2	SO4	T	501	5/5	0.99	0.16	40,43,43,46	0
2	SO4	K	501	5/5	0.99	0.12	54,58,61,62	0
2	SO4	H	501	5/5	0.99	0.15	50,52,54,60	0
2	SO4	A	501	5/5	0.99	0.12	58,61,63,70	0
2	SO4	R	501	5/5	0.99	0.13	35,37,39,45	0
2	SO4	O	501	5/5	0.99	0.14	47,49,51,57	0
2	SO4	M	501	5/5	0.99	0.09	54,56,59,64	0
2	SO4	D	501	5/5	0.99	0.13	41,44,44,48	0
2	SO4	W	501	5/5	1.00	0.12	49,49,51,60	0

6.5 Other polymers ⓘ

There are no such residues in this entry.