



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 01:12 PM EDT

PDB ID : 6U7T / pdb_00006u7t
Title : MutY adenine glycosylase bound to DNA containing a transition state analog (1N) paired with d(8-oxo-G)
Authors : O'Shea Murray, V.L.; Cao, S.; Horvath, M.P.; David, S.S.
Deposited on : 2019-09-03
Resolution : 2.00 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

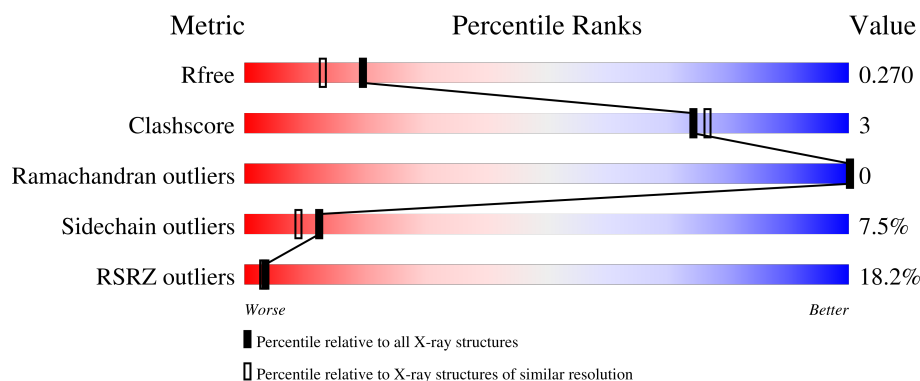
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 ≥ 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	366	18% 83% 12% • 5%
2	B	11	91% 9%
3	C	11	82% 9% 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6145 atoms, of which 2893 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 Adenine DNA glycosylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	349	Total	C	H	N	O	S	0	2	0
			5402	1766	2656	469	500	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	PRO	ARG	variant	UNP P83847
A	366	PRO	ASP	variant	UNP P83847

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	11	Total	C	H	N	O	P	0	0	0
			352	108	124	48	62	10			

- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*TP*CP*CP*AP*(NR1)P*GP*TP*CP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	10	Total	C	H	N	O	P	0	0	0
			306	92	113	31	60	10			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		

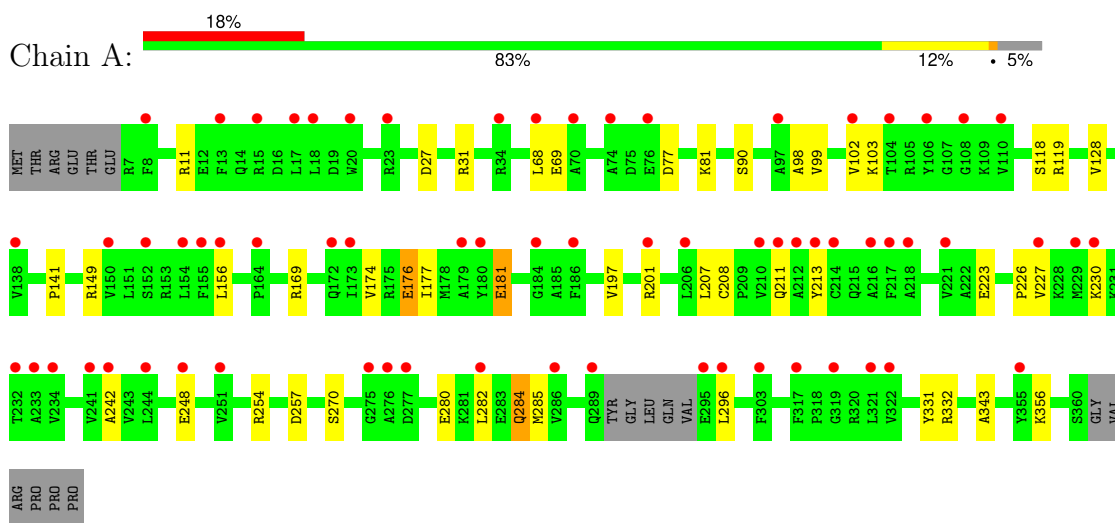
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	45	Total	O	0	0
			45	45		
6	B	16	Total	O	0	0
			16	16		
6	C	14	Total	O	0	0
			14	14		

