



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:37 PM GMT

PDB ID : 1HTQ  
Title : Multicopy crystallographic structure of a relaxed glutamine synthetase from Mycobacterium tuberculosis  
Authors : Gill, H.S.; Pfluegl, G.M.; Eisenberg, D.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2001-01-01  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : **NOT EXECUTED**  
Mogul : **NOT EXECUTED**  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

## 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 2.40 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 978720 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 glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-A	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-B	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-C	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-D	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	8-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-D	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-E	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-F	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	9-F	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-F	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-G	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	10-H	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-I	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-J	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-K	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-L	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	2-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-M	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-N	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-O	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-O	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	3-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-O	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	4-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	5-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	6-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	7-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	8-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	9-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	10-P	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	1-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	2-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0
1	3-Q	477	Total 3778	C 2406	N 633	O 727	S 12	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	4-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-Q	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-R	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	5-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-S	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-T	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	6-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-U	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-V	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	7-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-W	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	1-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	2-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	3-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	4-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	5-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	6-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	7-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	8-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	9-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			
1	10-X	477	Total	C	N	O	S	0	0	0
			3778	2406	633	727	12			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-V	1	Total	Mn	0	0
			1	1		
2	7-U	1	Total	Mn	0	0
			1	1		
2	6-J	1	Total	Mn	0	0
			1	1		
2	3-D	1	Total	Mn	0	0
			1	1		
2	8-R	1	Total	Mn	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-C	1	Total 1	Mn 1	0	0
2	7-O	1	Total 1	Mn 1	0	0
2	10-I	1	Total 1	Mn 1	0	0
2	6-T	1	Total 1	Mn 1	0	0
2	10-F	1	Total 1	Mn 1	0	0
2	4-M	1	Total 1	Mn 1	0	0
2	5-E	1	Total 1	Mn 1	0	0
2	3-U	1	Total 1	Mn 1	0	0
2	5-L	1	Total 1	Mn 1	0	0
2	10-T	1	Total 1	Mn 1	0	0
2	5-W	1	Total 1	Mn 1	0	0
2	2-G	1	Total 1	Mn 1	0	0
2	3-C	1	Total 1	Mn 1	0	0
2	8-S	1	Total 1	Mn 1	0	0
2	9-G	1	Total 1	Mn 1	0	0
2	2-P	1	Total 1	Mn 1	0	0
2	7-N	1	Total 1	Mn 1	0	0
2	9-N	1	Total 1	Mn 1	0	0
2	1-A	1	Total 1	Mn 1	0	0
2	4-J	1	Total 1	Mn 1	0	0
2	1-V	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-T	1	Total 1	Mn 1	0	0
2	8-B	1	Total 1	Mn 1	0	0
2	4-X	1	Total 1	Mn 1	0	0
2	6-D	1	Total 1	Mn 1	0	0
2	3-B	1	Total 1	Mn 1	0	0
2	8-P	1	Total 1	Mn 1	0	0
2	7-M	1	Total 1	Mn 1	0	0
2	10-O	1	Total 1	Mn 1	0	0
2	6-V	1	Total 1	Mn 1	0	0
