



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 11, 2024 – 09:01 PM EST

PDB ID : 3EPL  
Title : Crystallographic snapshots of eukaryotic dimethylallyltransferase acting on tRNA: Insight into tRNA recognition and reaction mechanism  
Authors : Huang, R.H.; Zhou, C.  
Deposited on : 2008-09-29  
Resolution : 3.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.36  
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) : 2.36

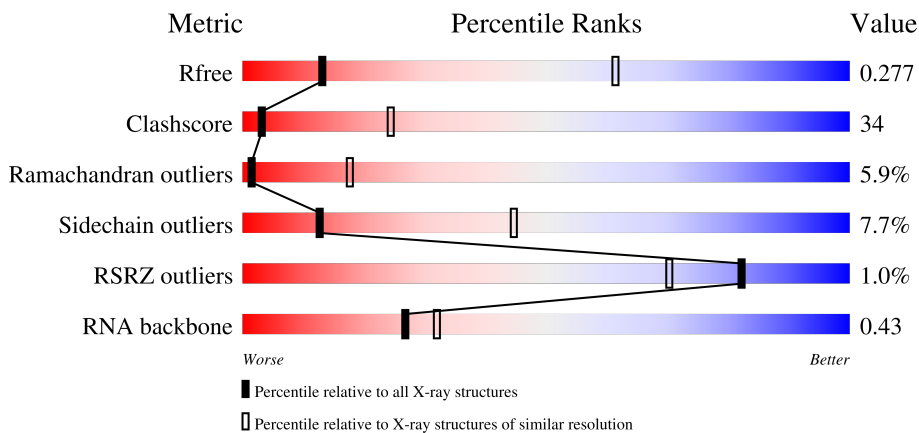
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	409	 4% 38% 51% 9%
1	B	409	 4% 35% 53% 9%
2	E	69	 4% 32% 55% 10%
3	F	69	 30% 42% 19% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	MG	F	73	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9775 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 tRNA isopentenyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3339	2119	589	617	14	0	0	0
1	B	402	3339	2119	589	617	14	0	0	0

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	69	1478	661	258	490	69	0	0	0

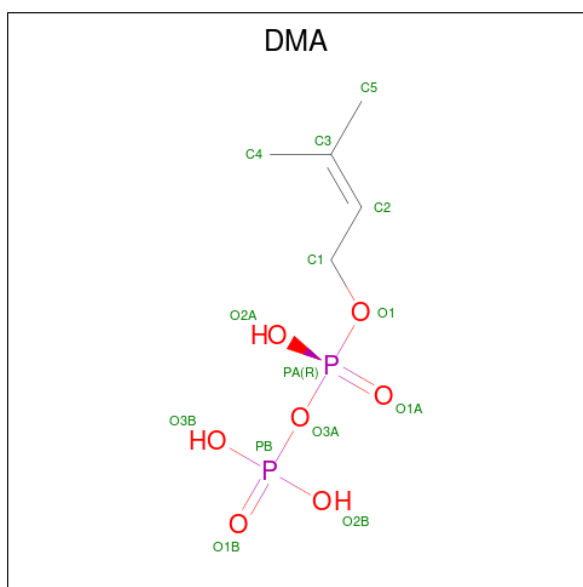
- Molecule 3 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	69	1473	656	258	490	69	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		

- Molecule 5 is DIMETHYLALLYL DIPHOSPHATE (three-letter code: DMA) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0
5	B	1	Total O P 9 7 2	0	0

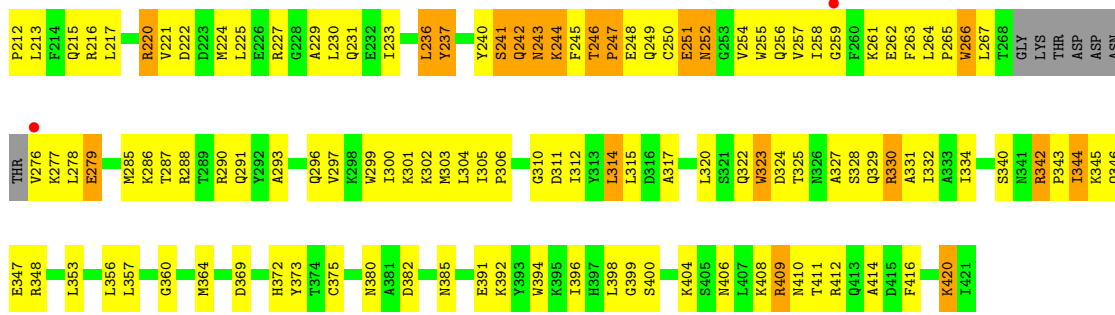
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	F	2	Total Mg 2 2	0	0

