



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 02:26 AM UTC

PDB ID : 4CG3 / pdb_00004cg3
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

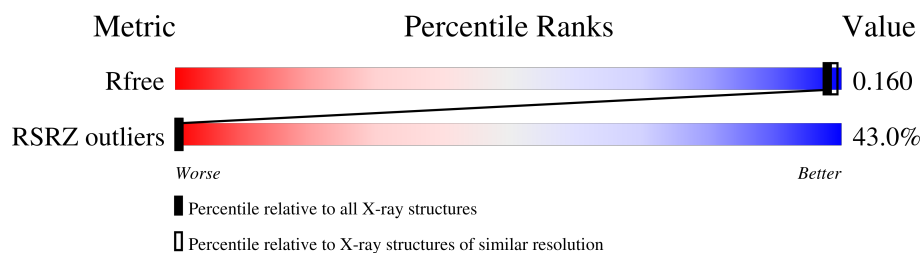
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 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	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	2-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	3-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	4-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	5-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	6-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	7-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	8-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	9-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	10-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	11-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	12-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	13-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	14-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	15-A	263	Total	C	H	N	O	S	0	0	0
			3980	1269	1969	352	385	5			
1	16-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	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 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	39-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	40-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	41-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	42-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	43-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	44-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	45-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	46-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	47-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	48-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	49-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	50-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	51-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	52-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	53-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	54-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	55-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	56-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	57-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	58-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	59-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	60-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	61-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	62-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	63-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	64-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	65-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	66-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	67-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	68-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	69-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	70-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	71-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	72-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	73-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	74-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	75-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	76-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0
1	77-A	263	Total 3980	C 1269	H 1969	N 352	O 385	S 5	0	0	0

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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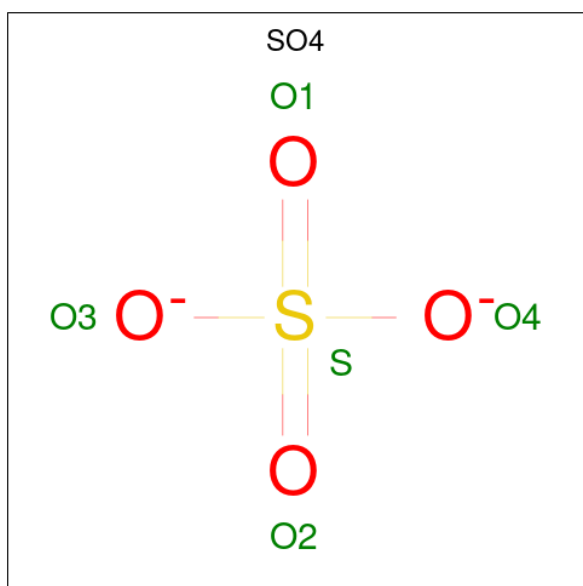
Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	LYS	-	expression tag	UNP E5BBQ3
A	-28	TYR	-	expression tag	UNP E5BBQ3
A	-27	LEU	-	expression tag	UNP E5BBQ3
A	-26	LEU	-	expression tag	UNP E5BBQ3
A	-25	PRO	-	expression tag	UNP E5BBQ3
A	-24	THR	-	expression tag	UNP E5BBQ3
A	-23	ALA	-	expression tag	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 (CCD ID: SO4) (formula: O₄S).



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 94	O 94	0	1
3	35-A	97	Total 98	O 98	0	1
3	36-A	98	Total 98	O 98	0	0
3	37-A	97	Total 97	O 97	0	0
3	38-A	91	Total 91	O 91	0	0
3	39-A	103	Total 104	O 104	0	1
3	40-A	89	Total 89	O 89	0	0
3	41-A	103	Total 104	O 104	0	1
3	42-A	111	Total 112	O 112	0	1
3	43-A	102	Total 102	O 102	0	0
3	44-A	83	Total 83	O 83	0	0
3	45-A	95	Total 96	O 96	0	1
3	46-A	98	Total 99	O 99	0	1
3	47-A	99	Total 100	O 100	0	1
3	48-A	83	Total 83	O 83	0	0
3	49-A	92	Total 93	O 93	0	1
3	50-A	94	Total 95	O 95	0	1
3	51-A	98	Total 99	O 99	0	1
3	52-A	98	Total 98	O 98	0	0
3	53-A	90	Total 90	O 90	0	0
3	54-A	94	Total 95	O 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 failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	117.90Å 117.90Å 36.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.12 – 1.55 23.12 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (23.12-1.55) 99.9 (23.12-1.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.55Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.117 , 0.149 0.130 , 0.160	Depositor DCC
R_{free} test set	3279 reflections (8.93%)	wwPDB-VP
Wilson B-factor (Å ²)	16.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	314292	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