2	10-D	1	Total 1	Mn 1	0	0
2	1-Q	1	Total 1	Mn 1	0	0
2	4-K	1	Total 1	Mn 1	0	0
2	5-G	1	Total 1	Mn 1	0	0
2	3-S	1	Total 1	Mn 1	0	0
2	8-C	1	Total 1	Mn 1	0	0
2	5-N	1	Total 1	Mn 1	0	0
2	1-R	1	Total 1	Mn 1	0	0
2	5-Q	1	Total 1	Mn 1	0	0
2	2-I	1	Total 1	Mn 1	0	0
2	3-A	1	Total 1	Mn 1	0	0
2	8-Q	1	Total 1	Mn 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9-I	1	Total 1	Mn 1	0	0
2	5-X	1	Total 1	Mn 1	0	0
2	2-R	1	Total 1	Mn 1	0	0
2	7-L	1	Total 1	Mn 1	0	0
2	1-W	1	Total 1	Mn 1	0	0
2	1-H	1	Total 1	Mn 1	0	0
2	1-C	1	Total 1	Mn 1	0	0
2	7-R	1	Total 1	Mn 1	0	0
2	4-H	1	Total 1	Mn 1	0	0
2	3-R	1	Total 1	Mn 1	0	0
2	6-M	1	Total 1	Mn 1	0	0
2	9-U	1	Total 1	Mn 1	0	0
2	6-F	1	Total 1	Mn 1	0	0
2	8-V	1	Total 1	Mn 1	0	0
2	7-C	1	Total 1	Mn 1	0	0
2	9-S	1	Total 1	Mn 1	0	0
2	9-V	1	Total 1	Mn 1	0	0
2	10-M	1	Total 1	Mn 1	0	0
2	6-P	1	Total 1	Mn 1	0	0
2	7-Q	1	Total 1	Mn 1	0	0
2	4-I	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	5-A	1	Total 1	Mn 1	0	0
2	10-S	1	Total 1	Mn 1	0	0
2	3-Q	1	Total 1	Mn 1	0	0
2	8-A	1	Total 1	Mn 1	0	0
2	5-H	1	Total 1	Mn 1	0	0
2	2-B	1	Total 1	Mn 1	0	0
2	1-X	1	Total 1	Mn 1	0	0
2	5-S	1	Total 1	Mn 1	0	0
2	2-K	1	Total 1	Mn 1	0	0
2	8-W	1	Total 1	Mn 1	0	0
2	9-K	1	Total 1	Mn 1	0	0
2	2-T	1	Total 1	Mn 1	0	0
2	7-B	1	Total 1	Mn 1	0	0
2	1-J	1	Total 1	Mn 1	0	0
2	1-E	1	Total 1	Mn 1	0	0
2	7-P	1	Total 1	Mn 1	0	0
2	4-V	1	Total 1	Mn 1	0	0
2	3-P	1	Total 1	Mn 1	0	0
2	8-F	1	Total 1	Mn 1	0	0
2	6-O	1	Total 1	Mn 1	0	0
2	8-T	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	10-J	1	Total 1	Mn 1	0	0
2	7-A	1	Total 1	Mn 1	0	0
2	10-C	1	Total 1	Mn 1	0	0
2	6-R	1	Total 1	Mn 1	0	0
2	10-X	1	Total 1	Mn 1	0	0
2	7-W	1	Total 1	Mn 1	0	0
2	4-W	1	Total 1	Mn 1	0	0
2	5-C	1	Total 1	Mn 1	0	0
2	10-Q	1	Total 1	Mn 1	0	0
2	3-O	1	Total 1	Mn 1	0	0
2	8-G	1	Total 1	Mn 1	0	0
2	5-J	1	Total 1	Mn 1	0	0
2	2-D	1	Total 1	Mn 1	0	0
2	9-B	1	Total 1	Mn 1	0	0
2	2-M	1	Total 1	Mn 1	0	0
2	8-U	1	Total 1	Mn 1	0	0
2	9-M	1	Total 1	Mn 1	0	0
2	2-V	1	Total 1	Mn 1	0	0
2	4-F	1	Total 1	Mn 1	0	0
2	1-L	1	Total 1	Mn 1	0	0
2	1-G	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	7-V	1	Total 1	Mn 1	0	0
2	4-T	1	Total 1	Mn 1	0	0
2	3-N	1	Total 1	Mn 1	0	0
2	8-D	1	Total 1	Mn 1	0	0
2	6-I	1	Total 1	Mn 1	0	0
2	6-B	1	Total 1	Mn 1	0	0
2	10-H	1	Total 1	Mn 1	0	0
2	7-G	1	Total 1	Mn 1	0	0
2	4-G	1	Total 1	Mn 1	0	0
2	10-A	1	Total 1	Mn 1	0	0
2	1-P	1	Total 1	Mn 1	0	0
2	4-U	1	Total 1	Mn 1	0	0
2	5-M	1	Total 1	Mn 1	0	0
2	10-W	1	Total 1	Mn 1	0	0
2	3-M	1	Total 1	Mn 1	0	0
2	8-E	1	Total 1	Mn 1	0	0
2	5-T	1	Total 1	Mn 1	0	0
2	2-F	1	Total 1	Mn 1	0	0
2	1-U	1	Total 1	Mn 1	0	0
2	9-D	1	Total 1	Mn 1	0	0
2	2-O	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	9-O	1	Total 1	Mn 1	0	0
2	2-X	1	Total 1	Mn 1	0	0
2	7-F	1	Total 1	Mn 1	0	0
2	4-D	1	Total 1	Mn 1	0	0
2	1-N	1	Total 1	Mn 1	0	0
2	7-T	1	Total 1	Mn 1	0	0
2	4-R	1	Total 1	Mn 1	0	0
2	3-L	1	Total 1	Mn 1	0	0
2	8-J	1	Total 1	Mn 1	0	0
2	6-K	1	Total 1	Mn 1	0	0
2	9-T	1	Total 1	Mn 1	0	0
2	8-X	1	Total 1	Mn 1	0	0
2	10-N	1	Total 1	Mn 1	0	0
2	6-U	1	Total 1	Mn 1	0	0
2	7-E	1	Total 1	Mn 1	0	0
2	4-E	1	Total 1	Mn 1	0	0
2	10-G	1	Total 1	Mn 1	0	0
2	5-D	1	Total 1	Mn 1	0	0
2	4-S	1	Total 1	Mn 1	0	0
2	5-O	1	Total 1	Mn 1	0	0
2	10-U	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	3-K	1	Total 1	Mn 1	0	0
2	8-K	1	Total 1	Mn 1	0	0
2	5-V	1	Total 1	Mn 1	0	0
2	2-H	1	Total 1	Mn 1	0	0
2	9-F	1	Total 1	Mn 1	0	0
2	2-Q	1	Total 1	Mn 1	0	0
2	9-Q	1	Total 1	Mn 1	0	0
2	1-I	1	Total 1	Mn 1	0	0
2	7-D	1	Total 1	Mn 1	0	0
2	4-B	1	Total 1	Mn 1	0	0
2	9-X	1	Total 1	Mn 1	0	0
2	4-P	1	Total 1	Mn 1	0	0
2	6-L	1	Total 1	Mn 1	0	0
2	3-J	1	Total 1	Mn 1	0	0
2	8-H	1	Total 1	Mn 1	0	0
2	6-E	1	Total 1	Mn 1	0	0
2	10-L	1	Total 1	Mn 1	0	0
2	6-W	1	Total 1	Mn 1	0	0
2	4-C	1	Total 1	Mn 1	0	0
2	10-E	1	Total 1	Mn 1	0	0
2	5-F	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	10-R	1	Total 1	Mn 1	0	0
2	4-Q	1	Total 1	Mn 1	0	0
2	5-I	1	Total 1	Mn 1	0	0
2	2-A	1	Total 1	Mn 1	0	0
2	3-I	1	Total 1	Mn 1	0	0
2	8-I	1	Total 1	Mn 1	0	0
2	9-A	1	Total 1	Mn 1	0	0
2	5-P	1	Total 1	Mn 1	0	0
2	2-J	1	Total 1	Mn 1	0	0
2	9-P	1	Total 1	Mn 1	0	0
2	9-H	1	Total 1	Mn 1	0	0
2	2-S	1	Total 1	Mn 1	0	0
2	1-K	1	Total 1	Mn 1	0	0
2	1-B	1	Total 1	Mn 1	0	0
2	6-N	1	Total 1	Mn 1	0	0
2	3-H	1	Total 1	Mn 1	0	0
2	8-N	1	Total 1	Mn 1	0	0
2	6-G	1	Total 1	Mn 1	0	0
2	7-K	1	Total 1	Mn 1	0	0
2	6-X	1	Total 1	Mn 1	0	0
2	10-B	1	Total 1	Mn 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-Q	1	Total 1	Mn 1	0	0
2	4-A	1	Total 1	Mn 1	0	0
2	10-P	1	Total 1	Mn 1	0	0
2	1-S	1	Total 1	Mn 1	0	0
2	5-K	1	Total 1	Mn 1	0	0
2	2-C	1	Total 1	Mn 1	0	0
2	3-G	1	Total 1	Mn 1	0	0
2	8-O	1	Total 1	Mn 1	0	0
2	9-C	1	Total 1	Mn 1	0	0
2	5-R	1	Total 1	Mn 1	0	0
2	2-L	1	Total 1	Mn 1	0	0
2	7-J	1	Total 1	Mn 1	0	0
2	1-T	1	Total 1	Mn 1	0	0
2	9-J	1	Total 1	Mn 1	0	0
2	2-U	1	Total 1	Mn 1	0	0
2	1-M	1	Total 1	Mn 1	0	0
2	7-X	1	Total 1	Mn 1	0	0
2	4-N	1	Total 1	Mn 1	0	0
2	1-D	1	Total 1	Mn 1	0	0
2	3-X	1	Total 1	Mn 1	0	0
2	9-R	1	Total 1	Mn 1	0	0

