



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:40 PM GMT

PDB ID : 4CG3  
Title : Structural and functional studies on a thermostable polyethylene terephthalate degrading hydrolase from *Thermobifida fusca*  
Authors : Roth, C.; Wei, R.; Oeser, T.; Then, J.; Foellner, C.; Zimmermann, W.; Straeter, N.  
Deposited on : 2013-11-20  
Resolution : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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 : **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 1.55 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 3 unique types of molecules in this entry. The entry contains 314292 atoms, of which 151613 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 CUTINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	2-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	3-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	4-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	5-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	6-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	7-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	8-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	9-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	10-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	11-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	12-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	13-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	14-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	15-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	16-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	18-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	19-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	20-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	21-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	22-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	23-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	24-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	25-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	26-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	27-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	28-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	29-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	30-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	31-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	32-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	33-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	34-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	35-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	36-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	37-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	39-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	40-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	41-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	42-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	43-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	44-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	45-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	46-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	47-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	48-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	49-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	50-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	51-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	52-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	53-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	54-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	55-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	56-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	57-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	58-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	60-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	61-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	62-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	63-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	64-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	65-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	66-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	67-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	68-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	69-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	70-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	71-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	72-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	73-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	74-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	75-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	76-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	77-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-30	MET	-	EXPRESSION TAG	UNP E5BBQ3

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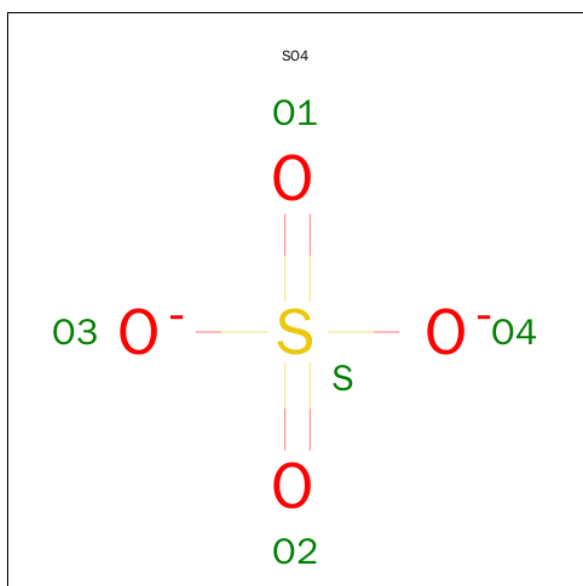
Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	LYS	-	EXPRESSION TAG	UNP E5BBQ3
A	-28	TYR	-	EXPRESSION TAG	UNP E5BBQ3
A	-27	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-26	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-25	PRO	-	EXPRESSION TAG	UNP E5BBQ3
A	-24	THR	-	EXPRESSION TAG	UNP E5BBQ3
A	-23	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-22	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-21	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-20	GLY	-	EXPRESSION TAG	UNP E5BBQ3
A	-19	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-18	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-17	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-16	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	-15	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-14	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-13	GLN	-	EXPRESSION TAG	UNP E5BBQ3
A	-12	PRO	-	EXPRESSION TAG	UNP E5BBQ3
A	-11	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-10	MET	-	EXPRESSION TAG	UNP E5BBQ3
A	-9	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	-8	MET	-	EXPRESSION TAG	UNP E5BBQ3
A	-7	ASP	-	EXPRESSION TAG	UNP E5BBQ3
A	-6	ILE	-	EXPRESSION TAG	UNP E5BBQ3
A	-5	GLY	-	EXPRESSION TAG	UNP E5BBQ3
A	-4	ILE	-	EXPRESSION TAG	UNP E5BBQ3
A	-3	ASN	-	EXPRESSION TAG	UNP E5BBQ3
A	-2	SER	-	EXPRESSION TAG	UNP E5BBQ3
A	-1	ASP	-	EXPRESSION TAG	UNP E5BBQ3
A	0	PRO	-	EXPRESSION TAG	UNP E5BBQ3
A	262	TYR	-	EXPRESSION TAG	UNP E5BBQ3
A	263	PRO	-	EXPRESSION TAG	UNP E5BBQ3
A	264	ASN	-	EXPRESSION TAG	UNP E5BBQ3
A	265	SER	-	EXPRESSION TAG	UNP E5BBQ3
A	266	SER	-	EXPRESSION TAG	UNP E5BBQ3
A	267	SER	-	EXPRESSION TAG	UNP E5BBQ3
A	268	VAL	-	EXPRESSION TAG	UNP E5BBQ3
A	269	ASP	-	EXPRESSION TAG	UNP E5BBQ3
A	270	LYS	-	EXPRESSION TAG	UNP E5BBQ3
A	271	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	272	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	273	ALA	-	EXPRESSION TAG	UNP E5BBQ3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	274	ALA	-	EXPRESSION TAG	UNP E5BBQ3
A	275	LEU	-	EXPRESSION TAG	UNP E5BBQ3
A	276	GLU	-	EXPRESSION TAG	UNP E5BBQ3
A	277	HIS	-	EXPRESSION TAG	UNP E5BBQ3
A	278	HIS	-	EXPRESSION TAG	UNP E5BBQ3
A	279	HIS	-	EXPRESSION TAG	UNP E5BBQ3
A	280	HIS	-	EXPRESSION TAG	UNP E5BBQ3
A	281	HIS	-	EXPRESSION TAG	UNP E5BBQ3
A	282	HIS	-	EXPRESSION TAG	UNP E5BBQ3

