



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:29 AM UTC

PDB ID : 4NU7 / pdb\_00004nu7  
Title : 2.05 Angstrom Crystal Structure of Ribulose-phosphate 3-epimerase from *Toxoplasma gondii*.  
Authors : Minasov, G.; Ruan, J.; Ngo, H.; Shuvalova, L.; Dubrovskaya, I.; Flores, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2013-12-03  
Resolution : 2.05 Å(reported)

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
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

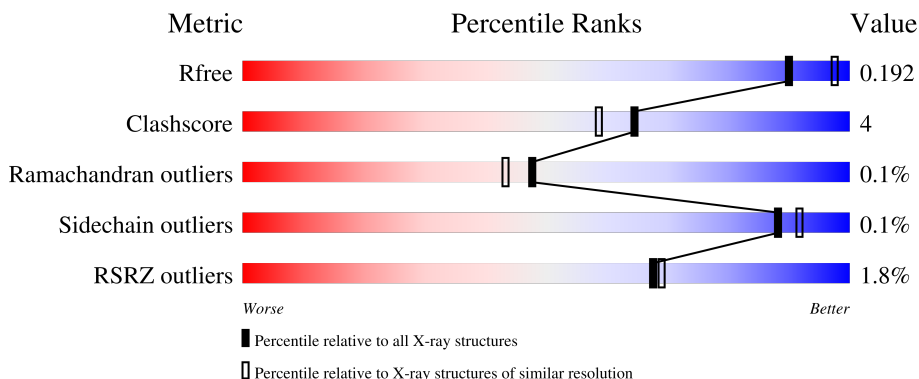
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	 2% 83% 9% 9%
1	B	246	 2% 85% 6% 9%
1	C	246	 2% 85% 7% 8%
1	D	246	 2% 85% 7% 8%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7648 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 Ribulose-phosphate 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	225	1798	1134	314	338	12	0	14	0
1	B	225	1725	1096	295	322	12	0	5	0
1	C	227	1772	1128	303	329	12	0	9	0
1	D	226	1754	1110	307	325	12	0	7	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	GLY	-	expression tag	UNP B9PPN9
A	232	GLU	-	expression tag	UNP B9PPN9
A	233	ASN	-	expression tag	UNP B9PPN9
A	234	LEU	-	expression tag	UNP B9PPN9
A	235	TYR	-	expression tag	UNP B9PPN9
A	236	PHE	-	expression tag	UNP B9PPN9
A	237	GLN	-	expression tag	UNP B9PPN9
A	238	SER	-	expression tag	UNP B9PPN9
A	239	ALA	-	expression tag	UNP B9PPN9
A	240	GLY	-	expression tag	UNP B9PPN9
A	241	HIS	-	expression tag	UNP B9PPN9
A	242	HIS	-	expression tag	UNP B9PPN9
A	243	HIS	-	expression tag	UNP B9PPN9
A	244	HIS	-	expression tag	UNP B9PPN9
A	245	HIS	-	expression tag	UNP B9PPN9
A	246	HIS	-	expression tag	UNP B9PPN9
B	231	GLY	-	expression tag	UNP B9PPN9
B	232	GLU	-	expression tag	UNP B9PPN9
B	233	ASN	-	expression tag	UNP B9PPN9
B	234	LEU	-	expression tag	UNP B9PPN9
B	235	TYR	-	expression tag	UNP B9PPN9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	236	PHE	-	expression tag	UNP B9PPN9
B	237	GLN	-	expression tag	UNP B9PPN9
B	238	SER	-	expression tag	UNP B9PPN9
B	239	ALA	-	expression tag	UNP B9PPN9
B	240	GLY	-	expression tag	UNP B9PPN9
B	241	HIS	-	expression tag	UNP B9PPN9
B	242	HIS	-	expression tag	UNP B9PPN9
B	243	HIS	-	expression tag	UNP B9PPN9
B	244	HIS	-	expression tag	UNP B9PPN9
B	245	HIS	-	expression tag	UNP B9PPN9
B	246	HIS	-	expression tag	UNP B9PPN9
C	231	GLY	-	expression tag	UNP B9PPN9
C	232	GLU	-	expression tag	UNP B9PPN9
C	233	ASN	-	expression tag	UNP B9PPN9
C	234	LEU	-	expression tag	UNP B9PPN9
C	235	TYR	-	expression tag	UNP B9PPN9
C	236	PHE	-	expression tag	UNP B9PPN9
C	237	GLN	-	expression tag	UNP B9PPN9
C	238	SER	-	expression tag	UNP B9PPN9
C	239	ALA	-	expression tag	UNP B9PPN9
C	240	GLY	-	expression tag	UNP B9PPN9
C	241	HIS	-	expression tag	UNP B9PPN9
C	242	HIS	-	expression tag	UNP B9PPN9
C	243	HIS	-	expression tag	UNP B9PPN9
C	244	HIS	-	expression tag	UNP B9PPN9
C	245	HIS	-	expression tag	UNP B9PPN9
C	246	HIS	-	expression tag	UNP B9PPN9
D	231	GLY	-	expression tag	UNP B9PPN9
D	232	GLU	-	expression tag	UNP B9PPN9
D	233	ASN	-	expression tag	UNP B9PPN9
D	234	LEU	-	expression tag	UNP B9PPN9
D	235	TYR	-	expression tag	UNP B9PPN9
D	236	PHE	-	expression tag	UNP B9PPN9
D	237	GLN	-	expression tag	UNP B9PPN9
D	238	SER	-	expression tag	UNP B9PPN9
D	239	ALA	-	expression tag	UNP B9PPN9
D	240	GLY	-	expression tag	UNP B9PPN9
D	241	HIS	-	expression tag	UNP B9PPN9
D	242	HIS	-	expression tag	UNP B9PPN9
D	243	HIS	-	expression tag	UNP B9PPN9
D	244	HIS	-	expression tag	UNP B9PPN9
D	245	HIS	-	expression tag	UNP B9PPN9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	246	HIS	-	expression tag	UNP B9PPN9

