



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:41 PM GMT

PDB ID : 4V99  
Title : The Crystallographic Structure of Panicum Mosaic Virus  
Authors : Makino, D.L.; Larson, S.B.; McPherson, A.  
Deposited on : 2012-07-04  
Resolution : 2.90 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.

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

MolProbity : **FAILED**  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
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 2.90 Å.

There are no percentiles available for this entry.

MolProbity failed to run properly; EDS was not executed - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 588120 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	AV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	AW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	AZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aa	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Ab	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Ae	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Af	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Ag	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Aj	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ak	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Al	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Ao	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Ap	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Aq	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	At	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Au	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Av	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Ay	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Az	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	A1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	A4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	A5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	A6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	BA	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	BV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	BW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	BZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ba	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Be	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Bk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Bt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Bv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	By	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Bz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	B4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	B5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	B6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	CL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	CV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	CW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	CZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ca	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ce	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ck	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Co	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ct	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Cu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Cv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Cy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Cz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	C4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	C5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	C6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	DQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	DV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	DW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	DZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Da	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Db	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	De	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Df	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Do	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Du	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Dv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Dy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Dz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	D4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	D6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	ER	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	EV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	EW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	EZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ea	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ee	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ef	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ej	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ek	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	El	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Eo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ep	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Eq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Et	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Eu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ev	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ey	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ez	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	E4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	E5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	E6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	FG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	FV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	FW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	FZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fa	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fe	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ff	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Fk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Fl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Fo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Fp	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fq	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Ft	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fu	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	Fv	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	Fy	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	Fz	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	F1	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	F4	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	F5	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	F6	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GA	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GB	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GC	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GF	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GG	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GH	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GK	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0
1	GL	189	Total 1451	C 915	N 253	O 278	S 5	0	0	0
1	GM	217	Total 1674	C 1049	N 304	O 316	S 5	0	0	0
1	GP	185	Total 1426	C 901	N 248	O 273	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	GQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	GV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	GW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	GZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ga	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ge	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Go	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Gu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Gv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Gy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Gz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	G4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	G5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	G6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	HV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	HW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	HZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ha	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	He	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ho	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ht	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Hv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Hy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Hz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	H4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	H5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	H6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	IB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	IV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	IW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	IZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ia	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ib	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ie	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	If	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Ig	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Ij	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ik	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Il	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Io	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ip	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Iq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	It	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Iu	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Iv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Iy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Iz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	I1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	I4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	I5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	I6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JA	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JB	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JC	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JF	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JG	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JH	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JK	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	JL	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JM	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JP	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JQ	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JR	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JU	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	JV	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	JW	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	JZ	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Ja	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jb	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Je	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jf	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jg	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jj	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jk	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jl	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jo	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jp	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jq	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jt	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ju	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	Jv	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	Jy	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	Jz	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J1	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			
1	J4	185	Total	C	N	O	S	0	0	0
			1426	901	248	273	4			
1	J5	189	Total	C	N	O	S	0	0	0
			1451	915	253	278	5			
1	J6	217	Total	C	N	O	S	0	0	0
			1674	1049	304	316	5			

