



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:16 AM UTC

PDB ID : 5YFE / pdb_00005yfe
Title : Enzymatic and structural characterization of the poly (ethylene terephthalate) hydrolase PETase from *I. sakaiensis*
Authors : Bao, R.; He, L.H.; Liu, B.
Deposited on : 2017-09-21
Resolution : 1.39 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

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	:	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

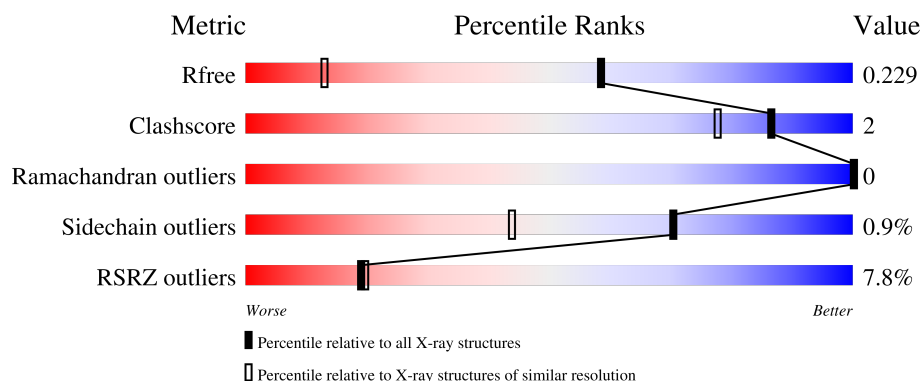
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 ≥ 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	272	8% 68% 28% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3971 atoms, of which 1906 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 Poly(ethylene terephthalate) hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	268	Total	C	H	N	O	S	0	0	0
			3865	1218	1891	354	391	11			

There are 11 discrepancies between the modelled and reference sequences:

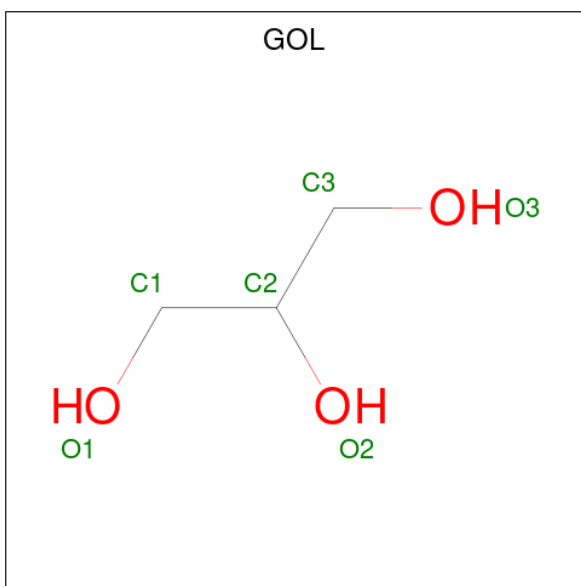
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	THR	engineered mutation	UNP A0A0K8P6T7
A	198	ALA	ARG	engineered mutation	UNP A0A0K8P6T7
A	261	ASN	ALA	engineered mutation	UNP A0A0K8P6T7
A	265	LEU	-	expression tag	UNP A0A0K8P6T7
A	266	GLU	-	expression tag	UNP A0A0K8P6T7
A	267	HIS	-	expression tag	UNP A0A0K8P6T7
A	268	HIS	-	expression tag	UNP A0A0K8P6T7
A	269	HIS	-	expression tag	UNP A0A0K8P6T7
A	270	HIS	-	expression tag	UNP A0A0K8P6T7
A	271	HIS	-	expression tag	UNP A0A0K8P6T7
A	272	HIS	-	expression tag	UNP A0A0K8P6T7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			13	3	7	3		

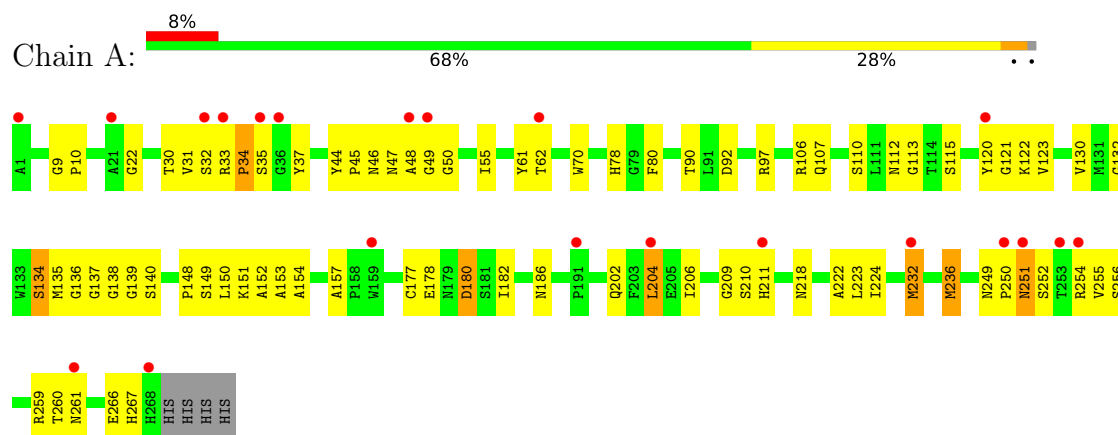
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Poly(ethylene terephthalate) hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.95Å 56.64Å 80.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.88 – 1.39 37.88 – 1.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.88-1.39) 100.0 (37.88-1.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.223 , 0.235 0.220 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	8.5	Xtriage
Anisotropy	0.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3971	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.71% 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.

