

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

#### Jan 24, 2023 - 03:19 pm GMT

PDB ID	:	6ZKZ
Title	:	Crystal structure of InhA:01 TCR in complex with HLA-E (F116C) bound to
		InhA (53-61 H4C)
Authors	:	Srikannathasan, V.; Karuppiah, V.; Robinson, R.A.
Deposited on		
Resolution	:	2.30  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 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:

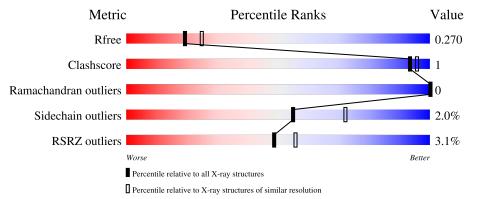
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

# 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 2.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 chain	
1	Δ	276	3%	
	A	270	92%	6% •
2	В	100	93%	7%
3	С	9	78%	22%
			6%	
4	D	199	91%	• 5%
5	Е	245	2% 95%	• •



#### 6ZKZ

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6582 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 HLA class I histocompatibility antigen, alpha chain E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	272	Total 2217	C 1385	N 396	O 428	S 8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	116	CYS	PHE	engineered mutation	UNP P13747

• Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	В	100	Total 837	C 533	N 141	O 159	$\frac{S}{4}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Enoyl-[acyl-carrier-protein] reductase [NADH].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	3 C 9	0	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
5		9	70	46	13	10	1			

• Molecule 4 is a protein called T-cell receptor alpha chain.

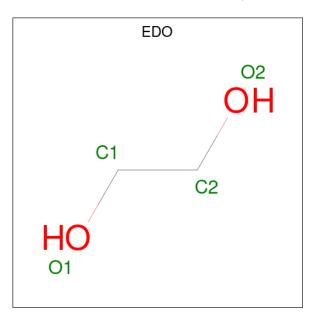
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	189	Total 1424	C 875	N 243	O 299	S 7	0	0	0

• Molecule 5 is a protein called T-cell receptor beta chain.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Е	243	Total 1919	C 1206	N 335	O 369	${ m S} 9$	0	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	D	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
6	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 7 is water.

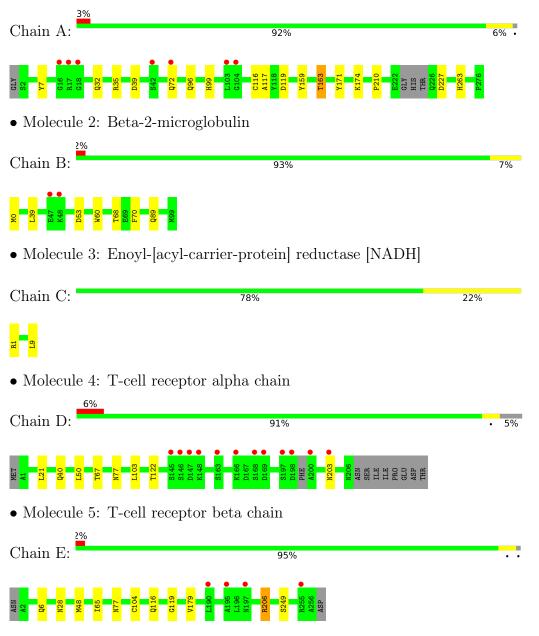
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	40	Total         O           40         40	0	0
7	В	10	Total         O           10         10	0	0
7	С	1	Total O 1 1	0	0
7	D	15	Total O 15 15	0	0
7	Е	33	Total         O           33         33	0	0



# 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: HLA class I histocompatibility antigen, alpha chain E





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.81Å 107.89Å 118.42Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	60.85 - 2.30	Depositor
Resolution (A)	60.77 - 2.30	EDS
% Data completeness	99.8 (60.85-2.30)	Depositor
(in resolution range)	99.8(60.77-2.30)	EDS
R <sub>merge</sub>	0.08	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.94 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D.	0.224 , $0.267$	Depositor
$R, R_{free}$	0.232 , $0.270$	DCC
$R_{free}$ test set	1928 reflections $(4.71\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	53.4	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, $34.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6582	wwPDB-VP
Average B, all atoms $(Å^2)$	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.11% 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: EDO,  $\rm QM8$ 

