

Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 03:31 PM BST

PDB ID : 4K29

Title: Crystal structure of an enoyl-CoA hydratase/isomerase from Xanthobacter

autotrophicus Py2

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Consortium (NYSGRC)

Deposited on : 2013-04-08

Resolution : 1.66 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 (i) symbol.

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 : 2.13.1

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)

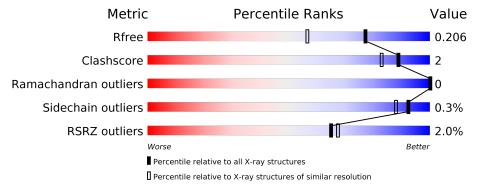
Validation Pipeline (wwPDB-VP) : 2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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 on 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 chain		
1	A	295	88%	•	9%
1	В	295	86%		9%
1	С	295	86%	•	9%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6703 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 Enoyl-CoA hydratase/isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	Λ	269	Total	С	N	О	S	Se	0	0	0
1	A	209	2037	1287	366	372	4	8	0	U	U
1	D	268	Total	С	N	О	S	Se	0	0	0
1	Б	200	2030	1283	365	370	4	8	0	U	
1	С	268	Total	С	N	О	S	Se	0	0	0
1		200	2030	1283	365	370	4	8	U	0	U

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	EXPRESSION TAG	UNP A7IKN6
A	-20	HIS	_	EXPRESSION TAG	UNP A7IKN6
A	-19	HIS	-	EXPRESSION TAG	UNP A7IKN6
A	-18	HIS	-	EXPRESSION TAG	UNP A7IKN6
A	-17	HIS	-	EXPRESSION TAG	UNP A7IKN6
A	-16	HIS	-	EXPRESSION TAG	UNP A7IKN6
A	-15	HIS	_	EXPRESSION TAG	UNP A7IKN6
A	-14	SER	-	EXPRESSION TAG	UNP A7IKN6
A	-13	SER	_	EXPRESSION TAG	UNP A7IKN6
A	-12	GLY	-	EXPRESSION TAG	UNP A7IKN6
A	-11	VAL	_	EXPRESSION TAG	UNP A7IKN6
A	-10	ASP	-	EXPRESSION TAG	UNP A7IKN6
A	-9	LEU	_	EXPRESSION TAG	UNP A7IKN6
A	-8	GLY	-	EXPRESSION TAG	UNP A7IKN6
A	-7	THR	-	EXPRESSION TAG	UNP A7IKN6
A	-6	GLU	-	EXPRESSION TAG	UNP A7IKN6
A	-5	ASN	-	EXPRESSION TAG	UNP A7IKN6
A	-4	LEU	-	EXPRESSION TAG	UNP A7IKN6
A	-3	TYR	-	EXPRESSION TAG	UNP A7IKN6
A	-2	PHE	-	EXPRESSION TAG	UNP A7IKN6
A	-1	GLN	-	EXPRESSION TAG	UNP A7IKN6
A	0	SER	-	EXPRESSION TAG	UNP A7IKN6
В	-21	MSE	-	EXPRESSION TAG	UNP A7IKN6

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Chain	Residue	Modelled	Actual	Comment	Reference
В	-20	HIS	-	EXPRESSION TAG	UNP A7IKN6
В	-19	HIS	-	EXPRESSION TAG	UNP A7IKN6
В	-18	HIS	-	EXPRESSION TAG	UNP A7IKN6
В	-17	HIS	_	EXPRESSION TAG	UNP A7IKN6
В	-16	HIS	_	EXPRESSION TAG	UNP A7IKN6
В	-15	HIS	_	EXPRESSION TAG	UNP A7IKN6
В	-14	SER	-	EXPRESSION TAG	UNP A7IKN6
В	-13	SER	_	EXPRESSION TAG	UNP A7IKN6
В	-12	GLY	_	EXPRESSION TAG	UNP A7IKN6
В	-11	VAL	_	EXPRESSION TAG	UNP A7IKN6
В	-10	ASP	_	EXPRESSION TAG	UNP A7IKN6
В	-9	LEU	-	EXPRESSION TAG	UNP A7IKN6
В	-8	GLY	_	EXPRESSION TAG	UNP A7IKN6
В	-7	THR	_	EXPRESSION TAG	UNP A7IKN6
В	-6	GLU	-	EXPRESSION TAG	UNP A7IKN6
В	-5	ASN	-	EXPRESSION TAG	UNP A7IKN6
В	-4	LEU	_	EXPRESSION TAG	UNP A7IKN6
В	-3	TYR	-	EXPRESSION TAG	UNP A7IKN6
В	-2	PHE	-	EXPRESSION TAG	UNP A7IKN6
В	-1	GLN	_	EXPRESSION TAG	UNP A7IKN6
В	0	SER	-	EXPRESSION TAG	UNP A7IKN6
С	-21	MSE	-	EXPRESSION TAG	UNP A7IKN6
С	-20	HIS	_	EXPRESSION TAG	UNP A7IKN6
С	-19	HIS	_	EXPRESSION TAG	UNP A7IKN6
С	-18	HIS	_	EXPRESSION TAG	UNP A7IKN6
С	-17	HIS	_	EXPRESSION TAG	UNP A7IKN6
С	-16	HIS	_	EXPRESSION TAG	UNP A7IKN6
С	-15	HIS	-	EXPRESSION TAG	UNP A7IKN6
С	-14	SER	-	EXPRESSION TAG	UNP A7IKN6
С	-13	SER	-	EXPRESSION TAG	UNP A7IKN6
С	-12	GLY	-	EXPRESSION TAG	UNP A7IKN6
С	-11	VAL	-	EXPRESSION TAG	UNP A7IKN6
С	-10	ASP	-	EXPRESSION TAG	UNP A7IKN6
С	-9	LEU	-	EXPRESSION TAG	UNP A7IKN6
С	-8	GLY	-	EXPRESSION TAG	UNP A7IKN6
С	-7	THR	-	EXPRESSION TAG	UNP A7IKN6
С	-6	GLU	-	EXPRESSION TAG	UNP A7IKN6
С	-5	ASN	-	EXPRESSION TAG	UNP A7IKN6
С	-4	LEU	-	EXPRESSION TAG	UNP A7IKN6
C	-3	TYR	-	EXPRESSION TAG	UNP A7IKN6
С	-2	PHE	-	EXPRESSION TAG	UNP A7IKN6
С	-1	GLN	_	EXPRESSION TAG	UNP A7IKN6