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: SO4, GOL

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	1.80	66/2021 (3.3%)	1.15	20/2754 (0.7%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	PRO	C-O	-12.72	1.11	1.23
1	A	134	SER	C-O	-12.44	1.12	1.24
1	A	206	ILE	C-O	-11.64	1.12	1.24
1	A	157	ALA	C-O	-11.10	1.18	1.23
1	A	223	LEU	C-O	-9.33	1.13	1.24
1	A	50	GLY	C-O	-9.17	1.14	1.23
1	A	148	PRO	C-O	-8.76	1.12	1.24
1	A	186	ASN	C-O	-8.72	1.13	1.24
1	A	135	MET	C-O	-8.61	1.13	1.24
1	A	149	SER	C-O	-8.23	1.13	1.24
1	A	46	ASN	C-O	-8.12	1.13	1.24
1	A	130	VAL	C-O	-8.02	1.16	1.24
1	A	178	GLU	C-O	-7.99	1.14	1.24
1	A	55	ILE	C-O	-7.99	1.15	1.24
1	A	222	ALA	C-O	-7.89	1.15	1.24
1	A	204	LEU	C-O	-7.69	1.15	1.24
1	A	152	ALA	C-O	-7.61	1.14	1.23
1	A	123	VAL	C-O	-7.56	1.15	1.24
1	A	232	MET	C-O	-7.17	1.15	1.24
1	A	136	GLY	C-O	-7.11	1.15	1.23
1	A	218	ASN	C-O	-7.00	1.14	1.23
1	A	138	GLY	C-O	-6.85	1.15	1.23
1	A	70	TRP	C-O	-6.82	1.15	1.24
1	A	30	THR	C-O	-6.82	1.15	1.23
1	A	122	LYS	C-O	-6.82	1.15	1.24
1	A	261	ASN	C-O	-6.80	1.15	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	GLY	C-O	-6.74	1.14	1.23
1	A	267	HIS	C-O	-6.64	1.16	1.24
1	A	255	VAL	C-O	-6.63	1.17	1.24
1	A	139	GLY	C-O	-6.61	1.15	1.23
1	A	150	LEU	C-O	-6.61	1.16	1.23
1	A	182	ILE	C-O	-6.58	1.16	1.24
1	A	209	GLY	C-O	-6.57	1.16	1.23
1	A	9	GLY	C-O	-6.42	1.15	1.24
1	A	250	PRO	C-N	-6.41	1.25	1.33
1	A	113	GLY	C-O	-6.39	1.18	1.24
1	A	34	PRO	C-O	-6.27	1.16	1.23
1	A	44	TYR	C-O	-6.25	1.17	1.24
1	A	180	ASP	C-O	-6.23	1.16	1.23
1	A	31	VAL	C-O	-6.16	1.17	1.24
1	A	80	PHE	C-O	-6.14	1.16	1.23
1	A	110	SER	C-O	-6.13	1.16	1.24
1	A	140	SER	C-O	-6.10	1.16	1.24
1	A	112	ASN	C-O	-6.08	1.16	1.24
1	A	137	GLY	C-O	-6.08	1.16	1.23
1	A	260	THR	C-N	-6.08	1.24	1.33
1	A	256	SER	C-O	-6.04	1.16	1.24
1	A	153	ALA	C-O	-5.87	1.17	1.23
1	A	249	ASN	C-O	-5.81	1.17	1.24
1	A	10	PRO	C-O	-5.80	1.16	1.23
1	A	33	ARG	C-O	-5.78	1.16	1.24
1	A	132	GLY	C-O	-5.57	1.16	1.23
1	A	97	ARG	CZ-NH2	-5.54	1.26	1.33
1	A	202	GLN	C-O	-5.50	1.17	1.23
1	A	259	ARG	C-O	-5.43	1.17	1.23
1	A	224	ILE	C-O	-5.42	1.17	1.24
1	A	46	ASN	N-CA	-5.33	1.39	1.46
1	A	107	GLN	C-O	-5.28	1.17	1.24
1	A	46	ASN	CA-CB	-5.24	1.45	1.53
1	A	22	GLY	N-CA	-5.23	1.37	1.44
1	A	92	ASP	C-O	-5.23	1.17	1.23
1	A	120	TYR	C-O	-5.16	1.17	1.24
1	A	78	HIS	C-O	-5.12	1.17	1.24
1	A	266	GLU	C-O	-5.05	1.17	1.23
1	A	236	MET	C-O	-5.05	1.17	1.24
1	A	151	LYS	C-O	-5.02	1.17	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLY	CA-C-O	8.16	126.77	119.83
1	A	210	SER	CA-C-O	-7.54	113.07	121.89
1	A	106	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	A	252	SER	N-CA-C	6.55	119.83	108.76
1	A	251	ASN	CB-CA-C	6.43	121.77	112.12
1	A	209	GLY	N-CA-C	6.42	120.27	111.54
1	A	250	PRO	N-CA-C	-6.27	100.33	110.55
1	A	106	ARG	CD-NE-CZ	6.20	133.07	124.40
1	A	35	SER	CA-C-O	-6.09	115.37	122.37
1	A	48	ALA	CA-C-N	5.97	129.63	123.30
1	A	48	ALA	C-N-CA	5.97	129.63	123.30
1	A	50	GLY	CA-C-O	-5.89	115.43	121.61
1	A	251	ASN	N-CA-C	-5.66	101.12	109.62
1	A	48	ALA	N-CA-C	5.57	118.11	111.71
1	A	154	ALA	CA-C-N	-5.27	114.81	120.03
1	A	154	ALA	C-N-CA	-5.27	114.81	120.03
1	A	115	SER	N-CA-C	5.17	117.66	111.71
1	A	249	ASN	N-CA-C	-5.11	101.86	109.42
1	A	130	VAL	N-CA-C	5.08	116.03	108.46
1	A	47	ASN	N-CA-CB	-5.05	104.03	111.51

