

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 12, 2023 – 10:51 AM EDT

PDB ID	:	4OGK
Title	:	X-ray structure of the uridine phosphorylase from Salmonella typhimurium in
		complex with thymidine at 2.40 A resolution
Authors	:	Sotnichenko, S.E.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Mikhailov, A.M.
Deposited on	:	2014-01-16
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 2.40 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 $(\#Entries, resolution range(Å))$
Rfree	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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 cl	hain	
1	А	253	2% <b>6</b> 2%	24%	
	11	200	5%	54 %	••
1	В	253	59%	36%	••
1	$\mathbf{C}$	253	67%	30%	••
1	D	253	55%	41%	
		252	2%		
	E	253	56%	40%	••



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Mol	Chain	Length	Quality of chain		
			4%		
1	F	253	70%	26%	•



#### 40GK

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11404 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	250	Total	С	Ν	Ο	S	0	0	0
	A	230	1877	1174	330	361	12	0	0	0
1	В	250	Total	С	Ν	Ο	S	0	0	0
1	D	230	1877	1174	330	361	12		0	0
1	С	250	Total	С	Ν	0	S	0	0	0
1		230	1877	1174	330	361	12	0		
1	Л	250	Total	С	Ν	0	S	0	0	0
1	D	230	1877	1174	330	361	12	0	0	
1	F	250	Total	С	Ν	Ο	S	0	0	0
1	Ľ	230	1877	1174	330	361	12	0	0	0
1	Б	245	Total	С	Ν	0	S	0	0	0
	Г	240	1837	1151	323	351	12	0	0	

• Molecule 1 is a protein called Uridine phosphorylase.

• Molecule 2 is THYMIDINE (three-letter code: THM) (formula:  $C_{10}H_{14}N_2O_5$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Δ	1	Total C N O	0	0
2	Л	I	17  10  2  5	0	0
2	В	1	Total C N O	0	0
2	D	1	17  10  2  5	0	0
2	Л	1	Total C N O	0	0
2	D	1	17  10  2  5	0	0
2	E	1	Total C N O	0	0
2	Ľ	1	17  10  2  5	0	0
2	F	1	Total C N O	0	0
	Г	I	17  10  2  5	0	0

• Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula:  $C_3H_8O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 4	С 3	0 1	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	Ε	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 7	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	O 3	0	0

• Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Ε	1	Total 13	C 8	O 5	0	0

• Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total K 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	10	Total O 10 10	0	0
8	В	10	Total O 10 10	0	0
8	С	11	Total O 11 11	0	0
8	D	7	Total O 7 7	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	Е	13	Total O 13 13	0	0
8	F	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	0	0



# 3 Residue-property plots (i)

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: Uridine phosphorylase



# 1223 D117 1223 2120 1233 2120 1234 122 1235 123 1235 134 124 138 1253 138 1253 138 1253 138 1253 138 1253 138 1253 136 1253 136 1253 145 1253 145 1264 146 1265 146 1265 146 1265 146 1266 146 1261 146 1262 146 1263 146 1264 146 1265 146 1266 146 1267 146 1268 146 1269 146 1264 146 1464 146 1464 146 1464 146 1464 146 1464 146 1464 146 1464 146 1464 146 1464 146 1464 146

• Molecule 1: Uridine phosphorylase





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants	89.97Å 89.97Å 256.56Å	Deneriten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	9.99 - 2.40	Depositor
Resolution (A)	29.45 - 2.40	EDS
% Data completeness	97.7 (9.99-2.40)	Depositor
(in resolution range)	99.9 (29.45-2.40)	EDS
R <sub>merge</sub>	0.08	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	$2.88 (at 2.39 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
B B.	0.220 , $0.236$	Depositor
II, II, <i>free</i>	0.221 , $0.233$	DCC
$R_{free}$ test set	2283 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	48.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 38.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.30, < L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.459 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.480 for h,-h-k,-l	Depositor
Outliers	0  of  45659  reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11404	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: PG4, PEG, THM, EDO, K, IPA

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).

