



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:29 am GMT

PDB ID : 4G0W  
Title : Human topoisomerase iibeta in complex with DNA and ametantrone  
Authors : Wu, C.C.; Li, T.K.; Li, Y.C.; Chan, N.L.  
Deposited on : 2012-07-10  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

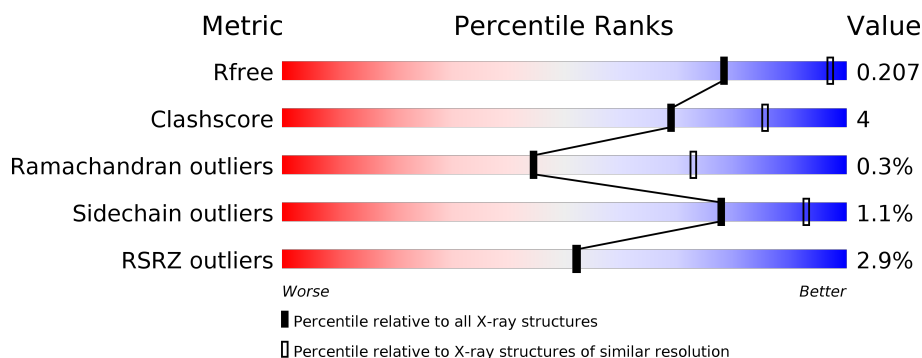
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	A	803	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>17%</div> </div> </div>
1	B	803	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>9%</div> <div>17%</div> </div> </div>
2	C	8	<div> <div>13%</div> <div> <div></div> <div>63%</div> <div>38%</div> </div> </div>
2	E	8	<div> <div>13%</div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
3	D	12	<div> <div></div> <div> <div></div> <div>50%</div> <div>50%</div> </div> </div>
3	F	12	<div> <div></div> <div> <div></div> <div>58%</div> <div>25%</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12185 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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	11	0
			5411	3448	935	1003	25			
1	B	664	Total	C	N	O	S	0	10	0
			5408	3449	936	999	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	EXPRESSION TAG	UNP Q02880
A	420	ALA	-	EXPRESSION TAG	UNP Q02880
A	421	SER	-	EXPRESSION TAG	UNP Q02880
A	422	TRP	-	EXPRESSION TAG	UNP Q02880
A	423	SER	-	EXPRESSION TAG	UNP Q02880
A	424	HIS	-	EXPRESSION TAG	UNP Q02880
A	425	PRO	-	EXPRESSION TAG	UNP Q02880
A	426	GLN	-	EXPRESSION TAG	UNP Q02880
A	427	PHE	-	EXPRESSION TAG	UNP Q02880
A	428	GLU	-	EXPRESSION TAG	UNP Q02880
A	429	LYS	-	EXPRESSION TAG	UNP Q02880
A	430	GLY	-	EXPRESSION TAG	UNP Q02880
A	431	ALA	-	EXPRESSION TAG	UNP Q02880
A	432	ASP	-	EXPRESSION TAG	UNP Q02880
A	433	ASP	-	EXPRESSION TAG	UNP Q02880
A	434	ASP	-	EXPRESSION TAG	UNP Q02880
A	435	ASP	-	EXPRESSION TAG	UNP Q02880
A	436	LYS	-	EXPRESSION TAG	UNP Q02880
A	437	VAL	-	EXPRESSION TAG	UNP Q02880
A	438	PRO	-	EXPRESSION TAG	UNP Q02880
A	439	ASP	-	EXPRESSION TAG	UNP Q02880
A	440	PRO	-	EXPRESSION TAG	UNP Q02880
A	441	THR	-	EXPRESSION TAG	UNP Q02880
A	442	SER	-	EXPRESSION TAG	UNP Q02880
A	443	VAL	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	EXPRESSION TAG	UNP Q02880
A	1202	GLY	-	EXPRESSION TAG	UNP Q02880
A	1203	ALA	-	EXPRESSION TAG	UNP Q02880
A	1204	PRO	-	EXPRESSION TAG	UNP Q02880
A	1205	GLY	-	EXPRESSION TAG	UNP Q02880
A	1206	PHE	-	EXPRESSION TAG	UNP Q02880
A	1207	SER	-	EXPRESSION TAG	UNP Q02880