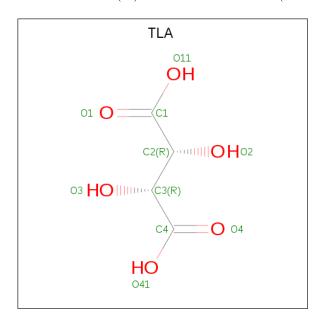
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Chain	Residue	Modelled	Actual	Comment	Reference
С	0	SER	-	EXPRESSION TAG	UNP A7IKN6

• Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	С	1	Total C O 10 4 6	0	0
2	С	1	Total C O 10 4 6	0	0

 \bullet Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

• Molecule 4 is water.

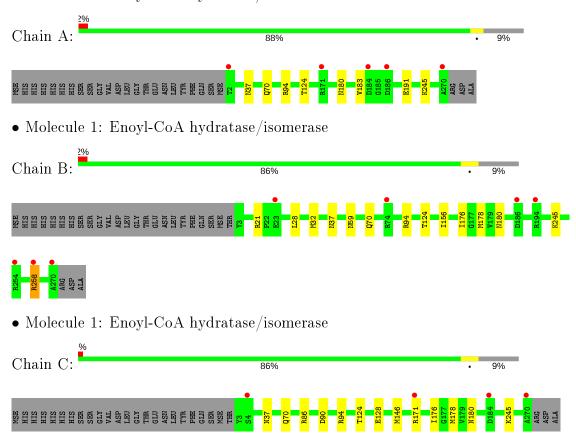
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	187	Total O 187 187	0	0
4	В	196	Total O 196 196	0	0
4	С	181	Total O 181 181	0	0



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: Enoyl-CoA hydratase/isomerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	115.05Å 144.58Å 129.57Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.49 - 1.66	Depositor
Resolution (A)	44.45 - 1.66	EDS
% Data completeness	99.6 (44.49-1.66)	Depositor
(in resolution range)	99.6 (44.45-1.66)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	7.83 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
D D.	0.181 , 0.198	Depositor
R, R_{free}	0.191 , 0.206	DCC
R_{free} test set	6360 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	11.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.39 , 40.9	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6703	wwPDB-VP
Average B, all atoms $(Å^2)$	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities 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: GOL, TLA

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		
IVIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.30	0/2064	0.57	0/2780	
1	В	0.30	0/2057	0.59	0/2770	
1	С	0.30	0/2057	0.59	0/2770	
All	All	0.30	0/6178	0.59	0/8320	

There are no bond length outliers.

There are no bond angle outliers.