*Continued on next page...*



*Continued from previous page...*

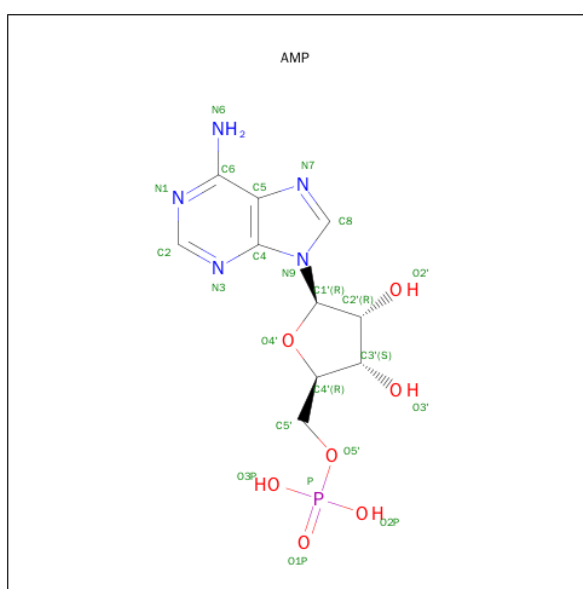
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	6-H	1	Total 1	Mn 1	0	0
2	3-F	1	Total 1	Mn 1	0	0
2	8-L	1	Total 1	Mn 1	0	0
2	6-A	1	Total 1	Mn 1	0	0
2	7-I	1	Total 1	Mn 1	0	0
2	9-W	1	Total 1	Mn 1	0	0
2	10-K	1	Total 1	Mn 1	0	0
2	6-S	1	Total 1	Mn 1	0	0
2	4-O	1	Total 1	Mn 1	0	0
2	3-W	1	Total 1	Mn 1	0	0
2	5-B	1	Total 1	Mn 1	0	0
2	10-V	1	Total 1	Mn 1	0	0
2	5-U	1	Total 1	Mn 1	0	0
2	2-E	1	Total 1	Mn 1	0	0
2	3-E	1	Total 1	Mn 1	0	0
2	8-M	1	Total 1	Mn 1	0	0
2	9-E	1	Total 1	Mn 1	0	0
2	2-N	1	Total 1	Mn 1	0	0
2	7-H	1	Total 1	Mn 1	0	0
2	7-S	1	Total 1	Mn 1	0	0
2	9-L	1	Total 1	Mn 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	2-W	1	Total	Mn	0	0
			1	1		
2	1-O	1	Total	Mn	0	0
			1	1		
2	4-L	1	Total	Mn	0	0
			1	1		
2	1-F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	2-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	3-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	4-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	5-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	6-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	7-A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-A	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-B	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-C	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-C	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-D	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-E	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	10-E	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-F	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-G	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-G	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-H	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-I	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-J	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	2-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-J	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-K	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-L	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	3-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-L	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-M	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-N	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	4-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-N	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-O	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-P	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	5-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-P	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-Q	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-R	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	6-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-R	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-S	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-T	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	7-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-T	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-U	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-V	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

