



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 1, 2019 – 05:12 PM EDT

PDB ID : 6KBZ  
Title : Crystal structure of yedK with ssDNA containing a tetrahydrofuran abasic site  
Authors : Wang, N.; Bao, H.; Huang, H.  
Deposited on : 2019-06-26  
Resolution : 1.65 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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

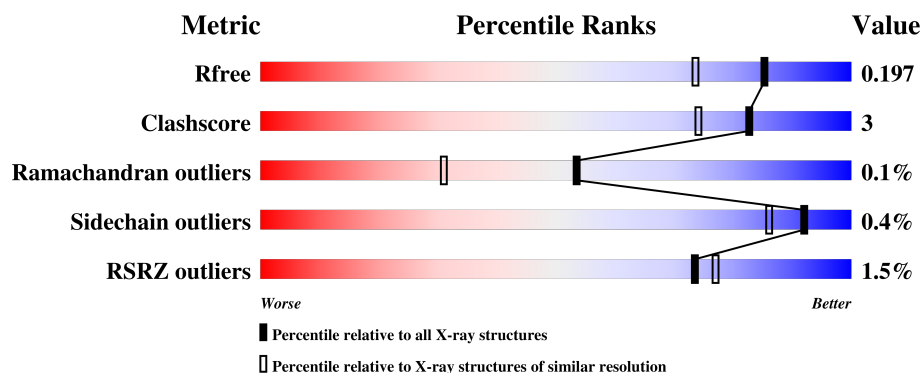
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	111664	1521 (1.66-1.66)
Clashscore	122126	1616 (1.66-1.66)
Ramachandran outliers	120053	1584 (1.66-1.66)
Sidechain outliers	120020	1584 (1.66-1.66)
RSRZ outliers	108989	1487 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	B	227	<div> <div>94%</div> <div>5%</div> </div>
1	D	227	<div> <div>%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	F	227	<div> <div>2%</div> <div>93%</div> <div>7%</div> </div>
1	H	227	<div> <div>3%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
2	A	10	<div> <div>90%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
2	C	10	 80%10%10%
2	E	10	 80%10%10%
2	G	10	 90%10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8909 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 SOS response-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	226	Total	C	N	O	S	0	0	0
			1800	1153	313	328	6			
1	D	223	Total	C	N	O	S	0	0	0
			1770	1131	310	323	6			
1	F	226	Total	C	N	O	S	0	0	0
			1800	1153	313	328	6			
1	H	220	Total	C	N	O	S	0	0	0
			1741	1114	307	314	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	223	LEU	-	expression tag	UNP A0A2S5ZH06
B	224	GLU	-	expression tag	UNP A0A2S5ZH06
B	225	VAL	-	expression tag	UNP A0A2S5ZH06
B	226	LEU	-	expression tag	UNP A0A2S5ZH06
B	227	PHE	-	expression tag	UNP A0A2S5ZH06
B	228	GLN	-	expression tag	UNP A0A2S5ZH06
D	223	LEU	-	expression tag	UNP A0A2S5ZH06
D	224	GLU	-	expression tag	UNP A0A2S5ZH06
D	225	VAL	-	expression tag	UNP A0A2S5ZH06
D	226	LEU	-	expression tag	UNP A0A2S5ZH06
D	227	PHE	-	expression tag	UNP A0A2S5ZH06
D	228	GLN	-	expression tag	UNP A0A2S5ZH06
F	223	LEU	-	expression tag	UNP A0A2S5ZH06
F	224	GLU	-	expression tag	UNP A0A2S5ZH06
F	225	VAL	-	expression tag	UNP A0A2S5ZH06
F	226	LEU	-	expression tag	UNP A0A2S5ZH06
F	227	PHE	-	expression tag	UNP A0A2S5ZH06
F	228	GLN	-	expression tag	UNP A0A2S5ZH06
H	223	LEU	-	expression tag	UNP A0A2S5ZH06
H	224	GLU	-	expression tag	UNP A0A2S5ZH06
H	225	VAL	-	expression tag	UNP A0A2S5ZH06

