



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 02:08 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](mailto: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>.

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

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

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 Å.

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

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

## 2 Entry composition

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

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

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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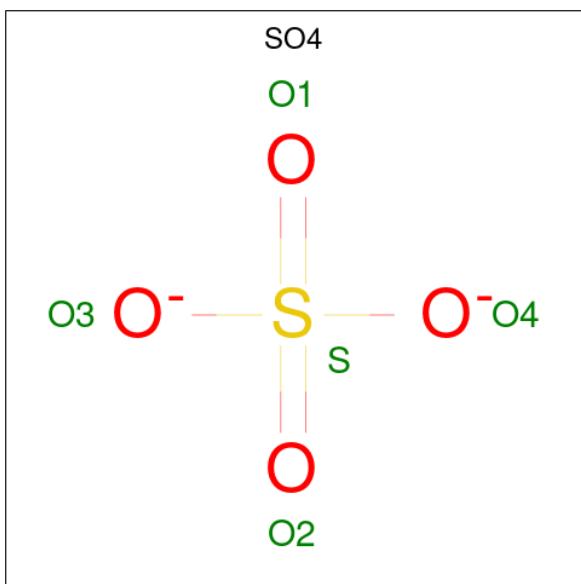
Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	SER	-	expression tag	UNP Q8U8L5
R	-8	SER	-	expression tag	UNP Q8U8L5
R	-7	GLY	-	expression tag	UNP Q8U8L5
R	-6	LEU	-	expression tag	UNP Q8U8L5
R	-5	VAL	-	expression tag	UNP Q8U8L5
R	-4	PRO	-	expression tag	UNP Q8U8L5
R	-3	ARG	-	expression tag	UNP Q8U8L5
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: O<sub>4</sub>S).



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	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	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	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	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	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	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	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	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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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
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

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

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.42Å 141.58Å 228.32Å 108.07° 101.85° 90.00°	Depositor
Resolution (Å)	72.70 – 2.29	Depositor
% Data completeness (in resolution range)	97.5 (72.70-2.29)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.208 , 0.254	Depositor
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtrriage
Anisotropy	0.316	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.56$ , $\langle L^2 \rangle = 0.40$	Xtrriage
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	Xtrriage
Total number of atoms	68292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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.

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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

### 4.2 Too-close contacts [i](#)

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

### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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