*Continued from previous page...*

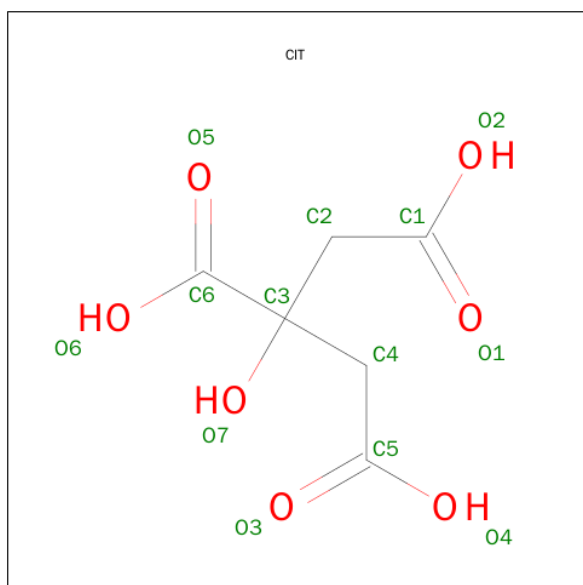
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	8-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-V	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	9-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	10-W	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	1-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	2-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	3-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	4-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	5-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	6-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	7-X	1	Total 23	C 10	N 5	O 7	P 1	0	0
3	8-X	1	Total 23	C 10	N 5	O 7	P 1	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	9-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	10-X	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-A	1	Total	C	O	0	0
			13	6	7		
4	2-A	1	Total	C	O	0	0
			13	6	7		
4	3-A	1	Total	C	O	0	0
			13	6	7		
4	4-A	1	Total	C	O	0	0
			13	6	7		
4	5-A	1	Total	C	O	0	0
			13	6	7		
4	6-A	1	Total	C	O	0	0
			13	6	7		
4	7-A	1	Total	C	O	0	0
			13	6	7		
4	8-A	1	Total	C	O	0	0
			13	6	7		
4	9-A	1	Total	C	O	0	0
			13	6	7		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-A	1	Total	C	O	0	0
			13	6	7		
4	1-B	1	Total	C	O	0	0
			13	6	7		
4	2-B	1	Total	C	O	0	0
			13	6	7		
4	3-B	1	Total	C	O	0	0
			13	6	7		
4	4-B	1	Total	C	O	0	0
			13	6	7		
4	5-B	1	Total	C	O	0	0
			13	6	7		
4	6-B	1	Total	C	O	0	0
			13	6	7		
4	7-B	1	Total	C	O	0	0
			13	6	7		
4	8-B	1	Total	C	O	0	0
			13	6	7		
4	9-B	1	Total	C	O	0	0
			13	6	7		
4	10-B	1	Total	C	O	0	0
			13	6	7		
4	1-C	1	Total	C	O	0	0
			13	6	7		
4	2-C	1	Total	C	O	0	0
			13	6	7		
4	3-C	1	Total	C	O	0	0
			13	6	7		
4	4-C	1	Total	C	O	0	0
			13	6	7		
4	5-C	1	Total	C	O	0	0
			13	6	7		
4	6-C	1	Total	C	O	0	0
			13	6	7		
4	7-C	1	Total	C	O	0	0
			13	6	7		
4	8-C	1	Total	C	O	0	0
			13	6	7		
4	9-C	1	Total	C	O	0	0
			13	6	7		
4	10-C	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	1-D	1	Total	C	O	0	0
			13	6	7		
4	2-D	1	Total	C	O	0	0
			13	6	7		
4	3-D	1	Total	C	O	0	0
			13	6	7		
4	4-D	1	Total	C	O	0	0
			13	6	7		
4	5-D	1	Total	C	O	0	0
			13	6	7		
4	6-D	1	Total	C	O	0	0
			13	6	7		
4	7-D	1	Total	C	O	0	0
			13	6	7		
4	8-D	1	Total	C	O	0	0
			13	6	7		
4	9-D	1	Total	C	O	0	0
			13	6	7		
4	10-D	1	Total	C	O	0	0
			13	6	7		
4	1-E	1	Total	C	O	0	0
			13	6	7		
4	2-E	1	Total	C	O	0	0
			13	6	7		
4	3-E	1	Total	C	O	0	0
			13	6	7		
4	4-E	1	Total	C	O	0	0
			13	6	7		
4	5-E	1	Total	C	O	0	0
			13	6	7		
4	6-E	1	Total	C	O	0	0
			13	6	7		
4	7-E	1	Total	C	O	0	0
			13	6	7		
4	8-E	1	Total	C	O	0	0
			13	6	7		
4	9-E	1	Total	C	O	0	0
			13	6	7		
4	10-E	1	Total	C	O	0	0
			13	6	7		
4	1-F	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	2-F	1	Total	C	O	0	0
			13	6	7		
4	3-F	1	Total	C	O	0	0
			13	6	7		
4	4-F	1	Total	C	O	0	0
			13	6	7		
4	5-F	1	Total	C	O	0	0
			13	6	7		
4	6-F	1	Total	C	O	0	0
			13	6	7		
4	7-F	1	Total	C	O	0	0
			13	6	7		
4	8-F	1	Total	C	O	0	0
			13	6	7		
4	9-F	1	Total	C	O	0	0
			13	6	7		
4	10-F	1	Total	C	O	0	0
			13	6	7		
4	1-G	1	Total	C	O	0	0
			13	6	7		
4	2-G	1	Total	C	O	0	0
			13	6	7		
4	3-G	1	Total	C	O	0	0
			13	6	7		
4	4-G	1	Total	C	O	0	0
			13	6	7		
4	5-G	1	Total	C	O	0	0
			13	6	7		
4	6-G	1	Total	C	O	0	0
			13	6	7		
4	7-G	1	Total	C	O	0	0
			13	6	7		
4	8-G	1	Total	C	O	0	0
			13	6	7		
4	9-G	1	Total	C	O	0	0
			13	6	7		
4	10-G	1	Total	C	O	0	0
			13	6	7		
4	1-H	1	Total	C	O	0	0
			13	6	7		
4	2-H	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	3-H	1	Total	C	O	0	0
			13	6	7		
4	4-H	1	Total	C	O	0	0
			13	6	7		
4	5-H	1	Total	C	O	0	0
			13	6	7		
4	6-H	1	Total	C	O	0	0
			13	6	7		
4	7-H	1	Total	C	O	0	0
			13	6	7		
4	8-H	1	Total	C	O	0	0
			13	6	7		
4	9-H	1	Total	C	O	0	0
			13	6	7		
4	10-H	1	Total	C	O	0	0
			13	6	7		
4	1-I	1	Total	C	O	0	0
			13	6	7		