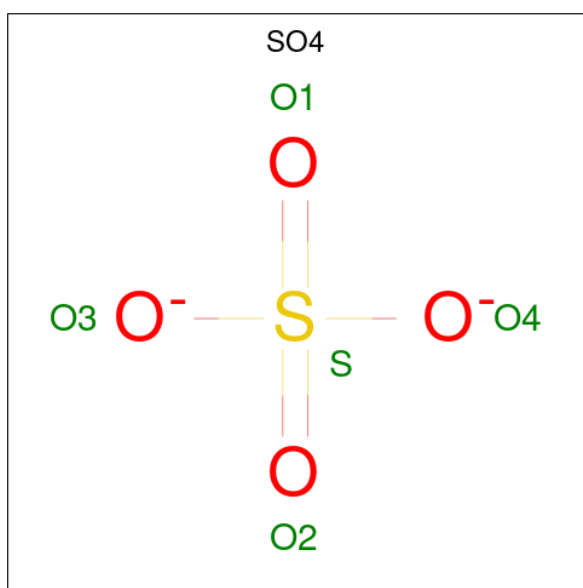
- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	1
2	B	2	Total Cl 2 2	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	1
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	1
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	129	Total O 135 135	0	6
5	B	119	Total O 124 124	0	6
5	C	126	Total O 131 131	0	6
5	D	139	Total O 140 140	0	4



## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.51Å 138.51Å 349.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.88 – 2.05 29.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-2.05) 99.9 (29.88-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 2.04Å)	Xtrriage
Refinement program	REFMAC 5.8.0046	Depositor
R, $R_{free}$	0.149 , 0.187 0.161 , 0.192	Depositor DCC
$R_{free}$ test set	4056 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for $-1/3^*h+1/3^*k+1/3^*l,-k,8/3^*h+4/3^*k+1/3^*l$ 0.015 for $-2/3^*h-1/3^*k-1/3^*l,-1/3^*h-2/3^*k+1/3^*l,-4/3^*h+4/3^*k+1/3^*l$ 0.002 for $-h,1/3^*h-1/3^*k-1/3^*l,-4/3^*h-8/3^*k+1/3^*l$	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7648	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, ZN

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  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.70	0/1833	0.85	0/2476
1	B	0.75	0/1759	0.90	2/2377 (0.1%)
1	C	0.75	0/1806	0.89	1/2442 (0.0%)
1	D	0.75	0/1788	0.86	2/2414 (0.1%)
All	All	0.74	0/7186	0.87	5/9709 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	LYS	N-CA-C	5.55	117.33	111.28
1	D	64	LYS	N-CA-C	5.35	117.86	111.71
1	B	21	LEU	N-CA-C	5.31	116.75	111.07
1	B	133	LEU	N-CA-C	5.30	119.30	112.41
1	D	46	VAL	N-CA-C	-5.07	103.29	109.01

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1798	0	1785	15	0
1	B	1725	0	1723	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1772	0	1783	18	0
1	D	1754	0	1757	10	0
2	A	2	0	0	1	0
2	B	2	0	0	1	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	25	0	0	0	0
4	B	15	0	0	1	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	135	0	0	1	0
5	B	124	0	0	0	0
5	C	131	0	0	1	0
5	D	140	0	0	1	0
All	All	7648	0	7048	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 56 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104[A]:GLN:HG2	5:A:500[A]:HOH:O	1.51	1.08
1:C:124[B]:ILE:HD11	1:C:128[B]:THR:O	1.73	0.89
1:B:104[A]:GLN:NE2	1:B:104[A]:GLN:H	1.87	0.72
1:B:221:ARG:HD2	4:B:306:SO4:O4	1.90	0.70
1:D:82:GLN:NE2	1:D:86:ASP:OD2	2.24	0.67