A	1208	SER	-	EXPRESSION TAG	UNP Q02880
A	1209	ILE	-	EXPRESSION TAG	UNP Q02880
A	1210	SER	-	EXPRESSION TAG	UNP Q02880
A	1211	ALA	-	EXPRESSION TAG	UNP Q02880
A	1212	HIS	-	EXPRESSION TAG	UNP Q02880
A	1213	HIS	-	EXPRESSION TAG	UNP Q02880
A	1214	HIS	-	EXPRESSION TAG	UNP Q02880
A	1215	HIS	-	EXPRESSION TAG	UNP Q02880
A	1216	HIS	-	EXPRESSION TAG	UNP Q02880
A	1217	HIS	-	EXPRESSION TAG	UNP Q02880
A	1218	HIS	-	EXPRESSION TAG	UNP Q02880
A	1219	HIS	-	EXPRESSION TAG	UNP Q02880
A	1220	HIS	-	EXPRESSION TAG	UNP Q02880
A	1221	HIS	-	EXPRESSION TAG	UNP Q02880
B	419	MET	-	EXPRESSION TAG	UNP Q02880
B	420	ALA	-	EXPRESSION TAG	UNP Q02880
B	421	SER	-	EXPRESSION TAG	UNP Q02880
B	422	TRP	-	EXPRESSION TAG	UNP Q02880
B	423	SER	-	EXPRESSION TAG	UNP Q02880
B	424	HIS	-	EXPRESSION TAG	UNP Q02880
B	425	PRO	-	EXPRESSION TAG	UNP Q02880
B	426	GLN	-	EXPRESSION TAG	UNP Q02880
B	427	PHE	-	EXPRESSION TAG	UNP Q02880
B	428	GLU	-	EXPRESSION TAG	UNP Q02880
B	429	LYS	-	EXPRESSION TAG	UNP Q02880
B	430	GLY	-	EXPRESSION TAG	UNP Q02880
B	431	ALA	-	EXPRESSION TAG	UNP Q02880
B	432	ASP	-	EXPRESSION TAG	UNP Q02880
B	433	ASP	-	EXPRESSION TAG	UNP Q02880
B	434	ASP	-	EXPRESSION TAG	UNP Q02880
B	435	ASP	-	EXPRESSION TAG	UNP Q02880
B	436	LYS	-	EXPRESSION TAG	UNP Q02880
B	437	VAL	-	EXPRESSION TAG	UNP Q02880
B	438	PRO	-	EXPRESSION TAG	UNP Q02880
B	439	ASP	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	EXPRESSION TAG	UNP Q02880
B	441	THR	-	EXPRESSION TAG	UNP Q02880
B	442	SER	-	EXPRESSION TAG	UNP Q02880
B	443	VAL	-	EXPRESSION TAG	UNP Q02880
B	444	ASP	-	EXPRESSION TAG	UNP Q02880
B	1202	GLY	-	EXPRESSION TAG	UNP Q02880
B	1203	ALA	-	EXPRESSION TAG	UNP Q02880
B	1204	PRO	-	EXPRESSION TAG	UNP Q02880
B	1205	GLY	-	EXPRESSION TAG	UNP Q02880
B	1206	PHE	-	EXPRESSION TAG	UNP Q02880
B	1207	SER	-	EXPRESSION TAG	UNP Q02880
B	1208	SER	-	EXPRESSION TAG	UNP Q02880
B	1209	ILE	-	EXPRESSION TAG	UNP Q02880
B	1210	SER	-	EXPRESSION TAG	UNP Q02880
B	1211	ALA	-	EXPRESSION TAG	UNP Q02880
B	1212	HIS	-	EXPRESSION TAG	UNP Q02880
B	1213	HIS	-	EXPRESSION TAG	UNP Q02880
B	1214	HIS	-	EXPRESSION TAG	UNP Q02880
B	1215	HIS	-	EXPRESSION TAG	UNP Q02880
B	1216	HIS	-	EXPRESSION TAG	UNP Q02880
B	1217	HIS	-	EXPRESSION TAG	UNP Q02880
B	1218	HIS	-	EXPRESSION TAG	UNP Q02880
B	1219	HIS	-	EXPRESSION TAG	UNP Q02880
B	1220	HIS	-	EXPRESSION TAG	UNP Q02880
B	1221	HIS	-	EXPRESSION TAG	UNP Q02880

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total 165	C 77	N 34	O 46	P 8	0	0	0
2	E	8	Total 165	C 77	N 34	O 46	P 8	0	0	0