- Molecule 2 is a RNA chain called 5'-R(P\*UP\*UP\*AP\*AP\*UP\*AP\*UP\*UP\*UP\*UP\*UP\*AP\*UP\*UP\*UP\*UP\*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AD	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AI	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AN	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AS	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	AX	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ac	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ah	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Am	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ar	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Aw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	A2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	BX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Br	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Bw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	B7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	CX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ch	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Cr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Cw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	C7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	DX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Dw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	D7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ED	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ES	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	EX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Ec	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Eh	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Em	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Er	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Ew	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	E2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	E7	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	FD	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	FI	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	FN	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	FS	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	FX	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Fc	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Fh	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Fm	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Fr	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Fw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	F2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	F7	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	GD	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	GI	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	GN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	GX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Gw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	G7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	HX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hr	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Hw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	H2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	ID	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	II	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	IX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ic	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ih	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Im	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Ir	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Iw	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I2	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	I7	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JD	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JI	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JN	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JS	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	JX	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jc	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jh	17	Total 349	C 157	N 46	O 129	P 17	0	0	0
2	Jm	17	Total 349	C 157	N 46	O 129	P 17	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Jr	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	Jw	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	J2	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			
2	J7	17	Total	C	N	O	P	0	0	0
			349	157	46	129	17			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Jt	1	Total	Ca	0	0
			1	1		
3	FU	1	Total	Ca	0	0
			1	1		
3	CA	1	Total	Ca	0	0
			1	1		
3	IZ	1	Total	Ca	0	0
			1	1		
3	Eo	1	Total	Ca	0	0
			1	1		
3	FK	1	Total	Ca	0	0
			1	1		
3	DZ	1	Total	Ca	0	0
			1	1		
3	Ce	1	Total	Ca	0	0
			1	1		
3	Af	1	Total	Ca	0	0
			1	1		
3	EF	1	Total	Ca	0	0
			1	1		
3	JL	1	Total	Ca	0	0
			1	1		
3	C4	1	Total	Ca	0	0
			1	1		
3	Gt	1	Total	Ca	0	0
			1	1		
3	Df	1	Total	Ca	0	0
			1	1		
3	HF	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Be	1	Total	Ca	0	0
			1	1		
3	AA	1	Total	Ca	0	0
			1	1		
3	Hj	1	Total	Ca	0	0
			1	1		
3	JA	1	Total	Ca	0	0
			1	1		
3	A4	1	Total	Ca	0	0
			1	1		
3	D4	1	Total	Ca	0	0
			1	1		
3	AL	1	Total	Ca	0	0
			1	1		
3	JZ	1	Total	Ca	0	0
			1	1		
3	DP	1	Total	Ca	0	0
			1	1		
3	Hg	1	Total	Ca	0	0
			1	1		
3	GK	1	Total	Ca	0	0
			1	1		
3	HZ	1	Total	Ca	0	0
			1	1		
3	JF	1	Total	Ca	0	0
			1	1		
3	EU	1	Total	Ca	0	0
			1	1		
3	AF	1	Total	Ca	0	0
			1	1		
3	CZ	1	Total	Ca	0	0
			1	1		
3	Ek	1	Total	Ca	0	0
			1	1		
3	Bo	1	Total	Ca	0	0
			1	1		
3	DK	1	Total	Ca	0	0
			1	1		
3	DF	1	Total	Ca	0	0
			1	1		
3	GA	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	DU	1	Total 1	Ca 1	0	0
3	Ao	1	Total 1	Ca 1	0	0
3	Jy	1	Total 1	Ca 1	0	0
3	CU	1	Total 1	Ca 1	0	0
3	Co	1	Total 1	Ca 1	0	0
3	Gj	1	Total 1	Ca 1	0	0
3	Et	1	Total 1	Ca 1	0	0
3	Cy	1	Total 1	Ca 1	0	0
3	BU	1	Total 1	Ca 1	0	0
3	Aj	1	Total 1	Ca 1	0	0
3	HP	1	Total 1	Ca 1	0	0
3	FF	1	Total 1	Ca 1	0	0
3	CP	1	Total 1	Ca 1	0	0
3	DA	1	Total 1	Ca 1	0	0
3	AU	1	Total 1	Ca 1	0	0
3	Ht	1	Total 1	Ca 1	0	0
3	GZ	1	Total 1	Ca 1	0	0
3	EK	1	Total 1	Ca 1	0	0
3	Fo	1	Total 1	Ca 1	0	0
3	Ct	1	Total 1	Ca 1	0	0
3	BZ	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	FP	1	Total 1	Ca 1	0	0
3	Bk	1	Total 1	Ca 1	0	0
3	GP	1	Total 1	Ca 1	0	0
3	AP	1	Total 1	Ca 1	0	0
3	I1	1	Total 1	Ca 1	0	0
3	Ft	1	Total 1	Ca 1	0	0
3	At	1	Total 1	Ca 1	0	0
3	B5	1	Total 1	Ca 1	0	0
3	IR	1	Total 1	Ca 1	0	0
3	BF	1	Total 1	Ca 1	0	0
3	BQ	1	Total 1	Ca 1	0	0
3	I4	1	Total 1	Ca 1	0	0
3	CG	1	Total 1	Ca 1	0	0
3	HK	1	Total 1	Ca 1	0	0
3	G1	1	Total 1	Ca 1	0	0
3	A1	1	Total 1	Ca 1	0	0
3	FZ	1	Total 1	Ca 1	0	0
3	AZ	1	Total 1	Ca 1	0	0
3	Ho	1	Total 1	Ca 1	0	0
3	BK	1	Total 1	Ca 1	0	0
3	If	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G4	1	Total 1	Ca 1	0	0
3	J4	1	Total 1	Ca 1	0	0
3	Jj	1	Total 1	Ca 1	0	0
3	Ey	1	Total 1	Ca 1	0	0
3	Je	1	Total 1	Ca 1	0	0
3	IA	1	Total 1	Ca 1	0	0
3	JP	1	Total 1	Ca 1	0	0
3	GF	1	Total 1	Ca 1	0	0
3	Dj	1	Total 1	Ca 1	0	0
3	EP	1	Total 1	Ca 1	0	0
3	Dy	1	Total 1	Ca 1	0	0
3	HA	1	Total 1	Ca 1	0	0
3	Dt	1	Total 1	Ca 1	0	0
3	H4	1	Total 1	Ca 1	0	0
3	Jo	1	Total 1	Ca 1	0	0
3	Go	1	Total 1	Ca 1	0	0
3	IK	1	Total 1	Ca 1	0	0
3	BB	1	Total 1	Ca 1	0	0
3	JU	1	Total 1	Ca 1	0	0
3	EZ	1	Total 1	Ca 1	0	0
3	Do	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Io	1	Total 1	Ca 1	0	0
3	Fk	1	Total 1	Ca 1	0	0
3	CK	1	Total 1	Ca 1	0	0
3	Ge	1	Total 1	Ca 1	0	0
3	IU	1	Total 1	Ca 1	0	0
3	FA	1	Total 1	Ca 1	0	0
3	Bt	1	Total 1	Ca 1	0	0
3	IF	1	Total 1	Ca 1	0	0
3	F4	1	Total 1	Ca 1	0	0
3	Fe	1	Total 1	Ca 1	0	0
3	HU	1	Total 1	Ca 1	0	0
3	Ij	1	Total 1	Ca 1	0	0
3	Cj	1	Total 1	Ca 1	0	0
3	Hy	1	Total 1	Ca 1	0	0
3	Ee	1	Total 1	Ca 1	0	0
3	By	1	Total 1	Ca 1	0	0
3	GU	1	Total 1	Ca 1	0	0
3	F1	1	Total 1	Ca 1	0	0
3	E4	1	Total 1	Ca 1	0	0
3	EC	1	Total 1	Ca 1	0	0
3	It	1	Total 1	Ca 1	0	0