77 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	64-A	1001	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	10-A	1001	-	4,4,4	0.25	0	6,6,6	0.31	0
2	SO4	68-A	1001	-	4,4,4	0.25	0	6,6,6	0.60	0
2	SO4	70-A	1001	-	4,4,4	0.37	0	6,6,6	0.44	0
2	SO4	33-A	1001	-	4,4,4	0.25	0	6,6,6	0.50	0
2	SO4	47-A	1001	-	4,4,4	0.37	0	6,6,6	0.62	0
2	SO4	8-A	1001	-	4,4,4	0.20	0	6,6,6	0.53	0
2	SO4	59-A	1001	-	4,4,4	0.23	0	6,6,6	0.52	0
2	SO4	52-A	1001	-	4,4,4	0.18	0	6,6,6	0.79	0
2	SO4	58-A	1001	-	4,4,4	0.24	0	6,6,6	0.33	0
2	SO4	20-A	1001	-	4,4,4	0.30	0	6,6,6	0.46	0
2	SO4	19-A	1001	-	4,4,4	0.30	0	6,6,6	0.40	0
2	SO4	40-A	1001	-	4,4,4	0.39	0	6,6,6	0.50	0
2	SO4	48-A	1001	-	4,4,4	0.29	0	6,6,6	0.61	0
2	SO4	22-A	1001	-	4,4,4	0.25	0	6,6,6	0.63	0
2	SO4	7-A	1001	-	4,4,4	0.37	0	6,6,6	0.36	0
2	SO4	39-A	1001	-	4,4,4	0.24	0	6,6,6	0.52	0
2	SO4	73-A	1001	-	4,4,4	0.29	0	6,6,6	0.53	0
2	SO4	34-A	1001	-	4,4,4	0.40	0	6,6,6	0.53	0
2	SO4	60-A	1001	-	4,4,4	0.28	0	6,6,6	0.38	0
2	SO4	27-A	1001	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	42-A	1001	-	4,4,4	0.38	0	6,6,6	0.53	0
2	SO4	50-A	1001	-	4,4,4	0.37	0	6,6,6	0.47	0
2	SO4	23-A	1001	-	4,4,4	0.09	0	6,6,6	0.57	0
2	SO4	18-A	1001	-	4,4,4	0.31	0	6,6,6	0.74	0
2	SO4	1-A	1001	-	4,4,4	0.29	0	6,6,6	0.67	0
2	SO4	62-A	1001	-	4,4,4	0.32	0	6,6,6	0.59	0
2	SO4	55-A	1001	-	4,4,4	0.25	0	6,6,6	0.48	0
2	SO4	72-A	1001	-	4,4,4	0.28	0	6,6,6	0.19	0
2	SO4	77-A	1001	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	66-A	1001	-	4,4,4	0.41	0	6,6,6	0.48	0
2	SO4	56-A	1001	-	4,4,4	0.28	0	6,6,6	0.69	0
2	SO4	67-A	1001	-	4,4,4	0.36	0	6,6,6	0.39	0
2	SO4	12-A	1001	-	4,4,4	0.33	0	6,6,6	0.64	0
2	SO4	5-A	1001	-	4,4,4	0.28	0	6,6,6	0.34	0
2	SO4	35-A	1001	-	4,4,4	0.42	0	6,6,6	0.65	0
2	SO4	65-A	1001	-	4,4,4	0.18	0	6,6,6	0.46	0
2	SO4	4-A	1001	-	4,4,4	0.51	0	6,6,6	0.62	0
