



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 02:12 PM EDT

PDB ID : 3CWA
Title : Crystal Structure of an AlkA Host/Guest Complex 8oxoGuanine:Cytosine Base Pair
Authors : Bowman, B.R.; Lee, S.; Wang, S.; Verdine, G.L.
Deposited on : unknown
Resolution : 2.40 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20030345
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) : rb-20030345

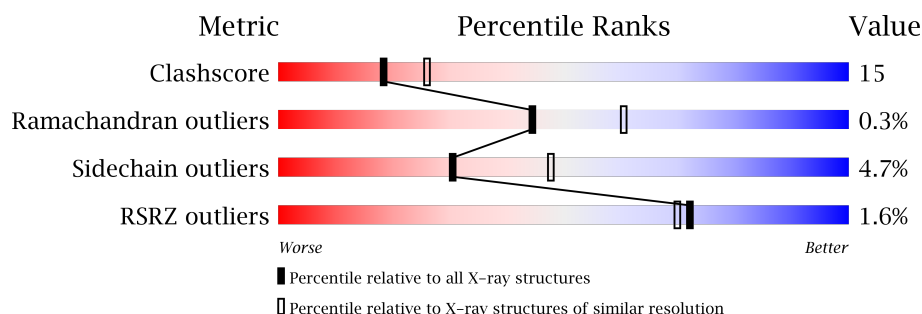
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 ≥ 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	282	 80% 18% .
1	B	282	 3% 74% 25% .
1	C	282	 1% 68% 29% .
1	D	282	 1% 73% 24% .
2	E	12	 17% 25% 58% 17%
2	G	12	 42% 58%
3	F	12	 17% 17% 83%

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Mol	Chain	Length	Quality of chain
3	H	12	 75% 25%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9900 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-3-methyladenine glycosylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	B	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	C	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			
1	D	282	Total	C	N	O	S	0	0	0
			2215	1427	387	389	12			

- Molecule 2 is a DNA chain called DNA (5'-D(*(8OG)P*DAP*DCP*DAP*DTP*DGP*DA P*DGP*DTP*DGP*DCP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			246	117	48	70	11			

- Molecule 3 is a DNA chain called DNA (5'-D(*DGP*DGP*DCP*DAP*DCP*DTP*DCP* DAP*DTP*DGP*DTP*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			
3	H	12	Total	C	N	O	P	0	0	0
			241	116	43	71	11			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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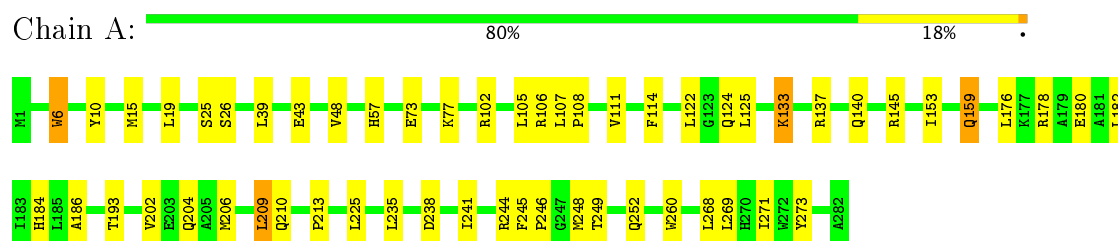
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	15	Total 15	O 15	0	0
4	C	16	Total 16	O 16	0	0
4	D	17	Total 17	O 17	0	0
4	H	1	Total 1	O 1	0	0

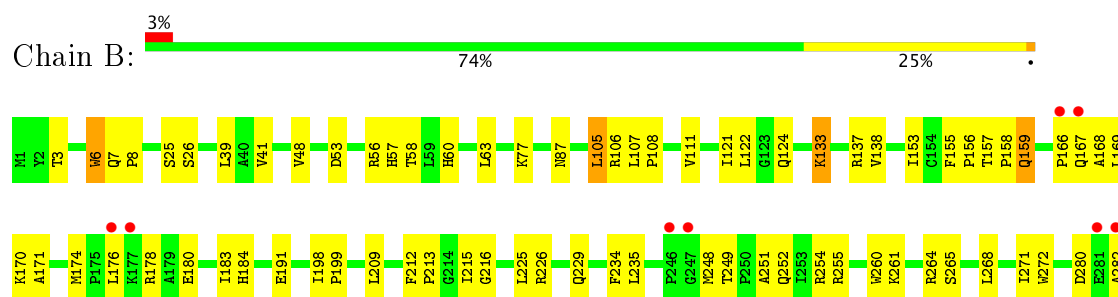
3 Residue-property plots [i](#)

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.