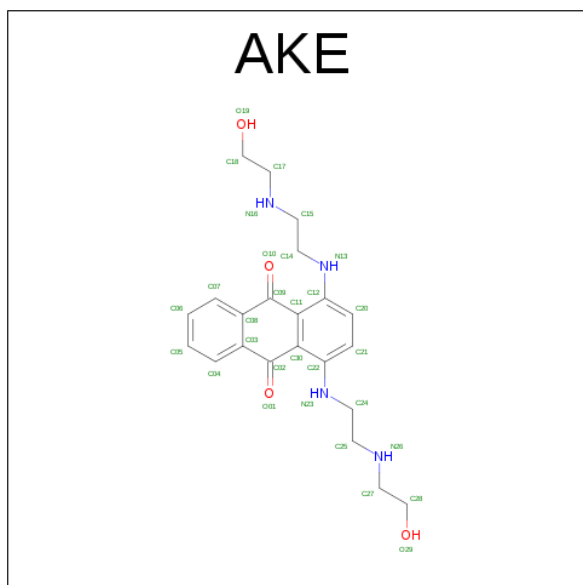
- Molecule 3 is a DNA chain called DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total 245	C 116	N 43	O 74	P 12	0	0	0
3	F	12	Total 245	C 116	N 43	O 74	P 12	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mg	0	0
			2	2		
4	A	2	Total	Mg	0	0
			2	2		
4	D	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 1,4-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMINO)ANTHRACEN E-9,10-DIONE (three-letter code: AKE) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	24	1
			60	44	8	8		
5	F	1	Total	C	N	O	24	1
			60	44	8	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	153	Total	O	0	0
			153	153		
6	B	172	Total	O	0	0
			172	172		

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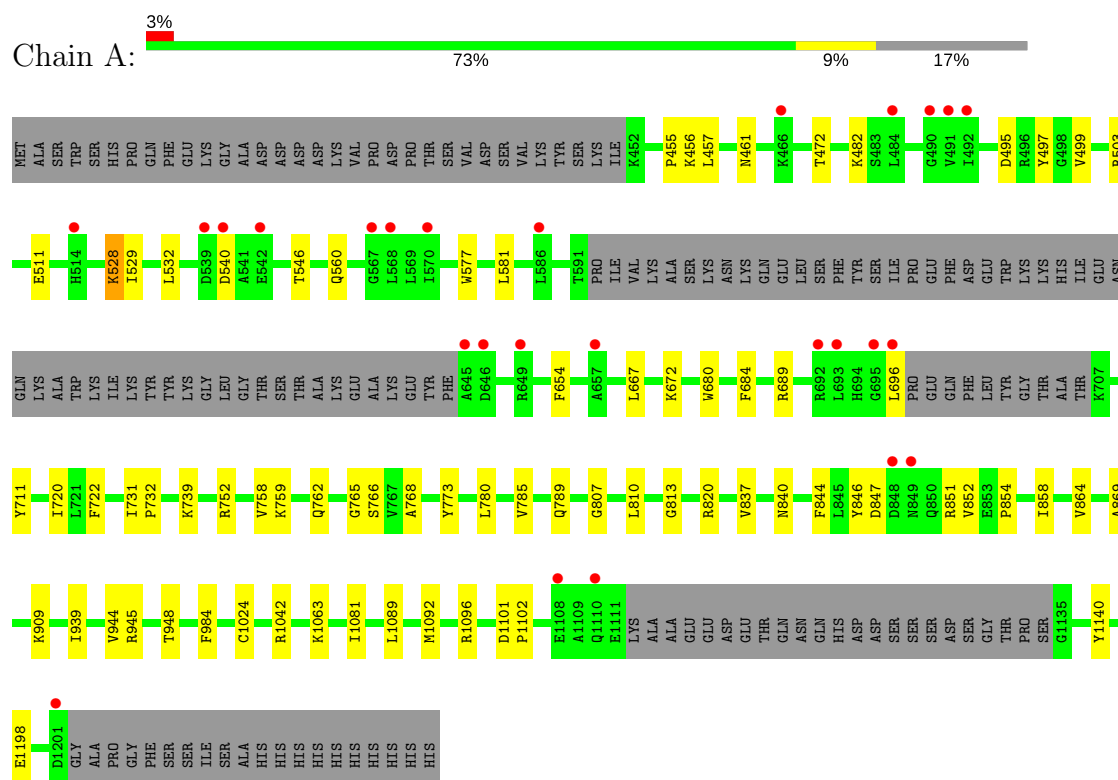
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	16	Total 16	O 16	0	0
6	D	32	Total 32	O 32	0	0
6	E	16	Total 16	O 16	0	0
6	F	31	Total 31	O 31	0	0