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	1-A	1	Total	O	S	0	0
			5	4	1		
2	2-A	1	Total	O	S	0	0
			5	4	1		
2	3-A	1	Total	O	S	0	0
			5	4	1		
2	4-A	1	Total	O	S	0	0
			5	4	1		
2	5-A	1	Total	O	S	0	0
			5	4	1		
2	6-A	1	Total	O	S	0	0
			5	4	1		
2	7-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	8-A	1	Total	O	S	0	0
			5	4	1		
2	9-A	1	Total	O	S	0	0
			5	4	1		
2	10-A	1	Total	O	S	0	0
			5	4	1		
2	11-A	1	Total	O	S	0	0
			5	4	1		
2	12-A	1	Total	O	S	0	0
			5	4	1		
2	13-A	1	Total	O	S	0	0
			5	4	1		
2	14-A	1	Total	O	S	0	0
			5	4	1		
2	15-A	1	Total	O	S	0	0
			5	4	1		
2	16-A	1	Total	O	S	0	0
			5	4	1		
2	17-A	1	Total	O	S	0	0
			5	4	1		
2	18-A	1	Total	O	S	0	0
			5	4	1		
2	19-A	1	Total	O	S	0	0
			5	4	1		
2	20-A	1	Total	O	S	0	0
			5	4	1		
2	21-A	1	Total	O	S	0	0
			5	4	1		
2	22-A	1	Total	O	S	0	0
			5	4	1		
2	23-A	1	Total	O	S	0	0
			5	4	1		
2	24-A	1	Total	O	S	0	0
			5	4	1		
2	25-A	1	Total	O	S	0	0
			5	4	1		
2	26-A	1	Total	O	S	0	0
			5	4	1		
2	27-A	1	Total	O	S	0	0
			5	4	1		
2	28-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	29-A	1	Total	O	S	0	0
			5	4	1		
2	30-A	1	Total	O	S	0	0
			5	4	1		
2	31-A	1	Total	O	S	0	0
			5	4	1		
2	32-A	1	Total	O	S	0	0
			5	4	1		
2	33-A	1	Total	O	S	0	0
			5	4	1		
2	34-A	1	Total	O	S	0	0
			5	4	1		
2	35-A	1	Total	O	S	0	0
			5	4	1		
2	36-A	1	Total	O	S	0	0
			5	4	1		
2	37-A	1	Total	O	S	0	0
			5	4	1		
2	38-A	1	Total	O	S	0	0
			5	4	1		
2	39-A	1	Total	O	S	0	0
			5	4	1		
2	40-A	1	Total	O	S	0	0
			5	4	1		
2	41-A	1	Total	O	S	0	0
			5	4	1		
2	42-A	1	Total	O	S	0	0
			5	4	1		
2	43-A	1	Total	O	S	0	0
			5	4	1		
2	44-A	1	Total	O	S	0	0
			5	4	1		
2	45-A	1	Total	O	S	0	0
			5	4	1		
2	46-A	1	Total	O	S	0	0
			5	4	1		
2	47-A	1	Total	O	S	0	0
			5	4	1		
2	48-A	1	Total	O	S	0	0
			5	4	1		
2	49-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	50-A	1	Total	O	S	0	0
			5	4	1		
2	51-A	1	Total	O	S	0	0
			5	4	1		
2	52-A	1	Total	O	S	0	0
			5	4	1		
2	53-A	1	Total	O	S	0	0
			5	4	1		
2	54-A	1	Total	O	S	0	0
			5	4	1		
2	55-A	1	Total	O	S	0	0
			5	4	1		
2	56-A	1	Total	O	S	0	0
			5	4	1		
2	57-A	1	Total	O	S	0	0
			5	4	1		
2	58-A	1	Total	O	S	0	0
			5	4	1		
2	59-A	1	Total	O	S	0	0
			5	4	1		
2	60-A	1	Total	O	S	0	0
			5	4	1		
2	61-A	1	Total	O	S	0	0
			5	4	1		
2	62-A	1	Total	O	S	0	0
			5	4	1		
2	63-A	1	Total	O	S	0	0
			5	4	1		
2	64-A	1	Total	O	S	0	0
			5	4	1		
2	65-A	1	Total	O	S	0	0
			5	4	1		
2	66-A	1	Total	O	S	0	0
			5	4	1		
2	67-A	1	Total	O	S	0	0
			5	4	1		
2	68-A	1	Total	O	S	0	0
			5	4	1		
2	69-A	1	Total	O	S	0	0
			5	4	1		
2	70-A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	71-A	1	Total	O	S	0	0
			5	4	1		
2	72-A	1	Total	O	S	0	0
			5	4	1		
2	73-A	1	Total	O	S	0	0
			5	4	1		
2	74-A	1	Total	O	S	0	0
			5	4	1		
2	75-A	1	Total	O	S	0	0
			5	4	1		
2	76-A	1	Total	O	S	0	0
			5	4	1		
2	77-A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	99	Total	O	0	0
			99	99		
3	2-A	101	Total	O	0	1
			102	102		
3	3-A	98	Total	O	0	0
			98	98		
3	4-A	85	Total	O	0	0
			85	85		
3	5-A	97	Total	O	0	1
			98	98		
3	6-A	98	Total	O	0	1