4	2-I	1	Total	C	O	0	0
			13	6	7		
4	3-I	1	Total	C	O	0	0
			13	6	7		
4	4-I	1	Total	C	O	0	0
			13	6	7		
4	5-I	1	Total	C	O	0	0
			13	6	7		
4	6-I	1	Total	C	O	0	0
			13	6	7		
4	7-I	1	Total	C	O	0	0
			13	6	7		
4	8-I	1	Total	C	O	0	0
			13	6	7		
4	9-I	1	Total	C	O	0	0
			13	6	7		
4	10-I	1	Total	C	O	0	0
			13	6	7		
4	1-J	1	Total	C	O	0	0
			13	6	7		
4	2-J	1	Total	C	O	0	0
			13	6	7		
4	3-J	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	4-J	1	Total	C	O	0	0
			13	6	7		
4	5-J	1	Total	C	O	0	0
			13	6	7		
4	6-J	1	Total	C	O	0	0
			13	6	7		
4	7-J	1	Total	C	O	0	0
			13	6	7		
4	8-J	1	Total	C	O	0	0
			13	6	7		
4	9-J	1	Total	C	O	0	0
			13	6	7		
4	10-J	1	Total	C	O	0	0
			13	6	7		
4	1-K	1	Total	C	O	0	0
			13	6	7		
4	2-K	1	Total	C	O	0	0
			13	6	7		
4	3-K	1	Total	C	O	0	0
			13	6	7		
4	4-K	1	Total	C	O	0	0
			13	6	7		
4	5-K	1	Total	C	O	0	0
			13	6	7		
4	6-K	1	Total	C	O	0	0
			13	6	7		
4	7-K	1	Total	C	O	0	0
			13	6	7		
4	8-K	1	Total	C	O	0	0
			13	6	7		
4	9-K	1	Total	C	O	0	0
			13	6	7		
4	10-K	1	Total	C	O	0	0
			13	6	7		
4	1-L	1	Total	C	O	0	0
			13	6	7		
4	2-L	1	Total	C	O	0	0
			13	6	7		
4	3-L	1	Total	C	O	0	0
			13	6	7		
4	4-L	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	5-L	1	Total	C	O	0	0
			13	6	7		
4	6-L	1	Total	C	O	0	0
			13	6	7		
4	7-L	1	Total	C	O	0	0
			13	6	7		
4	8-L	1	Total	C	O	0	0
			13	6	7		
4	9-L	1	Total	C	O	0	0
			13	6	7		
4	10-L	1	Total	C	O	0	0
			13	6	7		
4	1-M	1	Total	C	O	0	0
			13	6	7		
4	2-M	1	Total	C	O	0	0
			13	6	7		
4	3-M	1	Total	C	O	0	0
			13	6	7		
4	4-M	1	Total	C	O	0	0
			13	6	7		
4	5-M	1	Total	C	O	0	0
			13	6	7		
4	6-M	1	Total	C	O	0	0
			13	6	7		
4	7-M	1	Total	C	O	0	0
			13	6	7		
4	8-M	1	Total	C	O	0	0
			13	6	7		
4	9-M	1	Total	C	O	0	0
			13	6	7		
4	10-M	1	Total	C	O	0	0
			13	6	7		
4	1-N	1	Total	C	O	0	0
			13	6	7		
4	2-N	1	Total	C	O	0	0
			13	6	7		
4	3-N	1	Total	C	O	0	0
			13	6	7		
4	4-N	1	Total	C	O	0	0
			13	6	7		
4	5-N	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	6-N	1	Total	C	O	0	0
			13	6	7		
4	7-N	1	Total	C	O	0	0
			13	6	7		
4	8-N	1	Total	C	O	0	0
			13	6	7		
4	9-N	1	Total	C	O	0	0
			13	6	7		
4	10-N	1	Total	C	O	0	0
			13	6	7		
4	1-O	1	Total	C	O	0	0
			13	6	7		
4	2-O	1	Total	C	O	0	0
			13	6	7		
4	3-O	1	Total	C	O	0	0
			13	6	7		
4	4-O	1	Total	C	O	0	0
			13	6	7		
4	5-O	1	Total	C	O	0	0
			13	6	7		
4	6-O	1	Total	C	O	0	0
			13	6	7		
4	7-O	1	Total	C	O	0	0
			13	6	7		
4	8-O	1	Total	C	O	0	0
			13	6	7		
4	9-O	1	Total	C	O	0	0
			13	6	7		
4	10-O	1	Total	C	O	0	0
			13	6	7		
4	1-P	1	Total	C	O	0	0
			13	6	7		
4	2-P	1	Total	C	O	0	0
			13	6	7		
4	3-P	1	Total	C	O	0	0
			13	6	7		
4	4-P	1	Total	C	O	0	0
			13	6	7		
4	5-P	1	Total	C	O	0	0
			13	6	7		
4	6-P	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	7-P	1	Total	C	O	0	0
			13	6	7		
4	8-P	1	Total	C	O	0	0
			13	6	7		
4	9-P	1	Total	C	O	0	0
			13	6	7		
4	10-P	1	Total	C	O	0	0
			13	6	7		
4	1-Q	1	Total	C	O	0	0
			13	6	7		
4	2-Q	1	Total	C	O	0	0
			13	6	7		
4	3-Q	1	Total	C	O	0	0
			13	6	7		
4	4-Q	1	Total	C	O	0	0
			13	6	7		
4	5-Q	1	Total	C	O	0	0
			13	6	7		
4	6-Q	1	Total	C	O	0	0
			13	6	7		
4	7-Q	1	Total	C	O	0	0
			13	6	7		
4	8-Q	1	Total	C	O	0	0
			13	6	7		
4	9-Q	1	Total	C	O	0	0
			13	6	7		
4	10-Q	1	Total	C	O	0	0
			13	6	7		
4	1-R	1	Total	C	O	0	0
			13	6	7		
4	2-R	1	Total	C	O	0	0
			13	6	7		
4	3-R	1	Total	C	O	0	0
			13	6	7		
4	4-R	1	Total	C	O	0	0
			13	6	7		
4	5-R	1	Total	C	O	0	0
			13	6	7		
4	6-R	1	Total	C	O	0	0
			13	6	7		
4	7-R	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	8-R	1	Total	C	O	0	0
			13	6	7		
4	9-R	1	Total	C	O	0	0
			13	6	7		
4	10-R	1	Total	C	O	0	0
			13	6	7		
4	1-S	1	Total	C	O	0	0
			13	6	7		
4	2-S	1	Total	C	O	0	0
			13	6	7		
4	3-S	1	Total	C	O	0	0
			13	6	7		
4	4-S	1	Total	C	O	0	0
			13	6	7		
4	5-S	1	Total	C	O	0	0
			13	6	7		
4	6-S	1	Total	C	O	0	0
			13	6	7		
4	7-S	1	Total	C	O	0	0
			13	6	7		
4	8-S	1	Total	C	O	0	0
			13	6	7		
4	9-S	1	Total	C	O	0	0
			13	6	7		