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	
	Unam	RMSZ $ \# Z  > 5$		RMSZ	# Z  > 5
1	А	0.62	0/2281	0.71	0/3100
2	В	0.62	0/860	0.70	0/1162
3	С	0.52	0/61	0.69	0/82
4	D	0.66	0/1444	0.74	0/1958
5	Е	0.62	0/1971	0.71	0/2683
All	All	0.63	0/6617	0.71	0/8985

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)	H(added)	Clashes	Symm-Clashes
1	А	2217	0	2059	9	0
2	В	837	0	803	4	0
3	С	70	0	74	0	0
4	D	1424	0	1375	5	0
5	Е	1919	0	1822	5	0
6	А	4	0	6	0	0
6	В	4	0	6	0	0
6	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes						
6	Ε	4	0	6	0	0						
7	А	40	0	0	0	0						
7	В	10	0	0	0	0						
7	С	1	0	0	0	0						
7	D	15	0	0	0	0						
7	Ε	33	0	0	0	0						
All	All	6582	0	6157	18	0						

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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 1.

All (18) 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)
4:D:40:GLN:HE22	5:E:116:GLN:H	1.39	0.68
4:D:67:THR:HG22	4:D:77:ASN:HD22	1.75	0.52
1:A:72:GLN:HE21	5:E:65:ILE:HG22	1.76	0.51
4:D:21:LEU:HD22	4:D:122:THR:HG21	1.92	0.51
1:A:96:GLN:O	1:A:116:CYS:HA	2.13	0.49
5:E:6:GLN:HE21	5:E:119:GLY:HA3	1.78	0.48
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.50	0.47
2:B:39:LEU:HD13	2:B:68:THR:HG22	1.98	0.44
4:D:50:LEU:HD21	4:D:103:LEU:HD13	1.99	0.44
1:A:7:TYR:HB2	1:A:99:HIS:CE1	2.52	0.44
1:A:32:GLN:NE2	2:B:53:ASP:OD2	2.48	0.43
1:A:119:ASP:HB3	2:B:0:MET:HG3	1.99	0.43
4:D:67:THR:HG22	4:D:77:ASN:ND2	2.32	0.43
1:A:171:TYR:O	1:A:174:LYS:O	2.37	0.42
1:A:210:PRO:O	1:A:263:HIS:HE1	2.03	0.42
1:A:159:TYR:HA	1:A:163:THR:HG23	2.02	0.42
5:E:206:ARG:HD3	5:E:206:ARG:N	2.35	0.41
5:E:6:GLN:NE2	5:E:104:CYS:H	2.19	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	А	268/276~(97%)	259~(97%)	9~(3%)	0	100 100
2	В	98/100~(98%)	94 (96%)	4 (4%)	0	100 100
3	С	7/9~(78%)	7 (100%)	0	0	100 100
4	D	185/199~(93%)	175~(95%)	10~(5%)	0	100 100
5	Е	241/245~(98%)	235~(98%)	6(2%)	0	100 100
All	All	799/829~(96%)	770 (96%)	29~(4%)	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	А	235/237~(99%)	231~(98%)	4 (2%)	60 76		
2	В	95/95~(100%)	93~(98%)	2(2%)	53 70		
3	С	6/6~(100%)	5(83%)	1 (17%)	2 2		
4	D	163/173~(94%)	162~(99%)	1 (1%)	86 94		
5	Ε	210/212~(99%)	204~(97%)	6 (3%)	42 58		
All	All	709/723~(98%)	695~(98%)	14 (2%)	55 72		

All (14) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	35	ARG
1	А	39	ASP
1	А	163	THR
1	А	227	ASP
2	В	70	PHE
2	В	89	GLN
3	С	1	ARG
4	D	203	ASN
5	Е	28	ASN
5	Е	48	MET
5	Е	77	ASN
5	Е	179	VAL
5	Е	206	ARG
5	Е	249	SER