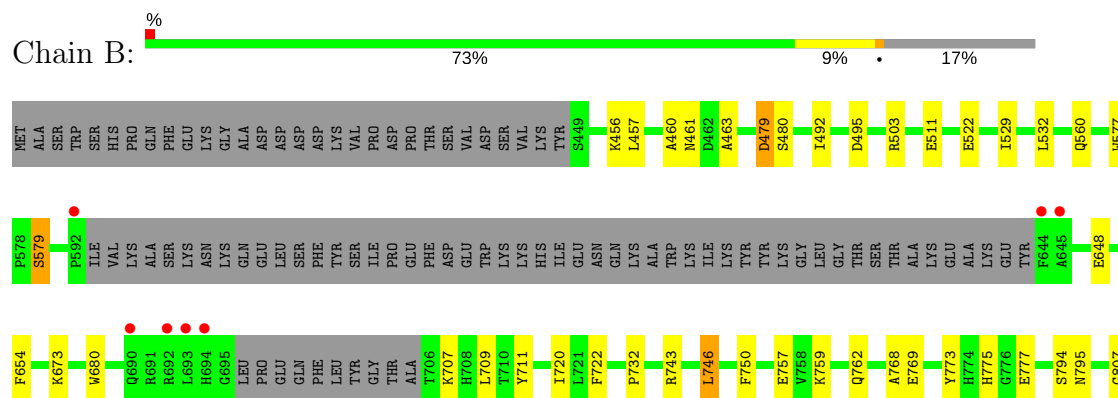
### 3 Residue-property plots [i](#)

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: DNA topoisomerase 2-beta



- Molecule 1: DNA topoisomerase 2-beta

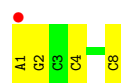




- Molecule 2: DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*AP\*GP\*C)-3')



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



- Molecule 3: DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3')



- Molecule 3: DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.66Å 176.42Å 93.64Å 90.00° 112.04° 90.00°	Depositor
Resolution (Å)	27.49 – 2.70 29.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.49-2.70) 98.8 (29.42-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.165 , 0.215 0.155 , 0.207	Depositor DCC
$R_{free}$ test set	3340 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AKE

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	0.41	0/5545	0.54	0/7467
1	B	0.41	0/5536	0.55	0/7455
2	C	0.81	0/185	1.44	2/283 (0.7%)
2	E	0.73	0/185	1.77	6/283 (2.1%)
3	D	0.84	0/273	1.66	6/419 (1.4%)
3	F	0.76	0/273	1.66	7/419 (1.7%)
All	All	0.45	0/11997	0.71	21/16326 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	DA	O4'-C1'-N9	9.69	114.78	108.00
2	E	2	DG	O4'-C1'-N9	9.33	114.53	108.00
2	E	1	DA	C3'-C2'-C1'	-9.00	91.69	102.50
2	E	1	DA	C1'-O4'-C4'	-8.64	101.46	110.10
3	F	10	DG	O4'-C1'-N9	8.37	113.86	108.00
3	D	19	DC	C1'-O4'-C4'	-8.26	101.84	110.10
3	D	10	DG	O4'-C1'-N9	8.12	113.68	108.00
3	F	19	DC	O4'-C1'-N1	7.77	113.44	108.00
3	D	19	DC	O4'-C4'-C3'	-7.76	101.34	106.00
3	F	14	DC	C4'-C3'-C2'	-7.31	96.52	103.10
2	E	8	DC	O4'-C1'-N1	7.19	113.03	108.00
3	F	16	DC	O4'-C1'-N1	7.15	113.01	108.00
3	D	20	DT	N3-C4-O4	5.61	123.27	119.90
3	F	19	DC	C1'-O4'-C4'	-5.57	104.53	110.10
3	F	14	DC	C1'-O4'-C4'	-5.43	104.67	110.10
2	C	2	DG	O4'-C1'-N9	5.39	111.77	108.00
3	F	14	DC	C5'-C4'-C3'	5.32	123.67	114.10
3	D	17	DG	C5-C6-O6	-5.25	125.45	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	20	DT	C5-C4-O4	-5.23	121.24	124.90
2	C	4	DC	C1'-O4'-C4'	-5.05	105.05	110.10
2	E	4	DC	C1'-O4'-C4'	-5.05	105.05	110.10

There are no chirality outliers.