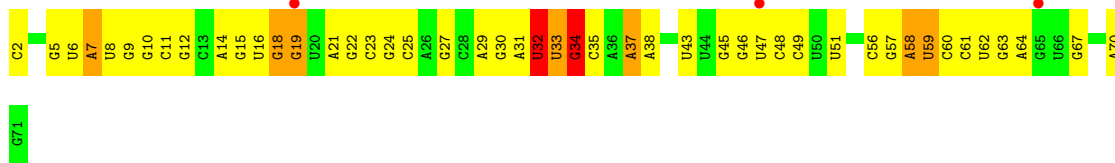
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	24	Total O 24 24	0	0
7	E	22	Total O 22 22	0	0
7	B	42	Total O 42 42	0	0
7	F	34	Total O 34 34	0	0

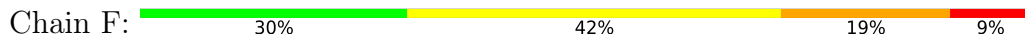




• Molecule 2: tRNA



• Molecule 3: tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.07Å 209.85Å 127.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 37.69 – 3.60	Depositor EDS
% Data completeness (in resolution range)	77.5 (50.00-3.60) 83.6 (37.69-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.91 (at 3.56Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.202 , 0.266 0.215 , 0.277	Depositor DCC
$R_{free}$ test set	1759 reflections (7.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	103.1	Xtrriage
Anisotropy	0.635	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 75.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9775	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: ZN, DMA, 6IA, MG

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	0.44	0/3411	0.58	4/4598 (0.1%)
1	B	0.46	0/3411	0.59	2/4598 (0.0%)
2	E	0.55	1/1619 (0.1%)	0.86	8/2518 (0.3%)
3	F	0.54	1/1645 (0.1%)	0.90	12/2561 (0.5%)
All	All	0.48	2/10086 (0.0%)	0.71	26/14275 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	C	OP3-P	-7.33	1.52	1.61
2	E	2	C	OP3-P	-7.24	1.52	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	32	U	C2'-C3'-O3'	9.05	129.41	109.50
3	F	32	U	C2'-C3'-O3'	9.02	129.35	109.50
3	F	18	G	C2'-C3'-O3'	8.07	127.25	109.50
3	F	46	G	N9-C1'-C2'	8.06	124.48	114.00
3	F	7	A	N9-C1'-C2'	8.03	124.44	114.00

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	3339	0	3346	275	0
1	B	3339	0	3346	253	0
2	E	1478	0	750	40	0
3	F	1473	0	741	50	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	9	0	0	2	0
5	B	9	0	0	2	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
7	A	24	0	0	7	0
7	B	42	0	0	9	0
7	E	22	0	0	0	0
7	F	34	0	0	8	0
All	All	9775	0	8183	598	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 34.

The worst 5 of 598 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:266:TRP:HE1	1:B:277:LYS:HG3	1.09	1.16
1:A:122:LYS:HD3	1:A:193:GLN:HE22	1.18	1.06
1:B:45:SER:HB3	1:B:110:GLY:HA3	1.33	1.05
1:A:45:SER:HB3	1:A:110:GLY:HA3	1.40	1.00
1:A:211:GLU:HB2	1:A:212:PRO:HD3	1.44	0.98

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	398/409 (97%)	312 (78%)	67 (17%)	19 (5%)	2	22
1	B	398/409 (97%)	303 (76%)	67 (17%)	28 (7%)	1	14
All	All	796/818 (97%)	615 (77%)	134 (17%)	47 (6%)	1	18

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	195	ILE
1	A	260	PHE
1	B	59	ASN
1	B	60	LYS

### 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	370/376 (98%)	340 (92%)	30 (8%)	11	43
1	B	370/376 (98%)	343 (93%)	27 (7%)	14	46
All	All	740/752 (98%)	683 (92%)	57 (8%)	13	45

