



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 07:04 pm GMT

PDB ID : 366D  
Title : 1.3 Å STRUCTURE DETERMINATION OF THE D(CG(5-BRU)ACG)2/6-BROMO-9-AMINO-DACA COMPLEX  
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Deposited on : 1997-12-19  
Resolution : 1.30 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](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

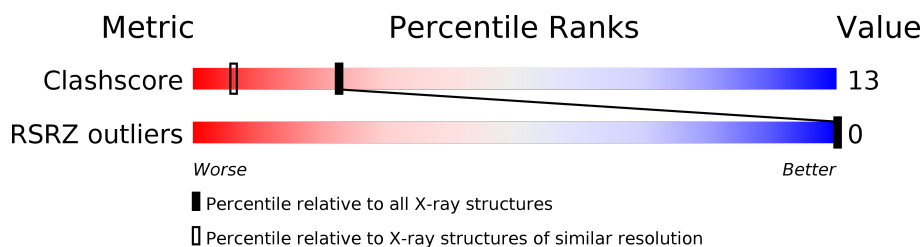
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 1.30 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1185 (1.32-1.28)
RSRZ outliers	101464	1133 (1.32-1.28)

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	6	 83% 17%

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DA6	A	3013	-	-	-	X

## 2 Entry composition [i](#)

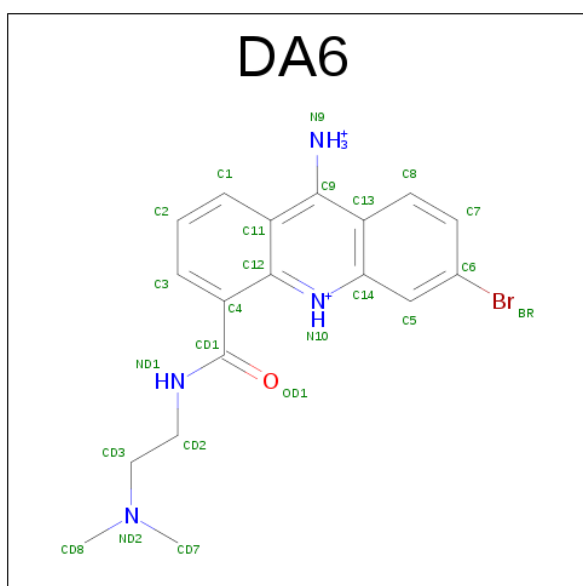
There are 3 unique types of molecules in this entry. The entry contains 336 atoms, of which 115 are hydrogens and 0 are deuteriums.

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 DNA chain called DNA (5'-D(\*CP\*GP\*(BRU)P\*AP\*CP\*G)-3').

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	6	Total	Br	C	H	N	O	P	0	2	0
			217	2	66	74	25	43	7			

- Molecule 2 is 6-BROMO-9-AMINO-N-ETHYL(DIAMINOMETHYL)ACRIDINE-4-CARB OXAMIDE (three-letter code: DA6) (formula: C<sub>18</sub>H<sub>21</sub>BrN<sub>4</sub>O).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	H	N	O		0	0
			45	1	18	21	4	1			
2	A	1	Total	Br	C	H	N	O		0	0
			44	1	18	20	4	1			


- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		

### 3 Residue-property plots

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 (5'-D(\*CP\*GP\*(BRU)P\*AP\*CP\*G)-3')

Chain A:  83% 17%

G1001
G1002
U1003
A1004
C1005
G1006

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	30.11Å 30.11Å 39.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.30 7.96 – 1.30	Depositor EDS
% Data completeness (in resolution range)	90.2 (8.00-1.30) 94.9 (7.96-1.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 1.30Å)	Xtriage
Refinement program	SHELXL-96	Depositor
R, $R_{free}$	0.185 , (Not available) 0.204 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	14.8	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.46 , 96.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.109 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	336	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.00% 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: DA6, BRU

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	2.68	8/135 (5.9%)	3.21	27/204 (13.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1002	DG	O4'-C1'	7.80	1.51	1.42
1	A	1006	DG	N9-C8	6.94	1.42	1.37
1	A	1004[A]	DA	P-OP1	6.89	1.60	1.49
1	A	1004[B]	DA	P-OP1	6.89	1.60	1.49
1	A	1006	DG	P-OP1	6.65	1.60	1.49
1	A	1001	DC	C2'-C1'	-5.88	1.46	1.52
1	A	1002	DG	N9-C8	-5.71	1.33	1.37
1	A	1006	DG	P-O5'	-5.68	1.54	1.59