There are no planarity outliers.

## 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	A	5411	0	5478	45	0
1	B	5408	0	5481	51	0
2	C	165	0	89	1	0
2	E	165	0	89	0	0
3	D	245	0	136	2	0
3	F	245	0	136	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	D	60	0	56	5	0
5	F	60	0	55	2	0
6	A	153	0	0	2	0
6	B	172	0	0	6	0
6	C	16	0	0	0	0
6	D	32	0	0	1	0
6	E	16	0	0	0	0
6	F	31	0	0	0	0
All	All	12185	0	11520	98	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 4.

All (98) 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:732:PRO:HG2	1:B:869:ALA:HB1	1.62	0.81
1:A:732:PRO:HG2	1:A:869:ALA:HB1	1.65	0.78
1:B:989:THR:HG22	1:B:992:LYS:H	1.49	0.78
1:A:762[B]:GLN:NE2	1:B:769:GLU:OE2	2.23	0.71
1:A:820[B]:ARG:HH12	1:B:820:ARG:HH22	1.35	0.71
1:B:880[B]:LEU:HD12	1:B:881:PRO:HD2	1.72	0.70
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.31	0.66
1:B:976:TYR:HB2	1:B:983:LYS:HD3	1.78	0.66
1:B:1170:ASP:OD1	1:B:1173[A]:ARG:NH2	2.33	0.62
1:B:456:LYS:NZ	1:B:479:ASP:OD2	2.24	0.61
1:A:461:ASN:HB2	1:A:495:ASP:HA	1.86	0.58
1:B:460:ALA:HB3	1:B:463:ALA:HB2	1.85	0.57
1:A:503:ARG:NH1	3:D:9:DT:O2	2.37	0.57
1:A:689:ARG:NH1	1:A:1024:CYS:SG	2.78	0.57
1:A:528:LYS:HD3	1:A:528:LYS:N	2.21	0.56
1:B:673:LYS:NZ	6:B:1571:HOH:O	2.38	0.56
1:B:757:GLU:HB2	1:B:823:PHE:HB3	1.87	0.56
1:B:865:LEU:HD23	1:B:880[B]:LEU:HD21	1.87	0.56
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.87	0.56
1:B:944:VAL:HG12	1:B:945:ARG:HG2	1.88	0.55
3:D:13:DG:O6	5:D:101[A]:AKE:H14	2.07	0.55
1:A:511:GLU:OE2	1:A:672:LYS:NZ	2.41	0.54
1:A:820[B]:ARG:NH1	1:B:820:ARG:HH22	2.06	0.52
1:B:511:GLU:HB2	6:B:1510:HOH:O	2.09	0.51
1:B:768:ALA:HA	1:B:773:TYR:HB3	1.91	0.51
1:A:768:ALA:HA	1:A:773:TYR:HB3	1.91	0.51
5:F:101[A]:AKE:N13	5:F:101[A]:AKE:O10	2.44	0.51
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.92	0.51
1:B:880[A]:LEU:HG	1:B:1016:MET:HG2	1.93	0.50
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.92	0.50
3:F:14:DC:H2''	3:F:15:DT:H5'	1.94	0.50
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.94	0.50
1:A:844:PHE:HA	1:A:854:PRO:HA	1.94	0.50
1:B:773:TYR:CE1	1:B:775:HIS:HB2	2.47	0.49
1:A:773:TYR:CE1	1:A:780:LEU:HG	2.48	0.49
1:A:654:PHE:HB3	1:A:711:TYR:CE1	2.48	0.49
1:A:807:GLY:HA3	1:A:813:GLY:HA2	1.95	0.49
1:A:765:GLY:HA3	1:B:762[A]:GLN:NE2	2.28	0.48
3:F:14:DC:H5'	5:F:101[A]:AKE:H14	1.96	0.48
1:B:870:GLU:OE2	1:B:945:ARG:NH2	2.46	0.48
1:B:903:PRO:HA	1:B:1032[A]:GLN:HE21	1.79	0.47
1:A:1092:MET:O	1:A:1096:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:ARG:NH2	6:B:1505:HOH:O	2.21	0.47
