



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 12:39 am GMT

PDB ID : 3RB4
Title : Dpo4 extension ternary complex with 3'-terminal primer G base opposite the 3-methylcytosine (m3c) lesion
Authors : Rechkoblit, O.; Patel, D.J.
Deposited on : 2011-03-28
Resolution : 2.81 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 : 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

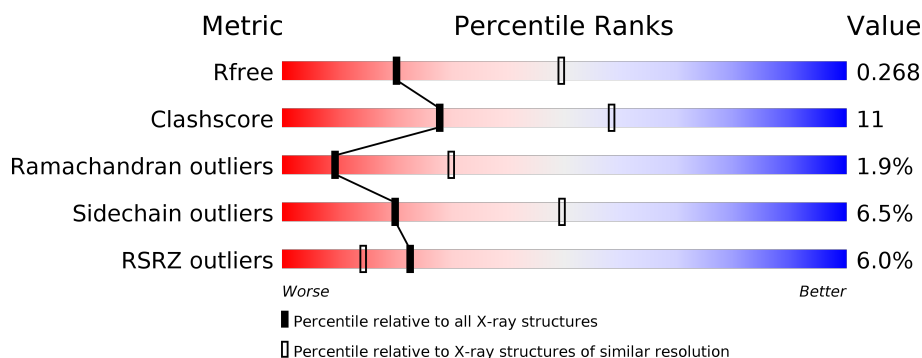
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	341	<div> <div>81%</div> <div>18%</div> <div>•</div> </div>
1	B	341	<div> <div>10%</div> <div>65%</div> <div>32%</div> <div>•</div> </div>
2	D	13	<div> <div>54%</div> <div>23%</div> <div>23%</div> </div>
2	H	13	<div> <div>15%</div> <div>15%</div> <div>62%</div> <div>23%</div> </div>
3	E	20	<div> <div>5%</div> <div>30%</div> <div>60%</div> <div>5%</div> <div>5%</div> </div>
3	J	20	<div> <div>35%</div> <div>20%</div> <div>30%</div> <div>10%</div> <div>40%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6700 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 polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2740	1757	472	505	6			
1	B	341	Total	C	N	O	S	0	0	0
			2740	1757	472	505	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q97W02
B	1001	GLY	-	EXPRESSION TAG	UNP Q97W02

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(DDG))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	13	Total	C	N	O	P	0	0	0
			272	130	53	77	12			
2	H	10	Total	C	N	O	P	0	0	0
			202	95	39	58	10			

- Molecule 3 is a DNA chain called DNA (5'-D(*C*CP*TP*AP*AP*CP*(ME6)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	19	Total	C	N	O	P	0	0	0
			374	181	66	109	18			
3	J	12	Total	C	N	O	P	0	0	0
			237	114	40	71	12			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Ca 3 3	0	0
5	A	3	Total Ca 3 3	0	0

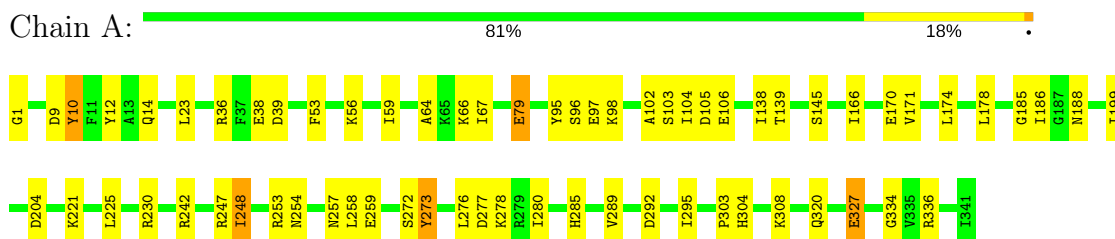
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	D	10	Total O 10 10	0	0
6	E	5	Total O 5 5	0	0
6	B	15	Total O 15 15	0	0
6	H	2	Total O 2 2	0	0

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 polymerase IV



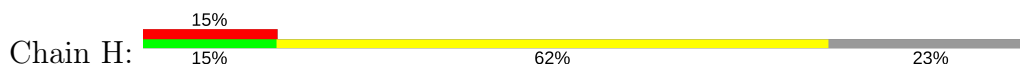
• Molecule 1: DNA polymerase IV

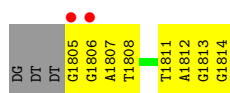


• Molecule 2: DNA (5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(DDG))-3')

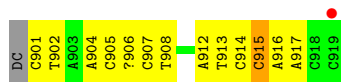


• Molecule 2: DNA (5'-D(*GP*TP*TP*GP*GP*AP*TP*GP*GP*TP*AP*GP*(DDG))-3')

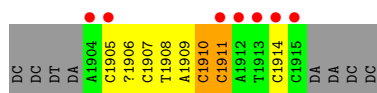




- Molecule 3: DNA (5'-D(*C*CP*TP*AP*AP*CP*(ME6)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*C)-3')