			99	99		
3	7-A	98	Total	O	0	0
			98	98		
3	8-A	100	Total	O	0	1
			101	101		
3	9-A	95	Total	O	0	0
			95	95		
3	10-A	90	Total	O	0	0
			90	90		
3	11-A	102	Total	O	0	1
			103	103		
3	12-A	97	Total	O	0	0
			97	97		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	13-A	87	Total 87	O 87	0	0
3	14-A	89	Total 90	O 90	0	1
3	15-A	111	Total 112	O 112	0	1
3	16-A	93	Total 93	O 93	0	0
3	17-A	82	Total 82	O 82	0	0
3	18-A	88	Total 89	O 89	0	1
3	19-A	89	Total 89	O 89	0	0
3	20-A	102	Total 103	O 103	0	1
3	21-A	101	Total 101	O 101	0	0
3	22-A	83	Total 83	O 83	0	0
3	23-A	102	Total 103	O 103	0	1
3	24-A	98	Total 98	O 98	0	0
3	25-A	98	Total 99	O 99	0	1
3	26-A	85	Total 85	O 85	0	0
3	27-A	99	Total 100	O 100	0	1
3	28-A	103	Total 104	O 104	0	1
3	29-A	104	Total 105	O 105	0	1
3	30-A	94	Total 94	O 94	0	0
3	31-A	91	Total 91	O 91	0	0
3	32-A	95	Total 96	O 96	0	1
3	33-A	90	Total 90	O 90	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	34-A	93	Total O 94 94	0	1
3	35-A	97	Total O 98 98	0	1
3	36-A	98	Total O 98 98	0	0
3	37-A	97	Total O 97 97	0	0
3	38-A	91	Total O 91 91	0	0
3	39-A	103	Total O 104 104	0	1
3	40-A	89	Total O 89 89	0	0
3	41-A	103	Total O 104 104	0	1
3	42-A	111	Total O 112 112	0	1
3	43-A	102	Total O 102 102	0	0
3	44-A	83	Total O 83 83	0	0
3	45-A	95	Total O 96 96	0	1
3	46-A	98	Total O 99 99	0	1
3	47-A	99	Total O 100 100	0	1
3	48-A	83	Total O 83 83	0	0
3	49-A	92	Total O 93 93	0	1
3	50-A	94	Total O 95 95	0	1
3	51-A	98	Total O 99 99	0	1
3	52-A	98	Total O 98 98	0	0
3	53-A	90	Total O 90 90	0	0
3	54-A	94	Total O 95 95	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	55-A	92	Total	O	0	0
			92	92		
3	56-A	94	Total	O	0	1
			95	95		
3	57-A	96	Total	O	0	1
			97	97		
3	58-A	91	Total	O	0	0
			91	91		
3	59-A	88	Total	O	0	0
			88	88		
3	60-A	97	Total	O	0	1
			98	98		
3	61-A	112	Total	O	0	1
			113	113		
3	62-A	103	Total	O	0	0
			103	103		
3	63-A	106	Total	O	0	1
			107	107		
3	64-A	100	Total	O	0	0
			100	100		
3	65-A	88	Total	O	0	0
			88	88		
3	66-A	103	Total	O	0	1
			104	104		
3	67-A	102	Total	O	0	0
			102	102		
3	68-A	104	Total	O	0	1
			105	105		
3	69-A	104	Total	O	0	0
			104	104		
3	70-A	103	Total	O	0	0
			103	103		
3	71-A	107	Total	O	0	1
			108	108		
3	72-A	101	Total	O	0	0
			101	101		
3	73-A	96	Total	O	0	0
			96	96		
3	74-A	95	Total	O	0	0
			95	95		
3	75-A	88	Total	O	0	0
			88	88		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	76-A	88	Total 88	O 88	0	0
3	77-A	101	Total 102	O 102	0	1

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	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.90 Å 117.90 Å 36.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.12 – 1.55	Depositor
% Data completeness (in resolution range)	99.9 (23.12-1.55)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.117 , 0.149	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	314292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	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 [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.