1:A:581:LEU:HD22	1:A:711:TYR:OH	2.15	0.46
1:A:739:LYS:HD3	2:C:6:DA:H5"	1.96	0.46
1:A:810[A]:LEU:HD12	1:A:948:THR:HB	1.97	0.46
1:B:1001:LEU:HA	1:B:1001:LEU:HD23	1.84	0.46
1:B:746:LEU:HD12	1:B:750:PHE:CZ	2.51	0.46
1:B:807:GLY:HA3	1:B:813:GLY:HA2	1.97	0.46
1:B:844:PHE:HA	1:B:854:PRO:HA	1.98	0.46
5:D:101[A]:AKE:N13	5:D:101[A]:AKE:O10	2.45	0.46
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.98	0.46
1:A:759:LYS:NZ	1:B:777:GLU:OE2	2.31	0.46
1:B:532:LEU:HD13	1:B:577:TRP:CZ3	2.52	0.46
5:D:101[A]:AKE:O01	5:D:101[A]:AKE:N23	2.48	0.45
1:B:879:LYS:HE2	6:D:208:HOH:O	2.17	0.45
1:A:909:LYS:NZ	1:A:1198:GLU:OE1	2.49	0.45
1:A:837:VAL:O	1:A:840:ASN:ND2	2.49	0.45
1:A:939:ILE:HB	1:A:984:PHE:HB2	1.99	0.45
1:B:492:ILE:HD12	1:B:492:ILE:H	1.82	0.45
1:A:851:ARG:NH2	6:A:1537:HOH:O	2.50	0.45
1:B:762[A]:GLN:HA	1:B:762[A]:GLN:HE21	1.81	0.44
1:A:532:LEU:HD13	1:A:577:TRP:CZ3	2.53	0.44
1:A:780:LEU:HD23	1:A:780:LEU:HA	1.80	0.44
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.99	0.44
1:B:842:LEU:HD21	1:B:858:ILE:HG22	1.99	0.44
1:A:581:LEU:HA	1:A:581:LEU:HD23	1.80	0.44
1:A:944:VAL:HG12	1:A:945:ARG:HG3	2.00	0.44
1:A:667:LEU:HD21	1:A:680:TRP:CG	2.53	0.44
1:B:759:LYS:HG3	1:B:823:PHE:CE2	2.53	0.44
1:A:1081:ILE:HG22	1:A:1089:LEU:HD11	1.99	0.43
1:A:482:LYS:HE2	1:A:499:VAL:HG13	1.99	0.43
1:B:654:PHE:HA	1:B:709:LEU:O	2.18	0.43
1:B:794:SER:OG	1:B:795:ASN:N	2.51	0.43
1:B:938:GLU:OE2	1:B:983:LYS:NZ	2.28	0.43
1:B:1056:MET:O	1:B:1060:GLU:HG3	2.19	0.43
1:B:503:ARG:O	5:D:101[A]:AKE:H22	2.18	0.43
1:A:752:ARG:HH11	1:A:758:VAL:HG21	1.83	0.43
1:A:1063:LYS:HG3	1:A:1140:TYR:CD1	2.54	0.43
1:A:455:PRO:O	1:A:456:LYS:HB2	2.18	0.43
1:B:1082:GLU:OE1	1:B:1082:GLU:N	2.41	0.43
1:B:648:GLU:O	1:B:707:LYS:NZ	2.52	0.42
1:A:785:VAL:O	1:A:789:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:PHE:HB3	1:B:711:TYR:CE1	2.55	0.42
1:A:820[B]:ARG:HD2	6:B:1544:HOH:O	2.20	0.42
1:A:864:VAL:HG12	6:A:1401:HOH:O	2.20	0.41
1:B:1154:VAL:O	1:B:1158:ILE:HG12	2.20	0.41
1:B:522:GLU:OE1	5:D:101[A]:AKE:H26	2.19	0.41
6:B:1508:HOH:O	3:F:10:DG:H5'	2.20	0.41
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	2.03	0.41
1:A:684:PHE:HB2	1:A:720:ILE:HD11	2.03	0.41
1:B:1030:THR:HB	1:B:1032[A]:GLN:OE1	2.21	0.41
1:B:1152:GLU:HB2	6:B:1466:HOH:O	2.21	0.41
1:A:472:THR:HB	1:A:497:TYR:CD1	2.56	0.41
1:A:731:ILE:HA	1:A:732:PRO:HD3	1.81	0.40
1:A:1101:ASP:HA	1:A:1102:PRO:HD3	1.85	0.40
1:B:1036:LYS:HE3	1:B:1040:ASP:OD2	2.22	0.40
1:B:680:TRP:CE2	1:B:720:ILE:HD12	2.56	0.40

There are no symmetry-related clashes.