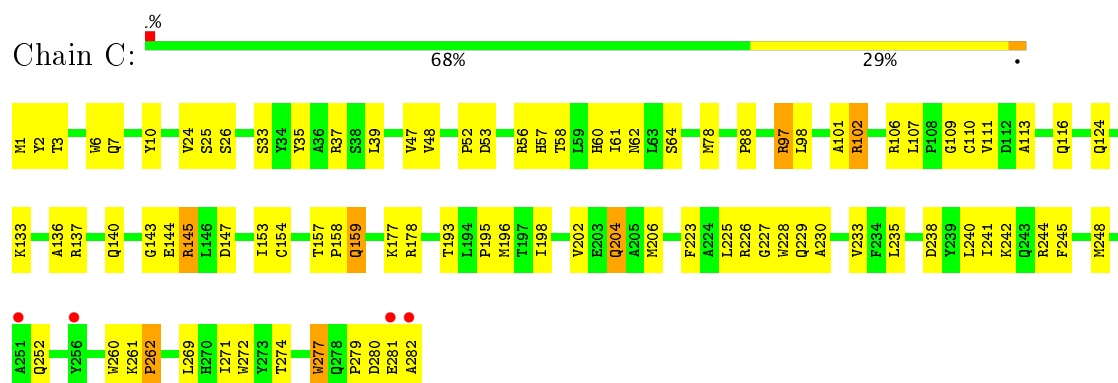
• Molecule 1: DNA-3-methyladenine glycosylase 2



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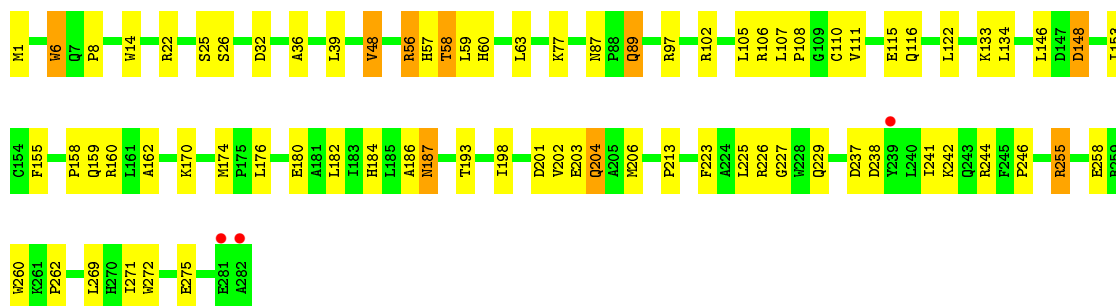


• Molecule 1: DNA-3-methyladenine glycosylase 2



• Molecule 1: DNA-3-methyladenine glycosylase 2





- Molecule 2: DNA (5'-D(*(8OG)P*DAP*DCP*DAP*DTP*DGP*DAP*DGP*DTP*DGP*DCP*DC)-3')



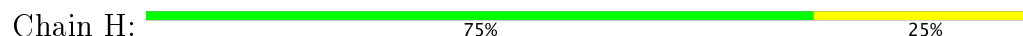
- Molecule 2: DNA (5'-D(*(8OG)P*DAP*DCP*DAP*DTP*DGP*DAP*DGP*DTP*DGP*DCP*DC)-3')



- Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DCP*DTP*DCP*DAP*DTP*DGP*DTP*D C)-3')



- Molecule 3: DNA (5'-D(*DGP*DGP*DCP*DAP*DCP*DTP*DCP*DAP*DTP*DGP*DTP*D C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.43Å 101.43Å 102.57Å 90.00° 94.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 45.66 – 2.37	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.40) 92.4 (45.66-2.37)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.37Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.260 0.222 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9900	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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: 8OG

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	0.37	0/2277	0.60	0/3104
1	B	0.37	0/2277	0.59	0/3104
1	C	0.37	0/2277	0.58	0/3104
1	D	0.39	0/2277	0.59	0/3104
2	E	0.94	1/253 (0.4%)	1.10	0/388
2	G	0.44	0/253	0.80	0/388
3	F	0.84	0/269	1.08	0/413
3	H	0.40	0/269	0.71	0/413
All	All	0.42	1/10152 (0.0%)	0.64	0/14018

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
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	10	DG	N9-C4	8.20	1.44	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	6	DG	Sidechain

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	2215	0	2209	47	0
1	B	2215	0	2209	77	0
1	C	2215	0	2209	68	0
1	D	2215	0	2209	53	0
2	E	246	0	135	11	0
2	G	246	0	135	10	0
3	F	241	0	137	28	0
3	H	241	0	137	5	0
4	A	17	0	0	0	0
4	B	15	0	0	0	0
4	C	16	0	0	1	0
4	D	17	0	0	0	0
4	H	1	0	0	0	0
All	All	9900	0	9380	287	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 15.