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1004[A]	DA	O4'-C1'-N9	-10.64	100.55	108.00
1	A	1004[B]	DA	O4'-C1'-N9	-10.64	100.55	108.00
1	A	1005	DC	C6-N1-C2	10.37	124.45	120.30
1	A	1005	DC	C5-C6-N1	-9.60	116.20	121.00
1	A	1006	DG	O4'-C1'-N9	-9.48	101.36	108.00
1	A	1002	DG	O4'-C1'-N9	-9.34	101.47	108.00
1	A	1006	DG	C5-N7-C8	7.39	108.00	104.30
1	A	1004[A]	DA	C4-C5-C6	7.37	120.69	117.00
1	A	1004[B]	DA	C4-C5-C6	7.37	120.69	117.00
1	A	1006	DG	N7-C8-N9	-6.60	109.80	113.10
1	A	1004[A]	DA	O5'-P-OP2	6.38	118.36	110.70
1	A	1004[B]	DA	O5'-P-OP2	6.38	118.36	110.70
1	A	1001	DC	C4-C5-C6	-6.19	114.30	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1001	DC	N3-C4-C5	5.97	124.29	121.90
1	A	1002	DG	C8-N9-C4	-5.95	104.02	106.40
1	A	1001	DC	N1-C1'-C2'	5.90	123.80	112.60
1	A	1006	DG	C5-C6-N1	5.71	114.36	111.50
1	A	1002	DG	C4-C5-C6	5.61	122.17	118.80
1	A	1005	DC	O4'-C1'-C2'	-5.54	101.47	105.90
1	A	1002	DG	N1-C6-O6	5.53	123.22	119.90
1	A	1001	DC	C5-C4-N4	-5.41	116.41	120.20
1	A	1001	DC	O4'-C4'-C3'	-5.35	102.36	104.50
1	A	1004[A]	DA	C2-N3-C4	5.24	113.22	110.60
1	A	1004[B]	DA	C2-N3-C4	5.24	113.22	110.60
1	A	1005	DC	N3-C4-C5	5.12	123.95	121.90
1	A	1001	DC	C2-N3-C4	5.06	122.43	119.90
1	A	1001	DC	N1-C2-N3	-5.04	115.67	119.20

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	143	74	64	4	0
2	A	48	41	42	3	0
3	A	30	0	0	1	0
All	All	221	115	106	4	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 13.

All (4) 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:A:1003[B]:BRU:H4'	3:A:4030:HOH:O	1.94	0.66
1:A:1006:DG:N7	2:A:3015:DA6:HD21	2.12	0.65
1:A:1006:DG:C5	2:A:3015:DA6:HD21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:DG:C6	2:A:3015:DA6:HD21	2.55	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 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
1	BRU	A	1003[A]	1	12,21,22	1.84	3 (25%)	14,30,33	3.19	5 (35%)
1	BRU	A	1003[B]	1	12,21,22	1.70	2 (16%)	14,30,33	2.79	5 (35%)

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
1	BRU	A	1003[A]	1	-	0/3/21/22	0/2/2/2
1	BRU	A	1003[B]	1	-	0/3/21/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1003[B]	BRU	O5'-C5'	-4.65	1.38	1.44
1	A	1003[A]	BRU	O5'-C5'	-4.13	1.39	1.44
1	A	1003[A]	BRU	C4-N3	2.44	1.40	1.36
1	A	1003[B]	BRU	O4'-C1'	2.89	1.48	1.42
1	A	1003[A]	BRU	O4'-C1'	3.42	1.50	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003[A]	BRU	O4'-C1'-N1	-8.03	94.24	107.78
1	A	1003[B]	BRU	O4'-C1'-N1	-7.19	95.66	107.78
1	A	1003[A]	BRU	BR-C5-C4	-4.94	114.00	121.50
1	A	1003[B]	BRU	BR-C5-C4	-4.66	114.43	121.50
1	A	1003[A]	BRU	O4'-C1'-C2'	-3.44	99.65	106.25
1	A	1003[B]	BRU	O4'-C1'-C2'	-2.77	100.93	106.25
1	A	1003[A]	BRU	O3'-C3'-C4'	-2.28	101.14	110.13
1	A	1003[B]	BRU	C5-C6-N1	2.04	122.55	119.56
1	A	1003[B]	BRU	C2'-C1'-N1	4.52	124.90	114.23
1	A	1003[A]	BRU	C2'-C1'-N1	5.67	127.63	114.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1003[B]	BRU	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DA6	A	3013	-	26,26,26	3.28	12 (46%)	33,37,37	2.27	7 (21%)
2	DA6	A	3015	-	26,26,26	3.40	13 (50%)	33,37,37	4.07	13 (39%)