4	10-S	1	Total	C	O	0	0
			13	6	7		
4	1-T	1	Total	C	O	0	0
			13	6	7		
4	2-T	1	Total	C	O	0	0
			13	6	7		
4	3-T	1	Total	C	O	0	0
			13	6	7		
4	4-T	1	Total	C	O	0	0
			13	6	7		
4	5-T	1	Total	C	O	0	0
			13	6	7		
4	6-T	1	Total	C	O	0	0
			13	6	7		
4	7-T	1	Total	C	O	0	0
			13	6	7		
4	8-T	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	9-T	1	Total	C	O	0	0
			13	6	7		
4	10-T	1	Total	C	O	0	0
			13	6	7		
4	1-U	1	Total	C	O	0	0
			13	6	7		
4	2-U	1	Total	C	O	0	0
			13	6	7		
4	3-U	1	Total	C	O	0	0
			13	6	7		
4	4-U	1	Total	C	O	0	0
			13	6	7		
4	5-U	1	Total	C	O	0	0
			13	6	7		
4	6-U	1	Total	C	O	0	0
			13	6	7		
4	7-U	1	Total	C	O	0	0
			13	6	7		
4	8-U	1	Total	C	O	0	0
			13	6	7		
4	9-U	1	Total	C	O	0	0
			13	6	7		
4	10-U	1	Total	C	O	0	0
			13	6	7		
4	1-V	1	Total	C	O	0	0
			13	6	7		
4	2-V	1	Total	C	O	0	0
			13	6	7		
4	3-V	1	Total	C	O	0	0
			13	6	7		
4	4-V	1	Total	C	O	0	0
			13	6	7		
4	5-V	1	Total	C	O	0	0
			13	6	7		
4	6-V	1	Total	C	O	0	0
			13	6	7		
4	7-V	1	Total	C	O	0	0
			13	6	7		
4	8-V	1	Total	C	O	0	0
			13	6	7		
4	9-V	1	Total	C	O	0	0
			13	6	7		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	10-V	1	Total	C	O	0	0
			13	6	7		
4	1-W	1	Total	C	O	0	0
			13	6	7		
4	2-W	1	Total	C	O	0	0
			13	6	7		
4	3-W	1	Total	C	O	0	0
			13	6	7		
4	4-W	1	Total	C	O	0	0
			13	6	7		
4	5-W	1	Total	C	O	0	0
			13	6	7		
4	6-W	1	Total	C	O	0	0
			13	6	7		
4	7-W	1	Total	C	O	0	0
			13	6	7		
4	8-W	1	Total	C	O	0	0
			13	6	7		
4	9-W	1	Total	C	O	0	0
			13	6	7		
4	10-W	1	Total	C	O	0	0
			13	6	7		
4	1-X	1	Total	C	O	0	0
			13	6	7		
4	2-X	1	Total	C	O	0	0
			13	6	7		
4	3-X	1	Total	C	O	0	0
			13	6	7		
4	4-X	1	Total	C	O	0	0
			13	6	7		
4	5-X	1	Total	C	O	0	0
			13	6	7		
4	6-X	1	Total	C	O	0	0
			13	6	7		
4	7-X	1	Total	C	O	0	0
			13	6	7		
4	8-X	1	Total	C	O	0	0
			13	6	7		
4	9-X	1	Total	C	O	0	0
			13	6	7		
4	10-X	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	261	Total O 261 261	0	0
5	2-A	262	Total O 262 262	0	0
5	3-A	261	Total O 261 261	0	0
5	4-A	263	Total O 263 263	0	0
5	5-A	261	Total O 261 261	0	0
5	6-A	257	Total O 257 257	0	0
5	7-A	265	Total O 265 265	0	0
5	8-A	259	Total O 259 259	0	0
5	9-A	265	Total O 265 265	0	0
5	10-A	262	Total O 262 262	0	0
5	1-B	264	Total O 264 264	0	0
5	2-B	261	Total O 261 261	0	0
5	3-B	263	Total O 263 263	0	0
5	4-B	262	Total O 262 262	0	0
5	5-B	261	Total O 261 261	0	0
5	6-B	265	Total O 265 265	0	0
5	7-B	264	Total O 264 264	0	0
5	8-B	264	Total O 264 264	0	0
5	9-B	258	Total O 258 258	0	0
5	10-B	263	Total O 263 263	0	0
5	1-C	261	Total O 261 261	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-C	264	Total 264	O 264	0	0
5	3-C	265	Total 265	O 265	0	0
5	4-C	261	Total 261	O 261	0	0
5	5-C	263	Total 263	O 263	0	0
5	6-C	262	Total 262	O 262	0	0
5	7-C	262	Total 262	O 262	0	0
5	8-C	263	Total 263	O 263	0	0
5	9-C	261	Total 261	O 261	0	0
5	10-C	262	Total 262	O 262	0	0
5	1-D	260	Total 260	O 260	0	0
5	2-D	269	Total 269	O 269	0	0
5	3-D	260	Total 260	O 260	0	0
5	4-D	263	Total 263	O 263	0	0
5	5-D	262	Total 262	O 262	0	0
5	6-D	265	Total 265	O 265	0	0
5	7-D	261	Total 261	O 261	0	0
5	8-D	265	Total 265	O 265	0	0
5	9-D	266	Total 266	O 266	0	0
5	10-D	262	Total 262	O 262	0	0
5	1-E	261	Total 261	O 261	0	0
5	2-E	254	Total 254	O 254	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	3-E	257	Total 257	O 257	0	0
5	4-E	263	Total 263	O 263	0	0
5	5-E	259	Total 259	O 259	0	0
5	6-E	262	Total 262	O 262	0	0
5	7-E	265	Total 265	O 265	0	0
5	8-E	257	Total 257	O 257	0	0
5	9-E	262	Total 262	O 262	0	0
5	10-E	257	Total 257	O 257	0	0
5	1-F	262	Total 262	O 262	0	0
5	2-F	263	Total 263	O 263	0	0
5	3-F	272	Total 272	O 272	0	0
5	4-F	264	Total 264	O 264	0	0
5	5-F	266	Total 266	O 266	0	0
5	6-F	263	Total 263	O 263	0	0
5	7-F	262	Total 262	O 262	0	0
5	8-F	268	Total 268	O 268	0	0
5	9-F	262	Total 262	O 262	0	0
5	10-F	261	Total 261	O 261	0	0
5	1-G	265	Total 265	O 265	0	0
5	2-G	262	Total 262	O 262	0	0