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Chain	Residue	Modelled	Actual	Comment	Reference
H	226	LEU	-	expression tag	UNP A0A2S5ZH06
H	227	PHE	-	expression tag	UNP A0A2S5ZH06
H	228	GLN	-	expression tag	UNP A0A2S5ZH06

- Molecule 2 is a DNA chain called 5'-D (\*CP\*GP\*GP\*TP\* (3DR) P\*GP\*AP\*TP\*TP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	9	Total	C	N	O	P	0	0	0
			177	84	29	55	9			
2	C	9	Total	C	N	O	P	0	0	0
			177	84	29	55	9			
2	E	9	Total	C	N	O	P	0	0	0
			177	84	29	55	9			
2	G	9	Total	C	N	O	P	0	0	0
			177	84	29	55	9			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	B	2	Total	Mg	0	0
			2	2		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	198	Total	O	0	0
			198	198		
4	A	47	Total	O	0	0
			47	47		
4	D	240	Total	O	0	0
			240	240		
4	C	44	Total	O	0	0
			44	44		
4	F	238	Total	O	0	0
			238	238		
4	E	43	Total	O	0	0
			43	43		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	219	Total 219	O 219	0	0
4	G	57	Total 57	O 57	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.

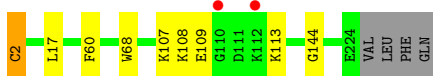
- Molecule 1: SOS response-associated protein

Chain B: 



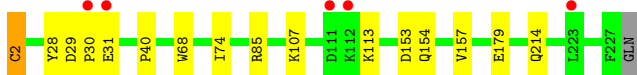
- Molecule 1: SOS response-associated protein

Chain D: 




- Molecule 1: SOS response-associated protein

Chain F: 



- Molecule 1: SOS response-associated protein

Chain H: 




- Molecule 2: 5'-D (\*CP\*GP\*GP\*TP\* (3DR) P\*GP\*AP\*TP\*TP\*C)-3'

Chain A: 



- Molecule 2: 5'-D (\*CP\*GP\*GP\*TP\* (3DR) P\*GP\*AP\*TP\*TP\*C)-3'

Chain C: 



- Molecule 2: 5'-D (\*CP\*GP\*GP\*TP\* (3DR) P\*GP\*AP\*TP\*TP\*C)-3'

Chain E: 80% 10% 10%



- Molecule 2: 5'-D (\*CP\*GP\*GP\*TP\* (3DR) P\*GP\*AP\*TP\*TP\*C)-3'

Chain G: 90% 10%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.53Å 111.39Å 104.10Å 90.00° 96.14° 90.00°	Depositor
Resolution (Å)	36.27 – 1.65 37.91 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.6 (36.27-1.65) 91.6 (37.91-1.65)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, $R_{free}$	0.160 , 0.196 0.160 , 0.197	Depositor DCC
$R_{free}$ test set	5192 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.0	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8590e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 3DR

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	B	0.35	0/1854	0.52	0/2522
1	D	0.36	0/1823	0.54	0/2480
1	F	0.37	0/1854	0.56	0/2522
1	H	0.37	0/1793	0.54	0/2438
2	A	0.71	0/184	1.00	0/280
2	C	0.77	0/184	0.98	0/280
2	E	0.84	0/184	1.00	0/280
2	G	0.86	0/184	1.02	0/280
All	All	0.42	0/8060	0.60	0/11082

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	B	1800	0	1735	7	0
1	D	1770	0	1702	8	0
1	F	1800	0	1735	11	0
1	H	1741	0	1676	16	0
2	A	177	0	100	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	177	0	100	1	0
2	E	177	0	100	1	0
2	G	177	0	100	0	0
3	B	2	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	47	0	0	0	0
4	B	198	0	0	1	0
4	C	44	0	0	0	0
4	D	240	0	0	4	1
4	E	43	0	0	0	0
4	F	238	0	0	3	1
4	G	57	0	0	0	0
4	H	219	0	0	8	1
All	All	8909	0	7248	40	2

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 3.

