



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 28, 2020 – 09:16 pm BST

PDB ID : 1YTU  
Title : Structural basis for 5'-end-specific recognition of the guide RNA strand by the A. fulgidus PIWI protein  
Authors : Ma, J.B.; Yuan, Y.R.; Meister, G.; Pei, Y.; Tuschl, T.; Patel, D.J.  
Deposited on : 2005-02-11  
Resolution : 2.50 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.

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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	:	2.11
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)	:	2.11

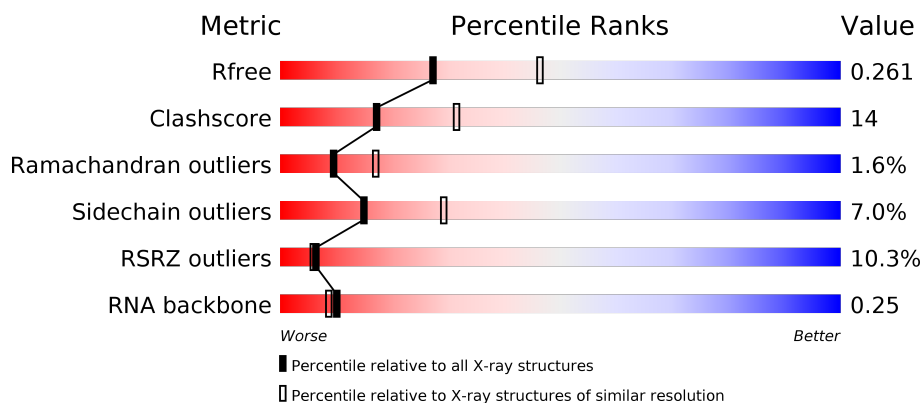
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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  $\geq 3$ , 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	C	6	
1	E	6	
2	D	4	
2	F	4	

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Mol	Chain	Length	Quality of chain
3	A	427	<div><div></div><div>11%</div><div>66%</div><div>26%</div><div></div><div></div></div>
3	B	427	<div><div></div><div>7%</div><div>72%</div><div>24%</div><div></div><div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7282 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 RNA chain called 5'-R(P\*AP\*GP\*AP\*CP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	5	Total	C	N	O	P	0	0	0
			110	49	23	33	5			
1	E	6	Total	C	N	O	P	0	0	0
			133	59	28	40	6			

- Molecule 2 is a RNA chain called 5'-R(P\*UP\*GP\*UP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			83	37	12	30	4			
2	F	4	Total	C	N	O	P	0	0	0
			83	37	12	30	4			

- Molecule 3 is a protein called hypothetical protein AF1318.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	410	Total	C	N	O	S	Se	0	0	0
			3336	2158	550	618	1	9			
3	B	427	Total	C	N	O	S	Se	0	0	0
			3478	2246	579	641	1	11			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O28951
A	2	MSE	MET	modified residue	UNP O28951
A	112	MSE	MET	modified residue	UNP O28951
A	139	MSE	MET	modified residue	UNP O28951
A	200	MSE	MET	modified residue	UNP O28951
A	208	MSE	MET	modified residue	UNP O28951
A	260	MSE	MET	modified residue	UNP O28951
A	280	MSE	MET	modified residue	UNP O28951

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Chain	Residue	Modelled	Actual	Comment	Reference
A	301	MSE	MET	modified residue	UNP O28951
A	339	MSE	MET	modified residue	UNP O28951
A	377	MSE	MET	modified residue	UNP O28951
B	1	MSE	MET	modified residue	UNP O28951
B	2	MSE	MET	modified residue	UNP O28951
B	112	MSE	MET	modified residue	UNP O28951
B	139	MSE	MET	modified residue	UNP O28951
B	200	MSE	MET	modified residue	UNP O28951
B	208	MSE	MET	modified residue	UNP O28951
B	260	MSE	MET	modified residue	UNP O28951
B	280	MSE	MET	modified residue	UNP O28951
B	301	MSE	MET	modified residue	UNP O28951
B	339	MSE	MET	modified residue	UNP O28951
B	377	MSE	MET	modified residue	UNP O28951

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

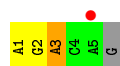
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	3	Total O 3 3	0	0
5	F	1	Total O 1 1	0	0
5	A	21	Total O 21 21	0	0
5	B	30	Total O 30 30	0	0

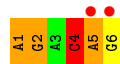
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 5'-R(P\*AP\*GP\*AP\*CP\*AP\*G)-3'