5	3-G	257	Total 257	O 257	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	4-G	261	Total 261	O 261	0	0
5	5-G	263	Total 263	O 263	0	0
5	6-G	267	Total 267	O 267	0	0
5	7-G	259	Total 259	O 259	0	0
5	8-G	265	Total 265	O 265	0	0
5	9-G	263	Total 263	O 263	0	0
5	10-G	264	Total 264	O 264	0	0
5	1-H	262	Total 262	O 262	0	0
5	2-H	263	Total 263	O 263	0	0
5	3-H	261	Total 261	O 261	0	0
5	4-H	266	Total 266	O 266	0	0
5	5-H	270	Total 270	O 270	0	0
5	6-H	263	Total 263	O 263	0	0
5	7-H	262	Total 262	O 262	0	0
5	8-H	261	Total 261	O 261	0	0
5	9-H	268	Total 268	O 268	0	0
5	10-H	264	Total 264	O 264	0	0
5	1-I	265	Total 265	O 265	0	0
5	2-I	265	Total 265	O 265	0	0
5	3-I	266	Total 266	O 266	0	0
5	4-I	263	Total 263	O 263	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	5-I	260	Total 260	O 260	0	0
5	6-I	263	Total 263	O 263	0	0
5	7-I	261	Total 261	O 261	0	0
5	8-I	265	Total 265	O 265	0	0
5	9-I	262	Total 262	O 262	0	0
5	10-I	263	Total 263	O 263	0	0
5	1-J	262	Total 262	O 262	0	0
5	2-J	258	Total 258	O 258	0	0
5	3-J	260	Total 260	O 260	0	0
5	4-J	260	Total 260	O 260	0	0
5	5-J	263	Total 263	O 263	0	0
5	6-J	259	Total 259	O 259	0	0
5	7-J	266	Total 266	O 266	0	0
5	8-J	263	Total 263	O 263	0	0
5	9-J	260	Total 260	O 260	0	0
5	10-J	264	Total 264	O 264	0	0
5	1-K	272	Total 272	O 272	0	0
5	2-K	271	Total 271	O 271	0	0
5	3-K	268	Total 268	O 268	0	0
5	4-K	267	Total 267	O 267	0	0
5	5-K	268	Total 268	O 268	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	6-K	270	Total 270	O 270	0	0
5	7-K	263	Total 263	O 263	0	0
5	8-K	264	Total 264	O 264	0	0
5	9-K	269	Total 269	O 269	0	0
5	10-K	271	Total 271	O 271	0	0
5	1-L	261	Total 261	O 261	0	0
5	2-L	264	Total 264	O 264	0	0
5	3-L	266	Total 266	O 266	0	0
5	4-L	263	Total 263	O 263	0	0
5	5-L	260	Total 260	O 260	0	0
5	6-L	260	Total 260	O 260	0	0
5	7-L	266	Total 266	O 266	0	0
5	8-L	262	Total 262	O 262	0	0
5	9-L	260	Total 260	O 260	0	0
5	10-L	263	Total 263	O 263	0	0
5	1-M	261	Total 261	O 261	0	0
5	2-M	264	Total 264	O 264	0	0
5	3-M	259	Total 259	O 259	0	0
5	4-M	264	Total 264	O 264	0	0
5	5-M	264	Total 264	O 264	0	0
5	6-M	262	Total 262	O 262	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	7-M	260	Total O 260 260	0	0
5	8-M	260	Total O 260 260	0	0
5	9-M	265	Total O 265 265	0	0
5	10-M	263	Total O 263 263	0	0
5	1-N	263	Total O 263 263	0	0
5	2-N	261	Total O 261 261	0	0
5	3-N	263	Total O 263 263	0	0
5	4-N	263	Total O 263 263	0	0
5	5-N	265	Total O 265 265	0	0
5	6-N	260	Total O 260 260	0	0
5	7-N	266	Total O 266 266	0	0
5	8-N	263	Total O 263 263	0	0
5	9-N	261	Total O 261 261	0	0
5	10-N	259	Total O 259 259	0	0
5	1-O	263	Total O 263 263	0	0
5	2-O	267	Total O 267 267	0	0
5	3-O	265	Total O 265 265	0	0
5	4-O	263	Total O 263 263	0	0
5	5-O	267	Total O 267 267	0	0
5	6-O	265	Total O 265 265	0	0
5	7-O	262	Total O 262 262	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	8-O	265	Total 265	O 265	0	0
5	9-O	263	Total 263	O 263	0	0
5	10-O	263	Total 263	O 263	0	0
5	1-P	261	Total 261	O 261	0	0
5	2-P	264	Total 264	O 264	0	0
5	3-P	260	Total 260	O 260	0	0
5	4-P	259	Total 259	O 259	0	0
5	5-P	262	Total 262	O 262	0	0
5	6-P	262	Total 262	O 262	0	0
5	7-P	261	Total 261	O 261	0	0
5	8-P	263	Total 263	O 263	0	0
5	9-P	265	Total 265	O 265	0	0
5	10-P	264	Total 264	O 264	0	0
5	1-Q	260	Total 260	O 260	0	0
5	2-Q	257	Total 257	O 257	0	0
5	3-Q	259	Total 259	O 259	0	0
5	4-Q	264	Total 264	O 264	0	0
5	5-Q	261	Total 261	O 261	0	0
5	6-Q	260	Total 260	O 260	0	0
5	7-Q	264	Total 264	O 264	0	0
5	8-Q	257	Total 257	O 257	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	9-Q	263	Total 263	O 263	0	0
5	10-Q	257	Total 257	O 257	0	0
5	1-R	261	Total 261	O 261	0	0
5	2-R	265	Total 265	O 265	0	0
5	3-R	268	Total 268	O 268	0	0
5	4-R	263	Total 263	O 263	0	0
5	5-R	265	Total 265	O 265	0	0
5	6-R	266	Total 266	O 266	0	0
5	7-R	264	Total 264	O 264	0	0
5	8-R	265	Total 265	O 265	0	0
5	9-R	264	Total 264	O 264	0	0
5	10-R	262	Total 262	O 262	0	0