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/246 (96%)	231 (98%)	6 (2%)	0	100	100
1	B	228/246 (93%)	219 (96%)	9 (4%)	0	100	100
1	C	234/246 (95%)	227 (97%)	6 (3%)	1 (0%)	30	22
1	D	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
All	All	930/984 (94%)	898 (97%)	31 (3%)	1 (0%)	48	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	134	GLY

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/193 (98%)	189 (100%)	0	100	100
1	B	180/193 (93%)	178 (99%)	2 (1%)	65	68
1	C	186/193 (96%)	186 (100%)	0	100	100
1	D	183/193 (95%)	183 (100%)	0	100	100
All	All	738/772 (96%)	736 (100%)	2 (0%)	88	90

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104[A]	GLN
1	B	104[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4	GLN
1	D	4	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z  > 2$
4	SO4	B	304	-	4,4,4	0.41	0	6,6,6	0.50	0
4	SO4	A	307	-	4,4,4	0.43	0	6,6,6	0.08	0
4	SO4	B	306	-	4,4,4	0.42	0	6,6,6	0.41	0
4	SO4	A	308[B]	-	4,4,4	0.48	0	6,6,6	0.20	0
4	SO4	A	306	-	4,4,4	0.31	0	6,6,6	0.37	0
4	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.42	0
4	SO4	C	304[A]	-	4,4,4	0.36	0	6,6,6	0.30	0
4	SO4	D	302	-	4,4,4	0.42	0	6,6,6	0.27	0
4	SO4	D	303	-	4,4,4	0.40	0	6,6,6	0.14	0
4	SO4	B	305	-	4,4,4	0.27	0	6,6,6	0.45	0
4	SO4	A	304	-	4,4,4	0.37	0	6,6,6	0.39	0
4	SO4	A	305	-	4,4,4	0.49	0	6,6,6	0.18	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	306	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	225/246 (91%)	-0.18	2 (0%) 81 83	13, 36, 60, 83	14 (6%)
1	B	225/246 (91%)	-0.16	5 (2%) 62 64	17, 35, 63, 82	5 (2%)
1	C	227/246 (92%)	-0.13	4 (1%) 67 69	15, 36, 64, 99	9 (3%)
1	D	226/246 (91%)	-0.18	5 (2%) 62 64	15, 35, 68, 103	7 (3%)
All	All	903/984 (91%)	-0.16	16 (1%) 67 69	13, 36, 64, 103	35 (3%)

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	THR	4.7
1	C	104[A]	GLN	3.7
1	D	156	GLY	3.6
1	C	230	LEU	3.5
1	D	139	GLY	3.2

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	308[B]	5/5	0.82	0.25	52,54,58,61	5
4	SO4	A	307	5/5	0.84	0.12	55,60,68,70	5
4	SO4	C	304[A]	5/5	0.86	0.16	48,53,60,62	5
4	SO4	A	306	5/5	0.89	0.12	44,50,52,59	5
4	SO4	A	305	5/5	0.89	0.12	55,66,67,80	5
4	SO4	D	303	5/5	0.89	0.12	37,44,47,49	5
2	CL	B	302	1/1	0.90	0.12	66,66,66,66	0
2	CL	A	302[A]	1/1	0.91	0.17	46,46,46,46	1
2	CL	B	301	1/1	0.92	0.14	78,78,78,78	0
4	SO4	B	306	5/5	0.93	0.16	49,51,59,60	5
2	CL	A	301	1/1	0.93	0.16	78,78,78,78	0
2	CL	C	301	1/1	0.93	0.10	63,63,63,63	0
4	SO4	B	305	5/5	0.94	0.12	40,43,49,52	5
4	SO4	D	302	5/5	0.96	0.07	57,58,65,73	0
4	SO4	A	304	5/5	0.97	0.09	43,47,58,71	0
4	SO4	C	303	5/5	0.98	0.07	43,46,53,56	0
4	SO4	B	304	5/5	0.98	0.06	46,49,50,57	0
3	ZN	A	303	1/1	0.99	0.04	35,35,35,35	1
3	ZN	B	303	1/1	0.99	0.07	38,38,38,38	1
3	ZN	C	302	1/1	0.99	0.03	36,36,36,36	1
3	ZN	D	301	1/1	0.99	0.09	37,37,37,37	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.