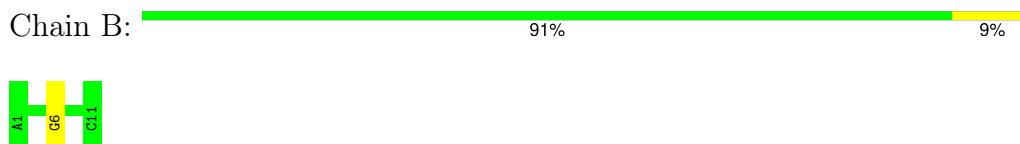
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

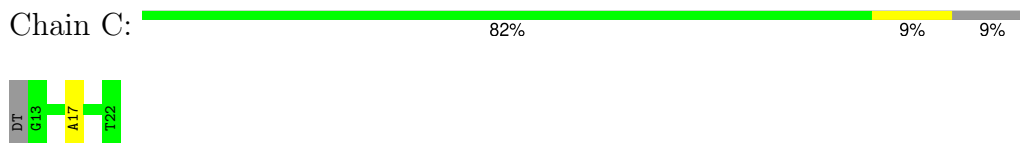
- Molecule 1: Adenine DNA glycosylase



- Molecule 2: DNA (5'-D(*AP*AP*GP*AP*CP*(8OG)P*TP*GP*GP*AP*C)-3')



- Molecule 3: DNA (5'-D(P*GP*TP*CP*CP*AP*(NR1)P*GP*TP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	37.80Å 86.49Å 140.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.33 – 2.00 41.33 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (41.33-2.00) 94.1 (41.33-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15rc2_3428	Depositor
R, R_{free}	0.261 , 0.270 0.262 , 0.270	Depositor DCC
R_{free} test set	1456 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6145	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NRI, SF4, 8OG, CA

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	0.19	0/2826	0.38	0/3850
2	B	0.26	0/230	0.54	0/351
3	C	0.30	0/201	0.63	0/305
All	All	0.21	0/3257	0.41	0/4506

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

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	2746	2656	2649	19	1
2	B	228	124	124	0	0
3	C	193	113	112	1	0
4	A	8	0	0	1	0
5	A	2	0	0	0	0
6	A	45	0	0	0	0
6	B	16	0	0	0	0
6	C	14	0	0	0	0
All	All	3252	2893	2885	19	1

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.

All (19) 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:98:ALA:O	1:A:102:VAL:HG23	2.07	0.53
1:A:181:GLU:N	1:A:181:GLU:OE2	2.44	0.51
1:A:176:GLU:HG2	1:A:177:ILE:HG23	1.91	0.51
1:A:181:GLU:CD	1:A:181:GLU:H	2.20	0.50
1:A:197:VAL:HG11	1:A:208:CYS:HA	1.94	0.49
1:A:211:GLN:HA	4:A:401:SF4:S3	2.52	0.49
1:A:141:PRO:HB3	1:A:174:VAL:HG11	1.96	0.47
1:A:242:ALA:HB2	1:A:282:LEU:HD22	1.95	0.46
1:A:257:ASP:OD1	1:A:257:ASP:N	2.48	0.46
1:A:285:MET:HE1	1:A:331:TYR:OH	2.16	0.46
1:A:149:ARG:NH1	3:C:17:DA:OP1	2.48	0.46
1:A:77:ASP:OD1	1:A:77:ASP:N	2.50	0.45
1:A:68:LEU:C	1:A:68:LEU:HD23	2.42	0.44
1:A:81:LYS:HA	1:A:343:ALA:HB2	1.99	0.44
1:A:69:GLU:HG3	1:A:103:LYS:HG3	2.02	0.42
1:A:149:ARG:HG3	1:A:226:PRO:HD3	2.01	0.41
1:A:254:ARG:NH2	1:A:270:SER:O	2.53	0.41
1:A:284:GLN:HG3	1:A:285:MET:N	2.36	0.40
1:A:207:LEU:O	1:A:208:CYS:C	2.65	0.40

All (1) 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)
1:A:230:LYS:HZ3	1:A:248:GLU:OE2[3_645]	1.57	0.03

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	347/366 (95%)	337 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	282/313 (90%)	261 (93%)	21 (7%)	13	9