Mal	Chain	Bond lengths		Bond angles	
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.49	2/1907~(0.1%)	0.55	0/2584
1	В	0.61	0/1907	0.59	0/2584
1	С	0.55	0/1907	0.57	0/2584
1	D	0.49	0/1907	0.56	0/2584
1	Е	0.47	0/1907	0.57	0/2584
1	F	0.49	0/1866	0.55	1/2528~(0.0%)
All	All	0.52	2/11401~(0.0%)	0.56	1/15448~(0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	167	GLU	CD-OE1	-5.56	1.19	1.25
1	А	253	LEU	C-OXT	5.01	1.32	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	F	44	LEU	CA-CB-CG	5.36	127.63	115.30

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.



40GN	400	GK
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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1877	0	1887	74	0
1	В	1877	0	1887	109	0
1	С	1877	0	1887	77	0
1	D	1877	0	1887	101	0
1	Е	1877	0	1887	106	0
1	F	1837	0	1847	60	0
2	А	17	0	14	4	0
2	В	17	0	14	1	0
2	D	17	0	14	0	0
2	Е	17	0	14	1	0
2	F	17	0	14	0	0
3	А	4	0	8	0	0
4	А	4	0	6	0	0
4	С	4	0	6	0	0
4	Е	4	0	6	0	0
4	F	4	0	6	0	0
5	D	7	0	10	0	0
6	Е	13	0	18	2	0
7	F	1	0	0	0	0
8	А	10	0	0	0	0
8	В	10	0	0	0	0
8	С	11	0	0	0	0
8	D	7	0	0	0	0
8	Е	13	0	0	0	0
8	F	5	0	0	0	0
All	All	11404	0	11412	493	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 22.

The worst 5 of 493 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:B:140:LEU:HD22	1:B:216:VAL:CG2	1.63	1.28
1:E:108:LEU:HD13	1:E:194:ASN:ND2	1.60	1.16
1:F:196:GLU:HG3	1:F:197:MET:H	1.08	1.10
1:B:140:LEU:HD22	1:B:216:VAL:HG21	1.23	1.08
1:F:15:ASP:HB3	1:F:44:LEU:HD13	1.37	1.03

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	А	248/253~(98%)	242 (98%)	6 (2%)	0	100 100
1	В	248/253~(98%)	241 (97%)	7 (3%)	0	100 100
1	С	248/253~(98%)	241 (97%)	6 (2%)	1 (0%)	34 48
1	D	248/253~(98%)	243~(98%)	5 (2%)	0	100 100
1	Е	248/253~(98%)	234 (94%)	14 (6%)	0	100 100
1	F	241/253~(95%)	235~(98%)	6 (2%)	0	100 100
All	All	1481/1518 (98%)	1436 (97%)	44 (3%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	163	TYR

#### 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	Perce	entiles
1	А	199/202~(98%)	190 (96%)	9 (4%)	27	44
1	В	199/202~(98%)	186 (94%)	13~(6%)	17	27
1	С	199/202~(98%)	193~(97%)	6 (3%)	41	61
1	D	199/202~(98%)	189~(95%)	10 (5%)	24	40
1	Ε	199/202~(98%)	190 (96%)	9 (4%)	27	44
1	F	194/202~(96%)	191 (98%)	3 (2%)	65	80



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1189/1212~(98%)	1139~(96%)	50~(4%)	30 47	

 $5~{\rm of}~50$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	D	73	SER
1	D	178	ARG
1	F	196	GLU
1	D	90	LEU
1	D	101	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	8	HIS
1	Е	222	ASN
1	В	222	ASN
1	В	236	GLN
1	С	230	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 monosaccharides in this entry.