5	1-S	265	Total 265	O 265	0	0
5	2-S	259	Total 259	O 259	0	0
5	3-S	264	Total 264	O 264	0	0
5	4-S	260	Total 260	O 260	0	0
5	5-S	263	Total 263	O 263	0	0
5	6-S	266	Total 266	O 266	0	0
5	7-S	263	Total 263	O 263	0	0
5	8-S	269	Total 269	O 269	0	0
5	9-S	259	Total 259	O 259	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	10-S	266	Total 266	O 266	0	0
5	1-T	261	Total 261	O 261	0	0
5	2-T	259	Total 259	O 259	0	0
5	3-T	262	Total 262	O 262	0	0
5	4-T	262	Total 262	O 262	0	0
5	5-T	258	Total 258	O 258	0	0
5	6-T	257	Total 257	O 257	0	0
5	7-T	263	Total 263	O 263	0	0
5	8-T	259	Total 259	O 259	0	0
5	9-T	265	Total 265	O 265	0	0
5	10-T	262	Total 262	O 262	0	0
5	1-U	263	Total 263	O 263	0	0
5	2-U	267	Total 267	O 267	0	0
5	3-U	267	Total 267	O 267	0	0
5	4-U	264	Total 264	O 264	0	0
5	5-U	263	Total 263	O 263	0	0
5	6-U	265	Total 265	O 265	0	0
5	7-U	262	Total 262	O 262	0	0
5	8-U	263	Total 263	O 263	0	0
5	9-U	265	Total 265	O 265	0	0
5	10-U	264	Total 264	O 264	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-V	265	Total 265	O 265	0	0
5	2-V	260	Total 260	O 260	0	0
5	3-V	258	Total 258	O 258	0	0
5	4-V	266	Total 266	O 266	0	0
5	5-V	261	Total 261	O 261	0	0
5	6-V	265	Total 265	O 265	0	0
5	7-V	265	Total 265	O 265	0	0
5	8-V	264	Total 264	O 264	0	0
5	9-V	259	Total 259	O 259	0	0
5	10-V	265	Total 265	O 265	0	0
5	1-W	269	Total 269	O 269	0	0
5	2-W	266	Total 266	O 266	0	0
5	3-W	266	Total 266	O 266	0	0
5	4-W	263	Total 263	O 263	0	0
5	5-W	262	Total 262	O 262	0	0
5	6-W	264	Total 264	O 264	0	0
5	7-W	265	Total 265	O 265	0	0
5	8-W	263	Total 263	O 263	0	0
5	9-W	261	Total 261	O 261	0	0
5	10-W	265	Total 265	O 265	0	0
5	1-X	264	Total 264	O 264	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-X	267	Total	O	0	0
			267	267		
5	3-X	265	Total	O	0	0
			265	265		
5	4-X	265	Total	O	0	0
			265	265		
5	5-X	265	Total	O	0	0
			265	265		
5	6-X	264	Total	O	0	0
			264	264		
5	7-X	261	Total	O	0	0
			261	261		
5	8-X	265	Total	O	0	0
			265	265		
5	9-X	266	Total	O	0	0
			266	266		
5	10-X	266	Total	O	0	0
			266	266		

MolProbity and EDS were not executed - this section will therefore be empty.

### 3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.72Å 257.69Å 274.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	99.6 (20.00-2.40)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.204 , 0.223	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	978720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

## 4 Model quality [i](#)

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

MolProbity was not executed - this section will therefore be empty.

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

MolProbity was not executed - this section will therefore be empty.

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

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

MolProbity was not executed - this section will therefore be empty.

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

MolProbity was not executed - this section will therefore be empty.

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

MolProbity was not executed - this section will therefore be empty.

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

validation-pack and Mogul were not executed - this section will therefore be empty.

### 4.5 Carbohydrates [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

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

validation-pack and Mogul were not executed - this section will therefore be empty.

### 4.7 Other polymers [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.



## 5 Fit of model and data ⓘ

### 5.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 5.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 5.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 5.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.