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	1974	1891	1891	8	0
2	A	10	0	0	0	0
3	A	12	15	16	0	0
4	A	69	0	0	0	0
All	All	2065	1906	1907	8	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 2.

All (8) 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:62:THR:HA	1:A:90:THR:HB	1.81	0.61
1:A:34:PRO:HB3	1:A:37:TYR:CZ	2.40	0.56
1:A:61:TYR:C	1:A:62:THR:HG23	2.36	0.51
1:A:204:LEU:C	1:A:204:LEU:HD23	2.36	0.49
1:A:134:SER:OG	1:A:211:HIS:CE1	2.66	0.48
1:A:232:MET:O	1:A:236:MET:HB2	2.19	0.43
1:A:254:ARG:HG3	1:A:254:ARG:HH11	1.84	0.41
1:A:177:CYS:O	1:A:180:ASP:HB2	2.22	0.40

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	266/272 (98%)	258 (97%)	8 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	213/217 (98%)	211 (99%)	2 (1%)	70	44

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

Mol	Chain	Res	Type
1	A	32	SER
1	A	251	ASN

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

Mol	Chain	Res	Type
1	A	147	ASN
1	A	179	ASN

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](#)

4 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	$\# Z > 2$
3	GOL	A	304	-	5,5,5	0.65	0	5,5,5	1.09	0
2	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.56	0
2	SO4	A	301	-	4,4,4	0.34	0	6,6,6	1.00	0
3	GOL	A	303	-	5,5,5	0.82	0	5,5,5	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	304	-	-	0/4/4/4	-
3	GOL	A	303	-	-	0/4/4/4	-

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	A	268/272 (98%)	0.48	21 (7%) 19 20	4, 11, 23, 48	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	49	GLY	5.5
1	A	32	SER	4.8
1	A	261	ASN	4.7
1	A	251	ASN	4.2
1	A	268	HIS	4.0
1	A	62	THR	3.2
1	A	191	PRO	3.2
1	A	253	THR	3.0
1	A	21	ALA	2.9
1	A	254	ARG	2.6
1	A	250	PRO	2.5
1	A	33	ARG	2.5
1	A	36	GLY	2.5
1	A	1	ALA	2.4
1	A	35	SER	2.3
1	A	211	HIS	2.3
1	A	204	LEU	2.3
1	A	232	MET	2.1
1	A	159	TRP	2.1
1	A	48	ALA	2.1
1	A	120	TYR	2.1

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, 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($\text{\AA}^2$)	Q<0.9
2	SO4	A	302	5/5	0.75	0.22	30,54,62,68	0
3	GOL	A	303	6/6	0.86	0.19	16,37,49,59	0
2	SO4	A	301	5/5	0.89	0.15	10,20,23,36	5
3	GOL	A	304	6/6	0.89	0.11	17,20,25,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.