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)	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	Α	2037	0	2068	5	0
1	В	2030	0	2061	10	0
1	С	2030	0	2061	8	0
2	A	10	0	4	0	0
2	С	20	0	8	0	0
3	A	6	0	8	0	0
3	С	6	0	8	0	0
4	A	187	0	0	0	0
4	В	196	0	0	1	0
4	С	181	0	0	0	0
All	All	6703	0	6218	23	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 (23) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${f distance} \; ({f \AA})$	overlap (Å)
1:B:37:ASN:HD22	1:B:94:ARG:HH11	1.42	0.67
1:C:37:ASN:HD22	1:C:94:ARG:HH11	1.40	0.67
1:A:37:ASN:HD22	1:A:94:ARG:HH11	1.43	0.66
1:C:176:ILE:HD11	1:C:178:MSE:HE3	1.83	0.58
1:A:124:THR:H	1:A:180:ASN:HD22	1.56	0.54
1:C:124:THR:H	1:C:180:ASN:HD22	1.55	0.53
1:B:156:ILE:HG12	4:B:377:HOH:O	2.07	0.53
1:A:70:GLN:HE22	1:A:245:LYS:NZ	2.07	0.52
1:B:124:THR:H	1:B:180:ASN:HD22	1.58	0.50
1:B:176:ILE:HD11	1:B:178:MSE:HE3	1.93	0.49
1:B:258:ARG:HH11	1:B:258:ARG:H	1.61	0.48
1:C:86:ARG:HD2	1:C:90:ASP:OD2	2.14	0.48
1:B:28:LEU:HD23	1:B:32:MSE:SE	2.64	0.47
1:C:70:GLN:HE22	1:C:245:LYS:NZ	2.13	0.47
1:B:21:ARG:CD	1:B:32:MSE:HE3	2.44	0.47
1:B:70:GLN:HE22	1:B:245:LYS:NZ	2.14	0.46
1:C:128:GLU:OE2	1:C:171:ARG:NH2	2.47	0.46
1:B:258:ARG:N	1:B:258:ARG:HD2	2.33	0.44
1:C:124:THR:H	1:C:180:ASN:ND2	2.16	0.44
1:C:146:MSE:HG3	1:C:146:MSE:O	2.18	0.44
1:B:124:THR:H	1:B:180:ASN:ND2	2.17	0.42
1:A:124:THR:H	1:A:180:ASN:ND2	2.16	0.42
1:A:183:VAL:HG11	1:A:191:GLU:HG2	2.02	0.42

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	Perce	$_{ m ntiles}$
1	A	$267/295 \; (90\%)$	260 (97%)	7 (3%)	0	100	100
1	В	266/295 (90%)	262 (98%)	4 (2%)	0	100	100
1	С	266/295 (90%)	262 (98%)	4 (2%)	0	100	100
All	All	799/885 (90%)	784 (98%)	15 (2%)	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	Perce	ntiles
1	A	201/214 (94%)	201 (100%)	0	100	100
1	В	200/214 (94%)	198 (99%)	2 (1%)	76	62
1	С	200/214 (94%)	200 (100%)	0	100	100
All	All	601/642 (94%)	599 (100%)	2 (0%)	92	88

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

Mol	Chain	${f Res}$	\mathbf{Type}
1	В	59	ASN
1	В	258	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	70	GLN
1	A	180	ASN
1	A	198	HIS
1	В	37	ASN
1	В	59	ASN
1	В	70	GLN
1	В	180	ASN

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Mol	Chain	Res	Type
1	С	37	ASN
1	С	70	GLN
1	С	180	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)

5 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	Mol Type Chain		Res Link	Bond lengths			Bond angles			
10101	Type	Chain	rtes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TLA	С	601	-	3,9,9	0.44	0	6,12,12	1.41	2 (33%)
2	TLA	A	301	-	3,9,9	0.51	0	6,12,12	0.77	0
3	GOL	A	302	_	5,5,5	0.28	0	5,5,5	0.25	0
2	TLA	С	602	-	3,9,9	0.46	0	6,12,12	1.04	1 (16%)
3	GOL	С	603	-	5,5,5	0.36	0	5,5,5	0.28	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	TLA	С	601	_	_	0/4/12/12	-
2	TLA	A	301	_	_	0/4/12/12	-
3	GOL	A	302	-	-	0/4/4/4	-
2	TLA	С	602	_	-	0/4/12/12	-
3	GOL	С	603	-	-	0/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^o)$
2	С	601	TLA	C4-C3-C2	-2.42	107.90	113.11
2	С	601	TLA	C1-C2-C3	-2.42	107.91	113.11
2	С	602	TLA	C4-C3-C2	-2.29	108.17	113.11

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 (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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	261/295~(88%)	-0.01	5 (1%) 66 69	6, 9, 19, 30	0
1	В	260/295~(88%)	-0.01	7 (2%) 54 55	6, 10, 22, 33	0
1	С	260/295 (88%)	-0.04	4 (1%) 73 77	5, 9, 18, 25	0
All	All	781/885 (88%)	-0.02	16 (2%) 65 67	5, 9, 20, 33	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ALA	6.8
1	A	2	THR	6.6
1	С	270	ALA	5.1
1	A	184	ASP	4.5
1	A	186	ASP	4.2
1	В	186	ASP	4.1
1	В	258	ARG	2.9
1	В	270	ALA	2.8
1	С	171	ARG	2.6
1	С	184	ASP	2.5
1	A	171	ARG	2.4
1	В	74	ARG	2.4
1	С	4	SER	2.3
1	В	194	ARG	2.2
1	В	254	ARG	2.1
1	В	23	GLU	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 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
2	TLA	С	601	10/10	0.85	0.16	17,18,18,18	10
3	GOL	A	302	6/6	0.86	0.14	24,25,25,25	0
2	TLA	С	602	10/10	0.86	0.20	19,21,23,23	0
3	GOL	С	603	6/6	0.88	0.11	18,18,19,19	0
2	TLA	A	301	10/10	0.91	0.15	25,26,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.