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	368	ASP
1	B	344	ILE
1	B	169	TYR
1	B	330	ARG
1	B	252	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	GLN
1	B	117	GLN
1	B	326	ASN
1	B	94	ASN
1	B	121	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	67/69 (97%)	15 (22%)	7 (10%)
3	F	68/69 (98%)	18 (26%)	7 (10%)
All	All	135/138 (97%)	33 (24%)	14 (10%)

5 of 33 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	7	A
2	E	9	G
2	E	10	G
2	E	18	G
2	E	19	G

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	F	18	G
3	F	32	U
3	F	58	A
3	F	37	A
3	F	48	C

## 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	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6IA	E	37	2	22,29,30	1.06	1 (4%)	22,41,44	1.63	5 (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
2	6IA	E	37	2	-	7/9/31/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	37	6IA	C13-C12	-3.25	1.40	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	37	6IA	O3'-C3'-C2'	4.44	126.17	111.82
2	E	37	6IA	C2'-C3'-C4'	2.57	107.63	102.64
2	E	37	6IA	C2-N1-C6	2.40	118.64	116.59
2	E	37	6IA	O3'-C3'-C4'	2.34	117.82	111.05
2	E	37	6IA	C16-C14-C15	2.02	119.84	110.51

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	37	6IA	N6-C12-C13-C14
2	E	37	6IA	C12-C13-C14-C15
2	E	37	6IA	O4'-C4'-C5'-O5'
2	E	37	6IA	C3'-C4'-C5'-O5'
2	E	37	6IA	C5-C6-N6-C12

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	37	6IA	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
5	DMA	A	422	-	6,8,13	2.42	2 (33%)	13,13,19	1.56	3 (23%)
5	DMA	B	422	-	6,8,13	2.36	2 (33%)	13,13,19	2.15	6 (46%)

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
5	DMA	A	422	-	-	1/6/6/13	-
5	DMA	B	422	-	-	0/6/6/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	422	DMA	PB-O1B	3.45	1.61	1.50
5	A	422	DMA	PB-O1B	3.45	1.61	1.50
5	A	422	DMA	PA-O1A	3.37	1.61	1.50
5	B	422	DMA	PA-O1A	3.25	1.61	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	422	DMA	O2A-PA-O1	3.71	121.83	107.64
5	A	422	DMA	PB-O3A-PA	-3.54	120.69	132.83
5	B	422	DMA	PB-O3A-PA	-3.20	121.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	422	DMA	O1-PA-O1A	2.95	122.25	110.68
5	B	422	DMA	O3A-PA-O1A	-2.95	94.85	111.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	422	DMA	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	422	DMA	2	0
5	B	422	DMA	2	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	402/409 (98%)	-0.23	3 (0%) 87 78	68, 121, 172, 193	0
1	B	402/409 (98%)	-0.19	3 (0%) 87 78	66, 122, 169, 187	0
2	E	68/69 (98%)	0.31	3 (4%) 34 21	80, 186, 212, 219	0
3	F	69/69 (100%)	-0.08	0 100 100	81, 155, 199, 206	0
All	All	941/956 (98%)	-0.17	9 (0%) 82 70	66, 126, 189, 219	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	47	U	3.0
2	E	65	G	2.9
1	A	110	GLY	2.3
1	B	259	GLY	2.3
2	E	19	G	2.3

### 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<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(Å <sup>2</sup> )	Q<0.9
2	6IA	E	37	27/28	0.96	0.31	109,112,120,122	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<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(Å <sup>2</sup> )	Q<0.9
6	MG	F	73	1/1	0.73	0.71	102,102,102,102	0
6	MG	E	72	1/1	0.76	0.16	132,132,132,132	0
6	MG	B	2	1/1	0.86	0.36	112,112,112,112	0
5	DMA	B	422	9/14	0.89	0.36	163,164,166,167	0
6	MG	F	72	1/1	0.90	0.12	106,106,106,106	0
5	DMA	A	422	9/14	0.92	0.37	175,175,177,177	0
4	ZN	B	1	1/1	0.98	0.17	98,98,98,98	0
4	ZN	A	1	1/1	1.00	0.15	96,96,96,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.