## 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	A	667/803 (83%)	640 (96%)	25 (4%)	2 (0%)	44 73
1	B	664/803 (83%)	635 (96%)	27 (4%)	2 (0%)	44 73
All	All	1331/1606 (83%)	1275 (96%)	52 (4%)	4 (0%)	44 73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	579	SER
1	A	540	ASP
1	B	848	ASP

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Mol	Chain	Res	Type
1	A	852	VAL

### 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	A	594/704 (84%)	589 (99%)	5 (1%)	85	95
1	B	593/704 (84%)	584 (98%)	9 (2%)	70	90
All	All	1187/1408 (84%)	1173 (99%)	14 (1%)	78	92

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

Mol	Chain	Res	Type
1	A	528	LYS
1	A	546	THR
1	A	696	LEU
1	A	766	SER
1	A	847	ASP
1	B	479	ASP
1	B	480	SER
1	B	579	SER
1	B	746	LEU
1	B	858	ILE
1	B	880[A]	LEU
1	B	880[B]	LEU
1	B	945	ARG
1	B	989	THR

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 [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	AKE	D	101[A]	-	32,32,32	2.03	7 (21%)	40,42,42	1.10	3 (7%)
5	AKE	D	101[B]	-	32,32,32	2.06	7 (21%)	40,42,42	1.15	4 (10%)
5	AKE	F	101[A]	-	32,32,32	2.03	7 (21%)	40,42,42	1.12	4 (10%)
5	AKE	F	101[B]	-	32,32,32	2.06	7 (21%)	40,42,42	1.18	5 (12%)

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	AKE	D	101[A]	-	-	0/14/30/30	0/3/3/3
5	AKE	D	101[B]	-	-	0/14/30/30	0/3/3/3
5	AKE	F	101[A]	-	-	0/14/30/30	0/3/3/3
5	AKE	F	101[B]	-	-	0/14/30/30	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	101[A]	AKE	C11-C09	-2.43	1.41	1.47
5	D	101[B]	AKE	C11-C09	-2.31	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101[B]	AKE	C11-C09	-2.31	1.42	1.47
5	F	101[A]	AKE	C11-C09	-2.08	1.42	1.47
5	D	101[A]	AKE	C11-C12	2.21	1.46	1.41
5	F	101[A]	AKE	C11-C12	2.28	1.46	1.41
5	F	101[B]	AKE	C11-C12	2.36	1.46	1.41
5	D	101[B]	AKE	C11-C12	2.43	1.46	1.41
5	F	101[B]	AKE	C06-C07	2.93	1.44	1.38
5	D	101[A]	AKE	C06-C07	2.96	1.44	1.38
5	D	101[B]	AKE	C06-C07	2.98	1.44	1.38
5	F	101[A]	AKE	C06-C07	3.18	1.45	1.38
5	D	101[A]	AKE	C12-N13	3.44	1.47	1.37
5	F	101[B]	AKE	C12-N13	3.66	1.47	1.37
5	F	101[A]	AKE	C12-N13	3.68	1.47	1.37
5	D	101[B]	AKE	C12-N13	3.74	1.47	1.37
5	F	101[A]	AKE	C22-N23	4.73	1.50	1.37
5	D	101[A]	AKE	C22-N23	4.76	1.50	1.37
5	D	101[B]	AKE	C22-N23	5.09	1.51	1.37
5	F	101[B]	AKE	C22-N23	5.10	1.51	1.37
5	D	101[A]	AKE	C20-C21	5.11	1.47	1.38
5	F	101[A]	AKE	C04-C03	5.13	1.48	1.39
5	D	101[B]	AKE	C04-C03	5.18	1.48	1.39
5	F	101[B]	AKE	C04-C03	5.20	1.48	1.39
5	D	101[B]	AKE	C20-C21	5.29	1.48	1.38
5	F	101[B]	AKE	C20-C21	5.29	1.48	1.38
5	F	101[A]	AKE	C20-C21	5.29	1.48	1.38
5	D	101[A]	AKE	C04-C03	5.55	1.48	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101[A]	AKE	C11-C12-N13	-2.42	118.51	121.35
5	D	101[A]	AKE	C30-C22-N23	-2.32	118.63	121.35
5	D	101[A]	AKE	C25-C24-N23	2.04	115.71	111.34
5	F	101[B]	AKE	C14-C15-N16	2.05	117.94	111.64
5	F	101[A]	AKE	O19-C18-C17	2.06	119.12	111.57
5	D	101[A]	AKE	O19-C18-C17	2.11	119.32	111.57
5	F	101[A]	AKE	C15-C14-N13	2.15	115.94	111.34
5	F	101[B]	AKE	C24-C25-N26	2.19	118.36	111.64
5	F	101[B]	AKE	O29-C28-C27	2.19	119.62	111.57
5	D	101[B]	AKE	C14-C15-N16	2.28	118.61	111.64
5	D	101[B]	AKE	O19-C18-C17	2.45	120.57	111.57
5	D	101[B]	AKE	C15-C14-N13	2.47	116.62	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101[B]	AKE	C25-C24-N23	2.90	117.54	111.34
5	F	101[A]	AKE	C25-C24-N23	2.94	117.64	111.34
5	F	101[B]	AKE	C15-C14-N13	2.97	117.69	111.34
5	F	101[B]	AKE	C25-C24-N23	3.05	117.87	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	101[A]	AKE	5	0
5	F	101[A]	AKE	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