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	27	ASP
1	A	31	ARG
1	A	90	SER
1	A	99	VAL
1	A	118	SER
1	A	119	ARG
1	A	128	VAL
1	A	156	LEU
1	A	169	ARG
1	A	176	GLU
1	A	181	GLU
1	A	201	ARG
1	A	213	TYR
1	A	223	GLU
1	A	227	VAL
1	A	280	GLU
1	A	284	GLN
1	A	296	LEU
1	A	332	ARG
1	A	356	LYS

Sometimes 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 ⓘ

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	$\# Z > 2$
3	NRI	C	18	3	7,11,12	0.59	0	3,14,17	0.64	0
2	8OG	B	6	2	22,25,26	0.61	0	26,37,40	1.03	3 (11%)

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
3	NRI	C	18	3	-	0/3/15/16	0/1/1/1
2	8OG	B	6	2	-	1/7/21/22	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	8OG	N7-C8-N9	3.06	110.02	106.61
2	B	6	8OG	C5-N7-C8	-2.40	106.16	109.47
2	B	6	8OG	C4-C5-N7	2.01	109.75	106.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	6	8OG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	SF4	A	401	1	0,12,12	-	-	-		

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
4	SF4	A	401	1	-	-	0/6/5/5

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	SF4	1	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, 95th 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 ²)	Q<0.9
1	A	349/366 (95%)	1.23	67 (19%) 3 3	20, 52, 71, 107	1 (0%)
2	B	10/11 (90%)	0.09	0 100 100	26, 39, 53, 59	0
3	C	9/11 (81%)	-0.14	0 100 100	24, 31, 50, 57	0
All	All	368/388 (94%)	1.17	67 (18%) 3 3	20, 52, 70, 107	1 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	5.0
1	A	286	VAL	4.1
1	A	213	TYR	4.1
1	A	108	GLY	4.0
1	A	289	GLN	4.0
1	A	275	GLY	4.0
1	A	106	TYR	3.9
1	A	217	PHE	3.8
1	A	295	GLU	3.4
1	A	155	PHE	3.3
1	A	201	ARG	3.2
1	A	68	LEU	3.1
1	A	17	LEU	3.1
1	A	214	CYS	3.0
1	A	102	VAL	3.0
1	A	296	LEU	3.0
1	A	218	ALA	2.9
1	A	110	VAL	2.9
1	A	227	VAL	2.9
1	A	282	LEU	2.8
1	A	212	ALA	2.8
1	A	229	MET	2.8
1	A	15	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	13	PHE	2.8
1	A	184	GLY	2.8
1	A	156	LEU	2.8
1	A	172	GLN	2.7
1	A	242	ALA	2.6
1	A	70	ALA	2.6
1	A	206	LEU	2.6
1	A	210	VAL	2.6
1	A	230	LYS	2.6
1	A	152	SER	2.6
1	A	321	LEU	2.6
1	A	317	PHE	2.5
1	A	232	THR	2.5
1	A	303	PHE	2.5
1	A	74	ALA	2.4
1	A	319	GLY	2.4
1	A	211	GLN	2.4
1	A	138	VAL	2.4
1	A	355	TYR	2.3
1	A	104	THR	2.3
1	A	8	PHE	2.3
1	A	322	VAL	2.3
1	A	97	ALA	2.3
1	A	180	TYR	2.3
1	A	233	ALA	2.2
1	A	18	LEU	2.2
1	A	234	VAL	2.2
1	A	179	ALA	2.2
1	A	277	ASP	2.2
1	A	221	VAL	2.2
1	A	241	VAL	2.2
1	A	76	GLU	2.1
1	A	173	ILE	2.1
1	A	150	VAL	2.1
1	A	216	ALA	2.1
1	A	248	GLU	2.1
1	A	164	PRO	2.1
1	A	34	ARG	2.1
1	A	251	VAL	2.1
1	A	186	PHE	2.1
1	A	20	TRP	2.1
1	A	154	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	244	LEU	2.0
1	A	23	ARG	2.0

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, 95th 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 ²)	Q<0.9
2	8OG	B	6	23/24	0.97	0.06	16,24,34,35	0
3	NRI	C	18	11/12	0.98	0.06	16,21,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
5	CA	A	403	1/1	0.91	0.09	61,61,61,61	0
5	CA	A	402	1/1	0.94	0.06	38,38,38,38	0
4	SF4	A	401	8/8	0.97	0.06	37,45,49,50	1

6.5 Other polymers [i](#)

There are no such residues in this entry.