2	SO4	76-A	1001	-	4,4,4	0.31	0	6,6,6	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	57-A	1001	-	4,4,4	0.30	0	6,6,6	0.47	0
2	SO4	16-A	1001	-	4,4,4	0.27	0	6,6,6	0.32	0
2	SO4	14-A	1001	-	4,4,4	0.38	0	6,6,6	0.41	0
2	SO4	36-A	1001	-	4,4,4	0.37	0	6,6,6	0.18	0
2	SO4	49-A	1001	-	4,4,4	0.35	0	6,6,6	0.79	0
2	SO4	51-A	1001	-	4,4,4	0.44	0	6,6,6	0.74	0
2	SO4	13-A	1001	-	4,4,4	0.22	0	6,6,6	0.30	0
2	SO4	71-A	1001	-	4,4,4	0.32	0	6,6,6	0.43	0
2	SO4	25-A	1001	-	4,4,4	0.40	0	6,6,6	0.36	0
2	SO4	75-A	1001	-	4,4,4	0.39	0	6,6,6	0.50	0
2	SO4	6-A	1001	-	4,4,4	0.40	0	6,6,6	0.47	0
2	SO4	53-A	1001	-	4,4,4	0.18	0	6,6,6	0.42	0
2	SO4	54-A	1001	-	4,4,4	0.24	0	6,6,6	0.64	0
2	SO4	2-A	1001	-	4,4,4	0.40	0	6,6,6	0.30	0
2	SO4	61-A	1001	-	4,4,4	0.36	0	6,6,6	0.38	0
2	SO4	11-A	1001	-	4,4,4	0.52	0	6,6,6	0.43	0
2	SO4	3-A	1001	-	4,4,4	0.50	0	6,6,6	0.74	0
2	SO4	46-A	1001	-	4,4,4	0.40	0	6,6,6	0.65	0
2	SO4	43-A	1001	-	4,4,4	0.40	0	6,6,6	0.63	0
2	SO4	17-A	1001	-	4,4,4	0.25	0	6,6,6	0.42	0
2	SO4	74-A	1001	-	4,4,4	0.36	0	6,6,6	0.66	0
2	SO4	45-A	1001	-	4,4,4	0.22	0	6,6,6	0.51	0
2	SO4	38-A	1001	-	4,4,4	0.24	0	6,6,6	0.70	0
2	SO4	29-A	1001	-	4,4,4	0.33	0	6,6,6	0.56	0
2	SO4	41-A	1001	-	4,4,4	0.27	0	6,6,6	0.79	0
2	SO4	15-A	1001	-	4,4,4	0.32	0	6,6,6	0.67	0
2	SO4	69-A	1001	-	4,4,4	0.22	0	6,6,6	0.61	0
2	SO4	26-A	1001	-	4,4,4	0.31	0	6,6,6	0.76	0
2	SO4	28-A	1001	-	4,4,4	0.39	0	6,6,6	0.39	0
2	SO4	37-A	1001	-	4,4,4	0.45	0	6,6,6	0.15	0
2	SO4	63-A	1001	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	44-A	1001	-	4,4,4	0.32	0	6,6,6	1.00	1 (16%)
2	SO4	9-A	1001	-	4,4,4	0.37	0	6,6,6	0.40	0
2	SO4	32-A	1001	-	4,4,4	0.31	0	6,6,6	0.54	0
2	SO4	24-A	1001	-	4,4,4	0.16	0	6,6,6	0.55	0
2	SO4	30-A	1001	-	4,4,4	0.44	0	6,6,6	0.48	0
2	SO4	21-A	1001	-	4,4,4	0.29	0	6,6,6	0.35	0
2	SO4	31-A	1001	-	4,4,4	0.20	0	6,6,6	0.53	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	44-A	1001	SO4	O4-S-O1	-2.01	99.03	109.56