The worst 5 of 287 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:F:14:DG:C4'	3:F:15:DG:H5''	1.72	1.20
3:F:14:DG:H4'	3:F:15:DG:C5'	1.72	1.18
3:H:21:DA:H2''	3:H:22:DT:H5'	1.12	1.07
2:G:5:DT:H2''	2:G:6:DG:H5'	1.34	1.06
1:B:77:LYS:HB3	1:B:111:VAL:HG23	1.34	1.04

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	280/282 (99%)	268 (96%)	12 (4%)	0	100	100
1	B	280/282 (99%)	262 (94%)	17 (6%)	1 (0%)	38	54
1	C	280/282 (99%)	262 (94%)	16 (6%)	2 (1%)	25	37
1	D	280/282 (99%)	268 (96%)	12 (4%)	0	100	100
All	All	1120/1128 (99%)	1060 (95%)	57 (5%)	3 (0%)	44	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	248	MET
1	C	277	TRP
1	C	281	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	A	222/222 (100%)	215 (97%)	7 (3%)	44	65
1	B	222/222 (100%)	216 (97%)	6 (3%)	50	71
1	C	222/222 (100%)	212 (96%)	10 (4%)	32	50
1	D	222/222 (100%)	203 (91%)	19 (9%)	12	18
All	All	888/888 (100%)	846 (95%)	42 (5%)	30	48

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	159	GLN
1	D	1	MET
1	D	255	ARG
1	C	204	GLN

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Mol	Chain	Res	Type
1	C	262	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	184	HIS
1	C	124	GLN
1	D	184	HIS
1	B	221	ASN
1	C	60	HIS

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
2	8OG	E	1	3,2	17,22,26	1.27	2 (11%)	22,33,40	2.51	5 (22%)
2	8OG	G	1	3,2	17,22,26	1.23	2 (11%)	22,33,40	2.47	5 (22%)

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	8OG	E	1	3,2	-	0/2/18/22	0/3/3/3
2	8OG	G	1	3,2	-	0/2/18/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	8OG	C8-N7	-3.29	1.30	1.34
2	E	1	8OG	C8-N7	-3.23	1.30	1.34
2	G	1	8OG	C6-N1	3.48	1.39	1.33
2	E	1	8OG	C6-N1	3.63	1.39	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	8OG	C5-C6-N1	-8.45	111.46	123.48
2	G	1	8OG	C5-C6-N1	-8.29	111.67	123.48
2	E	1	8OG	C2-N3-C4	-2.80	111.89	115.16
2	G	1	8OG	C2-N3-C4	-2.75	111.95	115.16
2	E	1	8OG	N3-C2-N1	-2.46	123.87	127.46

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	E	1	8OG	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	282/282 (100%)	-0.22	0 100 100	27, 45, 77, 101	0
1	B	282/282 (100%)	-0.13	8 (2%) 53 51	27, 47, 85, 130	0
1	C	282/282 (100%)	-0.14	4 (1%) 75 74	28, 46, 82, 157	0
1	D	282/282 (100%)	-0.10	3 (1%) 80 79	30, 46, 72, 143	0
2	E	11/12 (91%)	1.16	2 (18%) 1 1	58, 118, 149, 190	0
2	G	11/12 (91%)	-0.32	0 100 100	46, 67, 80, 89	0
3	F	12/12 (100%)	1.27	2 (16%) 2 2	78, 130, 143, 144	0
3	H	12/12 (100%)	-0.30	0 100 100	42, 60, 79, 85	0
All	All	1174/1176 (99%)	-0.12	19 (1%) 72 70	27, 47, 87, 190	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	282	ALA	7.4
1	D	282	ALA	5.6
1	C	281	GLU	4.3
2	E	12	DC	4.2
1	B	176	LEU	3.9

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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	8OG	G	1	20/24	0.91	0.16	-	77,83,88,90	0
2	8OG	E	1	20/24	0.89	0.15	-	77,83,88,90	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.