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	DA6	A	3013	-	-	0/10/10/10	0/3/3/3
2	DA6	A	3015	-	-	0/10/10/10	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3013	DA6	C2-C3	-7.44	1.24	1.38
2	A	3015	DA6	CD8-ND2	-6.59	1.25	1.46
2	A	3013	DA6	BR-C6	-6.50	1.76	1.90
2	A	3015	DA6	C13-C14	-5.00	1.33	1.41
2	A	3015	DA6	BR-C6	-4.74	1.80	1.90
2	A	3013	DA6	C4-CD1	-4.66	1.42	1.50
2	A	3013	DA6	C4-C12	-4.48	1.38	1.43
2	A	3015	DA6	CD3-CD2	-2.65	1.44	1.51
2	A	3015	DA6	CD2-ND1	-2.65	1.40	1.46
2	A	3015	DA6	C9-C13	-2.54	1.38	1.43
2	A	3013	DA6	C9-C13	-2.24	1.39	1.43
2	A	3013	DA6	C1-C11	-2.23	1.37	1.42
2	A	3015	DA6	CD3-ND2	2.13	1.54	1.46
2	A	3015	DA6	C5-C14	2.21	1.45	1.39
2	A	3015	DA6	C2-C1	2.30	1.42	1.36
2	A	3015	DA6	C8-C7	2.32	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3013	DA6	C11-C12	3.06	1.46	1.41
2	A	3013	DA6	CD2-ND1	3.29	1.53	1.46
2	A	3013	DA6	CD3-CD2	3.48	1.62	1.51
2	A	3013	DA6	C13-C14	3.49	1.47	1.41
2	A	3013	DA6	C3-C4	3.88	1.45	1.38
2	A	3015	DA6	CD7-ND2	4.47	1.60	1.46
2	A	3015	DA6	C12-N10	7.12	1.44	1.37
2	A	3013	DA6	CD1-ND1	7.24	1.49	1.33
2	A	3015	DA6	OD1-CD1	9.05	1.42	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3013	DA6	OD1-CD1-ND1	-7.00	108.12	122.59
2	A	3015	DA6	OD1-CD1-ND1	-6.91	108.31	122.59
2	A	3013	DA6	CD3-CD2-ND1	-6.83	99.27	111.67
2	A	3015	DA6	C8-C13-C9	-6.77	113.47	122.83
2	A	3015	DA6	C12-N10-C14	-4.40	115.69	122.92
2	A	3015	DA6	C7-C8-C13	-4.26	115.32	121.14
2	A	3015	DA6	OD1-CD1-C4	-3.67	116.39	121.66
2	A	3013	DA6	OD1-CD1-C4	-3.40	116.77	121.66
2	A	3015	DA6	BR-C6-C7	-2.25	115.95	119.30
2	A	3013	DA6	C13-C9-N9	-2.06	118.38	120.59
2	A	3013	DA6	C1-C11-C9	2.16	125.81	122.83
2	A	3015	DA6	C13-C14-N10	2.22	123.55	120.27
2	A	3015	DA6	C7-C6-C5	2.26	124.22	121.98
2	A	3013	DA6	C13-C9-C11	2.59	121.65	118.73
2	A	3015	DA6	C9-C13-C14	3.21	121.83	118.99
2	A	3013	DA6	C8-C13-C9	3.50	127.67	122.83
2	A	3015	DA6	C8-C13-C14	4.91	124.70	117.62
2	A	3015	DA6	CD8-ND2-CD7	6.38	126.83	109.72
2	A	3015	DA6	CD3-CD2-ND1	10.77	131.22	111.67
2	A	3015	DA6	C4-CD1-ND1	13.31	135.29	116.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3015	DA6	3	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	5/6 (83%)	-0.02	0 <a href="#">100</a> <a href="#">100</a>	16, 16, 19, 20	0

There are no RSRZ outliers to report.

### 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. 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
1	BRU	A	1003[A]	20/21	0.93	0.13	-	14,22,30,34	29
1	BRU	A	1003[B]	20/21	0.93	0.13	-	14,21,27,31	29

### 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( $\text{\AA}^2$ )	Q<0.9
2	DA6	A	3013	24/24	0.92	0.13	7.48	17,25,44,53	20
2	DA6	A	3015	24/24	0.76	0.19	-	1,21,43,45	44

## 6.5 Other polymers [i](#)

There are no such residues in this entry.