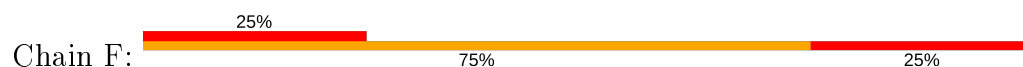
- Molecule 1: 5'-R(P\*AP\*GP\*AP\*CP\*AP\*G)-3'



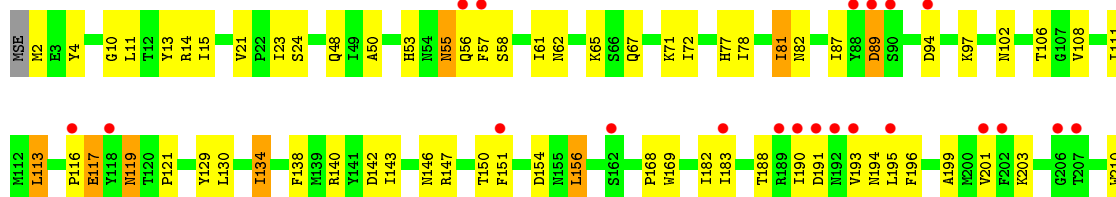
- Molecule 2: 5'-R(P\*UP\*GP\*UP\*C)-3'

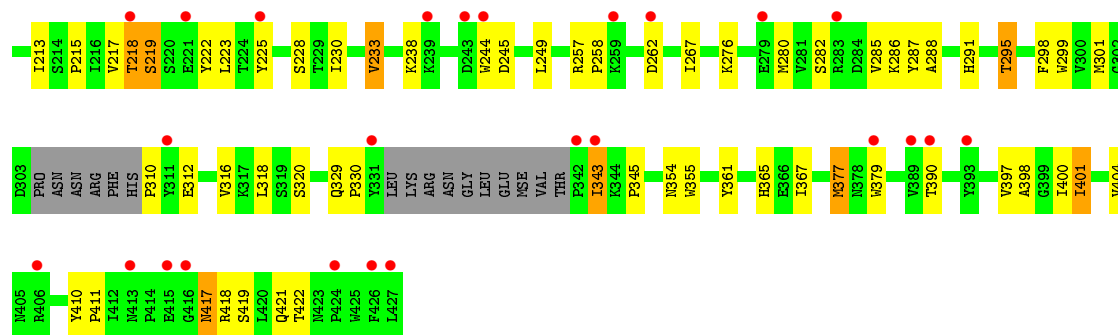


- Molecule 2: 5'-R(P\*UP\*GP\*UP\*C)-3'