The worst 5 of 40 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:H:29:ASP:O	4:H:401:HOH:O	2.05	0.74
1:F:214:GLN:O	4:F:401:HOH:O	2.12	0.67
1:B:177:ARG:HB2	1:B:180:ILE:HD13	1.77	0.67
1:D:2:CYS:N	4:D:301:HOH:O	2.28	0.65
1:D:108:LYS:NZ	1:H:68:TRP:O	2.33	0.62

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:427:HOH:O	4:H:459:HOH:O[1_655]	2.10	0.10
4:D:503:HOH:O	4:F:581:HOH:O[2_756]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	B	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
1	D	221/227 (97%)	214 (97%)	7 (3%)	0	100	100
1	F	224/227 (99%)	219 (98%)	5 (2%)	0	100	100
1	H	216/227 (95%)	209 (97%)	6 (3%)	1 (0%)	31	11
All	All	885/908 (98%)	861 (97%)	23 (3%)	1 (0%)	53	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	224	GLU

### 5.3.2 Protein sidechains

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	B	184/185 (100%)	184 (100%)	0	100	100
1	D	180/185 (97%)	179 (99%)	1 (1%)	87	78
1	F	184/185 (100%)	183 (100%)	1 (0%)	90	83
1	H	176/185 (95%)	175 (99%)	1 (1%)	87	78
All	All	724/740 (98%)	721 (100%)	3 (0%)	92	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	CYS
1	F	2	CYS
1	H	2	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	3DR	A	2	2	8,11,12	0.51	0	9,14,17	0.58	0
2	3DR	C	2	2	8,11,12	0.72	0	9,14,17	0.51	0
2	3DR	E	2	2	8,11,12	0.65	0	9,14,17	0.43	0
2	3DR	G	2	2	8,11,12	0.83	0	9,14,17	0.63	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	3DR	A	2	2	-	1/3/15/16	0/1/1/1
2	3DR	C	2	2	-	1/3/15/16	0/1/1/1
2	3DR	E	2	2	-	1/3/15/16	0/1/1/1
2	3DR	G	2	2	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2	3DR	O4'-C4'-C5'-O5'
2	A	2	3DR	O4'-C4'-C5'-O5'
2	C	2	3DR	O4'-C4'-C5'-O5'
2	G	2	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2	3DR	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	B	226/227 (99%)	-0.47	1 (0%) 92 93	8, 18, 37, 48	0
1	D	223/227 (98%)	-0.63	2 (0%) 84 86	7, 15, 35, 51	0
1	F	226/227 (99%)	-0.41	5 (2%) 62 63	5, 14, 37, 57	0
1	H	220/227 (96%)	-0.40	6 (2%) 54 55	6, 14, 41, 54	0
2	A	8/10 (80%)	-0.53	0 100 100	13, 18, 29, 53	0
2	C	8/10 (80%)	-0.56	0 100 100	12, 17, 29, 44	0
2	E	8/10 (80%)	-0.39	0 100 100	9, 18, 25, 53	0
2	G	8/10 (80%)	-0.50	0 100 100	9, 15, 22, 40	0
All	All	927/948 (97%)	-0.48	14 (1%) 73 77	5, 15, 38, 57	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	112	LYS	5.6
1	F	223	LEU	4.0
1	F	30	PRO	3.4
1	H	225	VAL	3.1
1	H	111	ASP	3.0

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

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	3DR	A	2	11/12	0.99	0.07	14,16,22,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	3DR	C	2	11/12	0.99	0.07	10,14,20,24	0
2	3DR	E	2	11/12	0.99	0.06	7,11,14,15	0
2	3DR	G	2	11/12	0.99	0.06	7,10,16,16	0

### 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
3	MG	H	301	1/1	0.93	0.13	32,32,32,32	0
3	MG	B	302	1/1	0.93	0.28	40,40,40,40	0
3	MG	F	301	1/1	0.94	0.18	33,33,33,33	0
3	MG	B	301	1/1	0.97	0.18	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.