# 5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 1 is 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).

Mal	Tuno	Chain	Dog	Link	Bo	ond leng	ths	B	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	THM	Е	301	-	18,18,18	2.22	5 (27%)	26,26,26	2.57	9 (34%)
6	PG4	Е	302	-	12,12,12	0.72	0	11,11,11	0.98	0
4	EDO	F	303	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	Е	303	-	3,3,3	0.49	0	2,2,2	0.28	0
2	THM	D	301	-	18,18,18	1.98	8 (44%)	26,26,26	2.35	8 (30%)
2	THM	А	301	-	18,18,18	1.90	8 (44%)	26,26,26	2.40	8 (30%)
2	THM	F	301	-	18,18,18	1.94	8 (44%)	26,26,26	2.32	8 (30%)
3	IPA	А	302	-	3,3,3	0.54	0	3,3,3	0.21	0
4	EDO	А	303	-	3,3,3	0.37	0	2,2,2	0.41	0
2	THM	В	301	-	18,18,18	1.94	7 (38%)	26,26,26	2.38	6 (23%)
4	EDO	С	301	-	3,3,3	0.45	0	2,2,2	0.35	0
5	PEG	D	302	-	6,6,6	0.63	0	$5,\!5,\!5$	0.76	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
2	THM	Е	301	-	-	0/6/18/18	0/2/2/2
6	PG4	Е	302	-	-	4/10/10/10	-
4	EDO	F	303	-	-	0/1/1/1	-
4	EDO	Е	303	-	-	0/1/1/1	-
2	THM	D	301	-	-	0/6/18/18	0/2/2/2
2	THM	А	301	-	-	2/6/18/18	0/2/2/2
2	THM	F	301	-	-	0/6/18/18	0/2/2/2
4	EDO	А	303	-	-	1/1/1/1	-
2	THM	В	301	-	-	0/6/18/18	0/2/2/2
4	EDO	C	301	-	-	0/1/1/1	-
5	PEG	D	302	-	_	4/4/4/4	-

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	301	THM	C6-N1	-5.38	1.28	1.38
2	Е	301	THM	C4-N3	-4.45	1.30	1.38



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
2	D	301	THM	C6-N1	3.88	1.44	1.38
2	В	301	THM	C6-N1	3.84	1.44	1.38
2	F	301	THM	C6-N1	3.80	1.44	1.38

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The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	301	THM	C5-C4-N3	6.30	120.69	115.31
2	А	301	THM	C4-N3-C2	-6.09	119.47	127.35
2	D	301	THM	C5-C4-N3	6.03	120.46	115.31
2	В	301	THM	C4-N3-C2	-6.01	119.56	127.35
2	А	301	THM	C5-C4-N3	5.94	120.38	115.31

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	303	EDO	O1-C1-C2-O2
2	А	301	THM	C3'-C4'-C5'-O5'
2	А	301	THM	O4'-C4'-C5'-O5'
5	D	302	PEG	O1-C1-C2-O2
6	Е	302	PG4	O2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Е	301	THM	1	0
6	Е	302	PG4	2	0
2	А	301	THM	4	0
2	В	301	THM	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,  $95^{th}$  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	А	250/253~(98%)	0.02	6 (2%) 59 57	44, 60, 61, 64	1 (0%)
1	В	250/253~(98%)	0.12	12 (4%) 30 29	51, 59, 60, 61	3(1%)
1	С	250/253~(98%)	0.04	6 (2%) 59 57	46, 59, 61, 62	5 (2%)
1	D	250/253~(98%)	-0.00	1 (0%) 92 91	56, 59, 61, 62	1 (0%)
1	Ε	250/253~(98%)	0.03	5 (2%) 65 63	50, 59, 60, 62	3 (1%)
1	F	245/253~(96%)	0.13	10 (4%) 37 36	56, 60, 61, 67	1 (0%)
All	All	1495/1518~(98%)	0.06	40 (2%) 54 52	44, 59, 61, 67	14 (0%)

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	253	LEU	4.7
1	В	237	THR	4.1
1	А	233	THR	3.8
1	В	10	GLY	3.6
1	В	234	MET	3.6

# 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 monosaccharides 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,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
5	PEG	D	302	7/7	0.55	0.29	$67,\!67,\!68,\!68$	0
4	EDO	F	303	4/4	0.65	0.21	$65,\!67,\!69,\!69$	0
4	EDO	С	301	4/4	0.70	0.22	62,62,63,64	0
6	PG4	Е	302	13/13	0.80	0.30	60,64,68,68	0
2	THM	В	301	17/17	0.82	0.24	54,59,60,60	0
3	IPA	А	302	4/4	0.82	0.20	60,60,60,60	0
4	EDO	E	303	4/4	0.85	0.21	$58,\!58,\!58,\!59$	0
2	THM	А	301	17/17	0.86	0.19	62,63,63,64	0
2	THM	D	301	17/17	0.86	0.21	$63,\!64,\!67,\!67$	0
2	THM	F	301	17/17	0.86	0.20	$59,\!63,\!67,\!68$	0
2	THM	Е	301	17/17	0.90	0.17	59,60,60,61	0
4	EDO	А	303	4/4	0.97	0.13	20,20,20,20	0
7	K	F	302	1/1	0.98	0.10	59,59,59,59	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