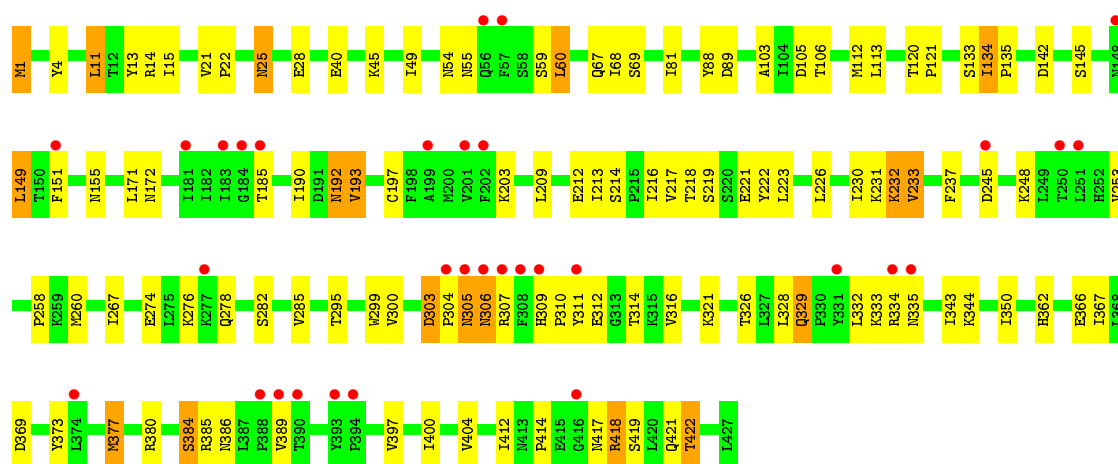


- Molecule 3: hypothetical protein AF1318





• Molecule 3: hypothetical protein AF1318



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	238.75Å 238.75Å 52.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 34.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.50) 99.2 (34.46-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.90 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.204 , 0.266 0.203 , 0.261	Depositor DCC
$R_{free}$ test set	1904 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7282	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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: 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	C	1.53	1/123 (0.8%)	1.90	2/188 (1.1%)
1	E	1.51	1/149 (0.7%)	1.95	6/229 (2.6%)
2	D	1.15	0/91	1.72	1/139 (0.7%)
2	F	1.29	0/91	2.05	4/139 (2.9%)
3	A	0.75	0/3411	0.81	2/4612 (0.0%)
3	B	0.86	0/3556	0.87	2/4808 (0.0%)
All	All	0.86	2/7421 (0.0%)	0.95	17/10115 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
3	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	A	OP3-P	-10.10	1.49	1.61
1	C	1	A	OP3-P	-9.55	1.49	1.61

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	4	C	O5'-P-OP1	-8.12	98.39	105.70
2	F	15	U	C4'-C3'-C2'	-7.92	94.68	102.60
3	B	369	ASP	CB-CG-OD1	6.95	124.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	15	U	O4'-C1'-N1	6.42	113.33	108.20
1	E	4	C	C6-N1-C2	-6.39	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	55	ASN	Peptide
3	B	306	ASN	Peptide

## 5.2 Too-close contacts

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	C	110	0	56	1	0
1	E	133	0	67	6	0
2	D	83	0	43	3	0
2	F	83	0	43	6	0
3	A	3336	0	3346	104	0
3	B	3478	0	3494	90	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	21	0	0	4	0
5	B	30	0	0	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
All	All	7282	0	7049	198	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 14.

The worst 5 of 198 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)
3:B:222:TYR:HD1	3:B:260:MSE:HE2	1.00	1.12
3:B:222:TYR:CD1	3:B:260:MSE:HE2	1.88	1.07
3:A:11:LEU:HD11	5:A:436:HOH:O	1.53	1.05
3:B:305:ASN:HA	3:B:307:ARG:HG3	1.37	1.01
3:A:301:MSE:HE1	3:B:314:THR:HG21	1.53	0.90

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	
3	A	404/427 (95%)	375 (93%)	23 (6%)	6 (2%)	10	18
3	B	425/427 (100%)	396 (93%)	22 (5%)	7 (2%)	9	17
All	All	829/854 (97%)	771 (93%)	45 (5%)	13 (2%)	9	17

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	193	VAL
3	B	219	SER
3	B	305	ASN
3	B	384	SER
3	A	57	PHE

### 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	
3	A	378/383 (99%)	352 (93%)	26 (7%)	15	30
3	B	394/383 (103%)	366 (93%)	28 (7%)	14	28
All	All	772/766 (101%)	718 (93%)	54 (7%)	15	29

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	401	ILE
3	B	55	ASN
3	B	367	ILE
3	A	417	ASN
3	B	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	47	ASN
3	B	56	GLN
3	B	306	ASN
3	B	25	ASN
3	B	309	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	4/6 (66%)	0	0
1	E	5/6 (83%)	2 (40%)	0
2	D	3/4 (75%)	1 (33%)	0
2	F	3/4 (75%)	2 (66%)	0
All	All	15/20 (75%)	5 (33%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	16	G
1	E	4	C
1	E	6	G
2	F	16	G
2	F	18	C

There are no RNA pucker outliers to report.

#### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

#### 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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, 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	C	5/6 (83%)	0.43	1 (20%) 1 0	61, 62, 73, 77	1 (20%)
1	E	6/6 (100%)	1.02	2 (33%) 0 0	51, 61, 84, 90	2 (33%)
2	D	4/4 (100%)	2.89	4 (100%) 0 0	97, 100, 102, 103	1 (25%)
2	F	4/4 (100%)	1.06	1 (25%) 0 0	93, 99, 102, 102	1 (25%)
3	A	401/427 (93%)	0.50	46 (11%) 4 4	40, 60, 82, 97	0
3	B	416/427 (97%)	0.41	32 (7%) 13 13	43, 56, 82, 95	0
All	All	836/874 (95%)	0.47	86 (10%) 6 6	40, 58, 83, 103	5 (0%)

The worst 5 of 86 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	305	ASN	6.7
1	E	6	G	5.3
3	A	283	ARG	5.3
3	A	57	PHE	5.1
2	D	15	U	4.8

### 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
4	MG	A	428	1/1	0.95	0.04	48,48,48,48	0
4	MG	B	428	1/1	0.97	0.04	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.