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 ⓘ

5.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	263/313 (84%)	2.39	113 (42%) 0 0	0, 0, 0, 0	263 (100%)
1	2-A	0/313	-	-	-	-
1	3-A	0/313	-	-	-	-
1	4-A	0/313	-	-	-	-
1	5-A	0/313	-	-	-	-
1	6-A	0/313	-	-	-	-
1	7-A	0/313	-	-	-	-
1	8-A	0/313	-	-	-	-
1	9-A	0/313	-	-	-	-
1	10-A	0/313	-	-	-	-
1	11-A	0/313	-	-	-	-
1	12-A	0/313	-	-	-	-
1	13-A	0/313	-	-	-	-
1	14-A	0/313	-	-	-	-
1	15-A	0/313	-	-	-	-
1	16-A	0/313	-	-	-	-
1	17-A	0/313	-	-	-	-
1	18-A	0/313	-	-	-	-
1	19-A	0/313	-	-	-	-
1	20-A	0/313	-	-	-	-
1	21-A	0/313	-	-	-	-
1	22-A	0/313	-	-	-	-
1	23-A	0/313	-	-	-	-
1	24-A	0/313	-	-	-	-
1	25-A	0/313	-	-	-	-
1	26-A	0/313	-	-	-	-
1	27-A	0/313	-	-	-	-
1	28-A	0/313	-	-	-	-
1	29-A	0/313	-	-	-	-
1	30-A	0/313	-	-	-	-
1	31-A	0/313	-	-	-	-
1	32-A	0/313	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/313	-	-	-	-
1	34-A	0/313	-	-	-	-
1	35-A	0/313	-	-	-	-
1	36-A	0/313	-	-	-	-
1	37-A	0/313	-	-	-	-
1	38-A	0/313	-	-	-	-
1	39-A	0/313	-	-	-	-
1	40-A	0/313	-	-	-	-
1	41-A	0/313	-	-	-	-
1	42-A	0/313	-	-	-	-
1	43-A	0/313	-	-	-	-
1	44-A	0/313	-	-	-	-
1	45-A	0/313	-	-	-	-
1	46-A	0/313	-	-	-	-
1	47-A	0/313	-	-	-	-
1	48-A	0/313	-	-	-	-
1	49-A	0/313	-	-	-	-
1	50-A	0/313	-	-	-	-
1	51-A	0/313	-	-	-	-
1	52-A	0/313	-	-	-	-
1	53-A	0/313	-	-	-	-
1	54-A	0/313	-	-	-	-
1	55-A	0/313	-	-	-	-
1	56-A	0/313	-	-	-	-
1	57-A	0/313	-	-	-	-
1	58-A	0/313	-	-	-	-
1	59-A	0/313	-	-	-	-
1	60-A	0/313	-	-	-	-
1	61-A	0/313	-	-	-	-
1	62-A	0/313	-	-	-	-
1	63-A	0/313	-	-	-	-
1	64-A	0/313	-	-	-	-
1	65-A	0/313	-	-	-	-
1	66-A	0/313	-	-	-	-
1	67-A	0/313	-	-	-	-
1	68-A	0/313	-	-	-	-
1	69-A	0/313	-	-	-	-
1	70-A	0/313	-	-	-	-
1	71-A	0/313	-	-	-	-
1	72-A	0/313	-	-	-	-
1	73-A	0/313	-	-	-	-
1	74-A	0/313	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	75-A	0/313	-	-	-	-
1	76-A	0/313	-	-	-	-
1	77-A	0/313	-	-	-	-
All	All	263/24101 (1%)	2.39	113 (42%) 0 0	0, 0, 0, 0	263 (100%)

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	248	LEU	20.0
1	1-A	213	ILE	18.7
1	1-A	246	ASP	15.4
1	1-A	62	GLY	14.7
1	1-A	244	PRO	14.0