#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

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

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

### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

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	R	504	-	4,4,4	0.16	0	6,6,6	0.20	0
2	SO4	W	505	-	4,4,4	0.13	0	6,6,6	0.09	0
2	SO4	Q	504	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	H	504	-	4,4,4	0.10	0	6,6,6	0.28	0
2	SO4	T	502	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	A	501	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	F	507	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	E	503	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	O	506	-	4,4,4	0.86	0	6,6,6	5.92	3 (50%)
2	SO4	E	506	-	4,4,4	0.14	0	6,6,6	0.16	0
2	SO4	G	503	-	4,4,4	0.11	0	6,6,6	0.13	0
2	SO4	L	503	-	4,4,4	0.13	0	6,6,6	0.19	0
2	SO4	O	501	-	4,4,4	0.13	0	6,6,6	0.35	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	K	505	-	4,4,4	0.39	0	6,6,6	0.58	0
2	SO4	A	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	I	501	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	A	502	-	4,4,4	0.12	0	6,6,6	0.08	0
2	SO4	N	506	-	4,4,4	0.13	0	6,6,6	0.18	0
2	SO4	T	503	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	O	502	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	R	501	-	4,4,4	0.27	0	6,6,6	0.59	0
2	SO4	P	1105	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	E	501	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	D	501	-	4,4,4	0.19	0	6,6,6	0.45	0
2	SO4	B	1204	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	Q	508	-	4,4,4	0.43	0	6,6,6	0.17	0
2	SO4	J	504	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	J	502	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	B	1203	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	L	504	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	A	506	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	L	502	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	L	506	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	H	501	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	Q	507	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	A	505	-	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	502	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	K	506	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	G	502	-	4,4,4	0.28	0	6,6,6	0.12	0
2	SO4	O	505	-	4,4,4	0.14	0	6,6,6	0.25	0
2	SO4	H	502	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	D	504	-	4,4,4	0.15	0	6,6,6	0.41	0
2	SO4	N	503	-	4,4,4	0.13	0	6,6,6	0.26	0
2	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	C	503	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	E	507	-	4,4,4	0.16	0	6,6,6	0.06	0
2	SO4	N	502	-	4,4,4	0.37	0	6,6,6	0.24	0
2	SO4	I	507	-	4,4,4	0.18	0	6,6,6	0.32	0
2	SO4	E	504	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	I	504	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	I	503	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	J	505	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	F	501	-	4,4,4	0.14	0	6,6,6	0.43	0
2	SO4	P	1104	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	L	505	-	4,4,4	0.13	0	6,6,6	0.13	0
2	SO4	P	1108	-	4,4,4	0.17	0	6,6,6	0.44	0
2	SO4	R	502	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	C	501	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	T	505	-	4,4,4	0.15	0	6,6,6	0.35	0
2	SO4	C	509	-	4,4,4	0.67	0	6,6,6	1.26	0
2	SO4	P	1102	-	4,4,4	0.17	0	6,6,6	0.49	0
2	SO4	O	504	-	4,4,4	0.19	0	6,6,6	0.11	0
2	SO4	Q	505	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	C	508	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	B	1207	-	4,4,4	0.12	0	6,6,6	0.12	0
2	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	G	504	-	4,4,4	0.15	0	6,6,6	0.14	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	P	1110	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	J	501	-	4,4,4	0.28	0	6,6,6	0.48	0
2	SO4	C	507	-	4,4,4	0.08	0	6,6,6	0.26	0
2	SO4	I	502	-	4,4,4	0.16	0	6,6,6	0.09	0
2	SO4	L	501	-	4,4,4	0.17	0	6,6,6	0.45	0
2	SO4	G	505	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	T	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	T	501	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	P	1103	-	4,4,4	0.14	0	6,6,6	0.17	0
2	SO4	E	505	-	4,4,4	0.14	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	R	506	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	W	503	-	4,4,4	0.12	0	6,6,6	0.13	0
2	SO4	M	501	-	4,4,4	0.18	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	D	506	-	4,4,4	0.13	0	6,6,6	0.17	0
2	SO4	P	1107	-	4,4,4	0.18	0	6,6,6	0.18	0
2	SO4	J	507	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	M	503	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	B	1201	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	J	506	-	4,4,4	0.12	0	6,6,6	0.19	0
2	SO4	P	1101	-	4,4,4	0.15	0	6,6,6	0.13	0
2	SO4	G	507	-	4,4,4	0.33	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	503	-	4,4,4	0.14	0	6,6,6	0.19	0
2	SO4	H	505	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	M	502	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	B	1206	-	4,4,4	0.10	0	6,6,6	0.17	0
2	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.22	0
2	SO4	F	506	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	C	504	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	F	504	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	H	503	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	F	502	-	4,4,4	0.74	0	6,6,6	2.13	3 (50%)
2	SO4	G	506	-	4,4,4	0.14	0	6,6,6	0.20	0
2	SO4	I	506	-	4,4,4	0.15	0	6,6,6	0.24	0
2	SO4	J	508	-	4,4,4	0.19	0	6,6,6	0.30	0
2	SO4	O	507	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	R	505	-	4,4,4	0.10	0	6,6,6	0.22	0
2	SO4	Q	502	-	4,4,4	0.15	0	6,6,6	0.34	0
2	SO4	Q	506	-	4,4,4	0.13	0	6,6,6	0.30	0
2	SO4	W	504	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	W	502	-	4,4,4	0.15	0	6,6,6	0.17	0
2	SO4	B	1205	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	R	503	-	4,4,4	0.13	0	6,6,6	0.21	0
2	SO4	K	501	-	4,4,4	0.21	0	6,6,6	0.44	0
2	SO4	C	506	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	N	501	-	4,4,4	0.11	0	6,6,6	0.32	0
2	SO4	Q	501	-	4,4,4	0.20	0	6,6,6	0.47	0
2	SO4	T	506	-	4,4,4	0.09	0	6,6,6	0.16	0
2	SO4	T	508	-	4,4,4	0.58	0	6,6,6	0.50	0
2	SO4	G	501	-	4,4,4	0.19	0	6,6,6	0.40	0
2	SO4	O	503	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	B	1202	-	4,4,4	0.19	0	6,6,6	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	K	504	-	4,4,4	0.65	0	6,6,6	0.30	0
2	SO4	F	503	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	K	502	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	N	504	-	4,4,4	0.14	0	6,6,6	0.11	0
2	SO4	I	505	-	4,4,4	0.16	0	6,6,6	0.22	0
2	SO4	M	504	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	P	1106	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	R	507	-	4,4,4	0.13	0	6,6,6	0.15	0
2	SO4	F	505	-	4,4,4	0.16	0	6,6,6	0.15	0
2	SO4	W	501	-	4,4,4	0.19	0	6,6,6	0.40	0
2	SO4	J	503	-	4,4,4	0.12	0	6,6,6	0.19	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.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	506	SO4	0	6

## 4.7 Other polymers [i](#)

There are no such residues in this entry.

## 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

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

### 5.2 Non-standard residues in protein, DNA, RNA chains

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

### 5.3 Carbohydrates

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

### 5.4 Ligands

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

### 5.5 Other polymers

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