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such side chains are listed below:

Mol	Chain	Res	Type
1	А	72	GLN
1	А	127	ASN
1	А	156	GLN
1	А	218	GLN
1	А	260	HIS
1	А	263	HIS
4	D	40	GLN
4	D	77	ASN
4	D	95	GLN
4	D	203	ASN
5	Е	6	GLN
5	Е	77	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)

1 non-standard protein/DNA/RNA residue is 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	Bos	Link	B	ond leng	gths	В	ond ang	gles
WIOI	Type	Ullaili	nes	LINK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	QM8	С	9	$1,\!3$	8,9,9	0.83	1 (12%)	9,10,10	1.26	2 (22%)

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	QM8	С	9	1,3	-	2/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	С	9	QM8	OXT-C	-2.12	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	9	QM8	OXT-C-O	-2.38	118.67	124.09
3	С	9	QM8	OXT-C-CA	2.19	120.83	113.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	9	QM8	CE-CD-CG-CB
3	С	9	QM8	CG-CD-CE-SZ

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no monosaccharides 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	Turne	Chain	Dec	Link	Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
6	EDO	В	101	-	3,3,3	0.08	0	2,2,2	0.12	0
6	EDO	D	301	-	3,3,3	0.08	0	2,2,2	0.21	0
6	EDO	А	301	-	3,3,3	0.06	0	2,2,2	0.14	0
6	EDO	Е	301	-	3,3,3	0.06	0	2,2,2	0.14	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
6	EDO	В	101	-	-	1/1/1/1	-
6	EDO	D	301	-	-	0/1/1/1	-
6	EDO	А	301	-	-	1/1/1/1	-
6	EDO	Е	301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	В	101	EDO	O1-C1-C2-O2
6	А	301	EDO	O1-C1-C2-O2

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 $>$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$\mathbf{Q}{<}0.9$
1	А	272/276~(98%)	0.30	7 (2%) 56 63	45, 54, 77, 84	0
2	В	100/100~(100%)	0.26	2 (2%) 65 71	45, 60, 77, 83	0
3	С	8/9~(88%)	0.55	0 100 100	48, 49, 52, 62	0
4	D	189/199~(94%)	0.60	12 (6%) 20 25	44, 62, 95, 105	0
5	Ε	243/245~(99%)	0.35	4 (1%) 72 77	47, 59, 79, 90	1 (0%)
All	All	812/829~(97%)	0.38	25 (3%) 49 56	44, 58, 83, 105	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	16	GLY	4.4
4	D	146	SER	4.4
4	D	198	ASP	3.9
5	Е	197	ASN	3.4
4	D	168	SER	3.3
4	D	169	ASP	3.3
4	D	203	ASN	3.0
5	Е	195	ALA	3.0
4	D	147	ASP	2.9
4	D	197	SER	2.7
4	D	163	SER	2.6
5	Е	190	LEU	2.6
2	В	48	LYS	2.4
1	А	42	SER	2.4
1	А	72	GLN	2.3
4	D	145	SER	2.3
5	Е	255	ARG	2.2
1	А	18	GLY	2.2
4	D	200	ALA	2.1
1	А	17	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	В	47	GLU	2.1
4	D	166	LYS	2.1
1	А	104	GLY	2.1
4	D	148	LYS	2.0
1	А	103	LEU	2.0

#### 6.2 Non-standard residues in protein, DNA, RNA chains (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	$B-factors(Å^2)$	Q<0.9
3	QM8	С	9	10/10	0.89	0.18	48,49,56,61	0

#### 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	B-factors(Å <sup>2</sup> )	Q<0.9
6	EDO	В	101	4/4	0.79	0.21	$66,\!66,\!66,\!67$	0
6	EDO	А	301	4/4	0.86	0.17	74,75,75,75	0
6	EDO	D	301	4/4	0.90	0.23	84,84,84,85	0
6	EDO	Е	301	4/4	0.94	0.13	72,72,73,73	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