### 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	A	664/803 (82%)	-0.37	26 (3%) 40 39	20, 42, 85, 116	0
1	B	664/803 (82%)	-0.43	11 (1%) 70 72	22, 39, 80, 112	0
2	C	8/8 (100%)	-0.36	1 (12%) 4 3	27, 30, 54, 86	0
2	E	8/8 (100%)	-0.49	1 (12%) 4 3	25, 28, 48, 87	0
3	D	12/12 (100%)	-0.88	0 100 100	25, 31, 36, 41	0
3	F	12/12 (100%)	-0.76	0 100 100	29, 35, 45, 65	0
All	All	1368/1646 (83%)	-0.41	39 (2%) 52 52	20, 40, 84, 116	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	645	ALA	4.4
1	B	693	LEU	4.3
1	B	592	PRO	4.3
1	A	1201	ASP	4.1
1	B	1201	ASP	4.0
1	B	692	ARG	3.9
1	A	849	ASN	3.6
1	A	542	GLU	3.5
1	B	644	PHE	3.4
2	C	1	DA	3.2
1	A	490	GLY	3.1
1	A	848	ASP	3.1
1	A	696	LEU	3.0
1	A	491	VAL	3.0
1	A	692	ARG	2.8
1	B	848	ASP	2.8
1	A	695	GLY	2.6
1	B	849	ASN	2.6
1	A	646	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	693	LEU	2.5
1	A	539	ASP	2.5
1	A	466	LYS	2.5
1	A	649	ARG	2.5
1	A	540	ASP	2.4
1	A	568	LEU	2.4
1	B	846	TYR	2.4
1	B	694	HIS	2.4
1	A	657	ALA	2.2
1	A	484	LEU	2.2
1	A	586	LEU	2.2
2	E	1	DA	2.2
1	B	690	GLN	2.2
1	A	567	GLY	2.1
1	A	492	ILE	2.1
1	A	514	HIS	2.1
1	A	570	ILE	2.1
1	A	1108	GLU	2.0
1	A	645	ALA	2.0
1	A	1110	GLN	2.0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	A	1302	1/1	0.96	0.23	1.92	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	AKE	F	101[B]	30/30	0.97	0.16	0.94	27,31,42,46	30
5	AKE	F	101[A]	30/30	0.97	0.16	0.88	26,31,43,52	6
5	AKE	D	101[B]	30/30	0.97	0.14	0.45	16,28,41,47	30
5	AKE	D	101[A]	30/30	0.97	0.14	0.43	21,27,41,51	6
4	MG	B	1302	1/1	0.98	0.14	-0.53	55,55,55,55	0
4	MG	D	102	1/1	0.98	0.07	-1.75	55,55,55,55	0
4	MG	F	102	1/1	0.99	0.05	-	41,41,41,41	0
4	MG	A	1301	1/1	0.97	0.07	-	34,34,34,34	0
4	MG	B	1301	1/1	0.98	0.08	-	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.