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

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	1-A	1001	5/5	0.49	0.37	24,24,24,26	5
2	SO4	2-A	1001	5/5	-	-	22,22,23,24	5
2	SO4	3-A	1001	5/5	-	-	24,25,25,26	5
2	SO4	4-A	1001	5/5	-	-	26,26,28,28	5
2	SO4	5-A	1001	5/5	-	-	27,28,29,30	5
2	SO4	6-A	1001	5/5	-	-	25,26,27,27	5
2	SO4	7-A	1001	5/5	-	-	24,24,26,26	5
2	SO4	8-A	1001	5/5	-	-	24,24,25,26	5
2	SO4	9-A	1001	5/5	-	-	20,22,22,23	5
2	SO4	10-A	1001	5/5	-	-	21,21,23,23	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	11-A	1001	5/5	-	-	21,22,23,24	5
2	SO4	12-A	1001	5/5	-	-	20,21,21,22	5
2	SO4	13-A	1001	5/5	-	-	22,23,23,24	5
2	SO4	14-A	1001	5/5	-	-	23,24,25,25	5
2	SO4	15-A	1001	5/5	-	-	21,23,23,23	5
2	SO4	16-A	1001	5/5	-	-	21,22,22,23	5
2	SO4	17-A	1001	5/5	-	-	21,21,22,23	5
2	SO4	18-A	1001	5/5	-	-	21,21,22,23	5
2	SO4	19-A	1001	5/5	-	-	20,20,22,22	5
2	SO4	20-A	1001	5/5	-	-	18,19,19,21	5
2	SO4	21-A	1001	5/5	-	-	18,19,19,20	5
2	SO4	22-A	1001	5/5	-	-	19,21,21,21	5
2	SO4	23-A	1001	5/5	-	-	23,23,24,25	5
2	SO4	24-A	1001	5/5	-	-	23,24,25,26	5
2	SO4	25-A	1001	5/5	-	-	21,22,22,23	5
2	SO4	26-A	1001	5/5	-	-	20,21,21,23	5
2	SO4	27-A	1001	5/5	-	-	22,22,23,24	5
2	SO4	28-A	1001	5/5	-	-	23,24,24,25	5
2	SO4	29-A	1001	5/5	-	-	24,25,26,26	5
2	SO4	30-A	1001	5/5	-	-	25,26,27,27	5
2	SO4	31-A	1001	5/5	-	-	26,28,28,29	5
2	SO4	32-A	1001	5/5	-	-	27,27,29,29	5
2	SO4	33-A	1001	5/5	-	-	27,28,29,29	5
2	SO4	34-A	1001	5/5	-	-	25,25,27,27	5
2	SO4	35-A	1001	5/5	-	-	24,24,24,26	5
2	SO4	36-A	1001	5/5	-	-	24,24,26,26	5
2	SO4	37-A	1001	5/5	-	-	23,24,24,25	5
2	SO4	38-A	1001	5/5	-	-	24,25,25,26	5
2	SO4	39-A	1001	5/5	-	-	25,27,27,28	5
2	SO4	40-A	1001	5/5	-	-	27,28,29,30	5
2	SO4	41-A	1001	5/5	-	-	26,27,28,28	5
2	SO4	42-A	1001	5/5	-	-	24,25,26,27	5
2	SO4	43-A	1001	5/5	-	-	23,24,25,25	5
2	SO4	44-A	1001	5/5	-	-	24,25,26,27	5
2	SO4	45-A	1001	5/5	-	-	24,24,25,26	5
2	SO4	46-A	1001	5/5	-	-	23,24,24,25	5
2	SO4	47-A	1001	5/5	-	-	21,21,22,23	5
2	SO4	48-A	1001	5/5	-	-	22,23,23,24	5
2	SO4	49-A	1001	5/5	-	-	22,23,24,24	5
2	SO4	50-A	1001	5/5	-	-	20,20,22,22	5
2	SO4	51-A	1001	5/5	-	-	18,19,19,20	5
2	SO4	52-A	1001	5/5	-	-	20,21,21,22	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	53-A	1001	5/5	-	-	20,21,21,22	5
2	SO4	54-A	1001	5/5	-	-	21,22,22,23	5
2	SO4	55-A	1001	5/5	-	-	22,22,23,24	5
2	SO4	56-A	1001	5/5	-	-	25,25,26,27	5
2	SO4	57-A	1001	5/5	-	-	25,26,26,28	5
2	SO4	58-A	1001	5/5	-	-	27,27,28,29	5
2	SO4	59-A	1001	5/5	-	-	29,30,31,32	5
2	SO4	60-A	1001	5/5	-	-	30,30,30,32	5
2	SO4	61-A	1001	5/5	-	-	28,28,29,30	5
2	SO4	62-A	1001	5/5	-	-	27,27,29,30	5
2	SO4	63-A	1001	5/5	-	-	26,27,27,28	5
2	SO4	64-A	1001	5/5	-	-	25,25,26,27	5
2	SO4	65-A	1001	5/5	-	-	24,24,25,26	5
2	SO4	66-A	1001	5/5	-	-	23,24,25,25	5
2	SO4	67-A	1001	5/5	-	-	26,26,26,28	5
2	SO4	68-A	1001	5/5	-	-	27,28,29,29	5
2	SO4	69-A	1001	5/5	-	-	31,31,32,33	5
2	SO4	70-A	1001	5/5	-	-	29,31,31,32	5
2	SO4	71-A	1001	5/5	-	-	29,31,31,32	5
2	SO4	72-A	1001	5/5	-	-	27,28,29,30	5
2	SO4	73-A	1001	5/5	-	-	25,27,28,28	5
2	SO4	74-A	1001	5/5	-	-	24,25,26,27	5
2	SO4	75-A	1001	5/5	-	-	23,24,25,25	5
2	SO4	76-A	1001	5/5	-	-	25,26,27,27	5
2	SO4	77-A	1001	5/5	-	-	26,26,28,28	5

5.5 Other polymers [i](#)

There are no such residues in this entry.