MolProbity failed to run properly; EDS was not executed - this section will therefore be empty.

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	411.74Å 403.90Å 412.46Å 90.00° 89.65° 90.00°	Depositor
Resolution (Å)	50.01 – 2.90	Depositor
% Data completeness (in resolution range)	74.9 (50.01-2.90)	Depositor
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.99 (at 2.91Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.251 , 0.285	Depositor
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.138	Xtriage
Estimated twinning fraction	0.025 for -l,k,h 0.034 for -h,-l,-k 0.024 for -h,l,k 0.044 for -k,-h,-l 0.024 for k,h,-l 0.017 for -l,-h,k 0.030 for -k,l,-h 0.038 for l,h,k 0.027 for k,-l,-h 0.035 for h,-k,-l 0.030 for -l,-k,-h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 2217465 reflections	Xtriage
Total number of atoms	588120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 4 Model quality [i](#)

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

MolProbity failed to run properly - this section will therefore be empty.

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

MolProbity failed to run properly - this section will therefore be empty.

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

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

MolProbity failed to run properly - this section will therefore be empty.

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

MolProbity failed to run properly - this section will therefore be empty.

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

MolProbity failed to run properly - this section will therefore be 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 carbohydrates in this entry.

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

Of 120 ligands modelled in this entry, 120 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 5 Fit of model and data [i](#)

### 5.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 5.3 Carbohydrates [i](#)

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

### 5.4 Ligands [i](#)

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

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

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