- Molecule 3: DNA (5'-D(*C*CP*TP*AP*AP*CP*(ME6)P*CP*TP*AP*CP*CP*AP*TP*CP*CP*AP*AP*CP*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	53.27Å 110.00Å 101.53Å 90.00° 101.35° 90.00°	Depositor
Resolution (Å)	20.00 – 2.81 19.99 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.81) 97.4 (19.99-2.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.205 , 0.256 0.215 , 0.268	Depositor DCC
R_{free} test set	1367 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6700	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ME6, DDG, DGT

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	0.54	0/2779	0.63	0/3731
1	B	0.35	0/2779	0.49	0/3731
2	D	0.83	0/282	1.96	11/436 (2.5%)
2	H	0.53	0/216	1.11	0/333
3	E	0.98	0/394	1.68	7/600 (1.2%)
3	J	0.61	0/240	1.24	2/363 (0.6%)
All	All	0.53	0/6690	0.85	20/9194 (0.2%)

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	803	DT	O3'-P-O5'	-11.87	81.44	104.00
3	E	901	DC	O4'-C1'-N1	-10.18	100.88	108.00
2	D	805	DG	O4'-C1'-N9	9.09	114.36	108.00
2	D	803	DT	O4'-C1'-N1	9.06	114.34	108.00
3	E	904	DA	O4'-C4'-C3'	-8.64	100.82	106.00

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	A	2740	0	2883	38	0
1	B	2740	0	2880	83	0
2	D	272	0	149	2	0
2	H	202	0	108	8	0
3	E	374	0	217	11	0
3	J	237	0	138	11	0
4	A	31	0	12	1	0
4	B	31	0	12	4	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	35	0	0	5	0
6	B	15	0	0	4	0
6	D	10	0	0	1	0
6	E	5	0	0	0	0
6	H	2	0	0	1	0
All	All	6700	0	6399	146	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 11.

The worst 5 of 146 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:14:GLN:HE22	1:A:139:THR:H	1.05	1.00
3:J:1905:DC:H2''	3:J:1906:ME6:H5'	1.50	0.91
1:A:277:ASP:O	1:A:278:LYS:HB2	1.76	0.86
1:B:1010:TYR:HD2	1:B:1048:TYR:HE1	1.27	0.82
1:B:1051:ARG:HH12	4:B:1414:DGT:PG	2.03	0.81

There are no symmetry-related clashes.

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	339/341 (99%)	322 (95%)	16 (5%)	1 (0%)	44	77
1	B	339/341 (99%)	292 (86%)	35 (10%)	12 (4%)	4	14
All	All	678/682 (99%)	614 (91%)	51 (8%)	13 (2%)	9	30

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1115	VAL
1	B	1161	ASN
1	B	1167	ASP
1	B	1277	ASP
1	B	1076	MET

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	299/299 (100%)	280 (94%)	19 (6%)	20	50
1	B	299/299 (100%)	279 (93%)	20 (7%)	19	48
All	All	598/598 (100%)	559 (94%)	39 (6%)	20	49

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ASP
1	B	1062	VAL
1	B	1297	SER
1	A	327	GLU
1	B	1019	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	GLN

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Mol	Chain	Res	Type
1	B	1130	ASN
1	B	1014	GLN
1	A	257	ASN
1	B	1020	ASN

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	DDG	D	814	2	16,23,24	1.56	3 (18%)	15,33,36	2.84	4 (26%)
3	ME6	E	906	3	14,21,22	0.61	0	18,30,33	1.45	1 (5%)
2	DDG	H	1814	2	7,10,24	0.50	0	6,12,36	0.46	0
3	ME6	J	1906	3	14,21,22	0.64	0	18,30,33	1.37	3 (16%)

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	DDG	D	814	2	-	0/3/18/19	0/3/3/3
3	ME6	E	906	3	-	0/3/21/22	0/2/2/2
2	DDG	H	1814	2	-	0/3/12/19	0/1/1/3
3	ME6	J	1906	3	-	0/3/21/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	814	DDG	C8-N7	-2.28	1.30	1.34
2	D	814	DDG	C2-N1	2.33	1.39	1.35
2	D	814	DDG	C6-N1	4.78	1.41	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	814	DDG	C5-C6-N1	-7.64	112.61	123.48
2	D	814	DDG	N3-C2-N1	-3.15	122.86	127.46
3	J	1906	ME6	C2'-C1'-N1	-2.43	108.48	114.23
2	D	814	DDG	C6-C5-C4	-2.10	118.76	120.84
3	J	1906	ME6	O4'-C1'-N1	2.30	111.66	107.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	906	ME6	5	0
2	H	1814	DDG	2	0
3	J	1906	ME6	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	DGT	A	414	5	26,33,33	1.07	1 (3%)	28,52,52	3.13	9 (32%)
4	DGT	B	1414	5	26,33,33	1.03	2 (7%)	28,52,52	3.22	10 (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
4	DGT	A	414	5	-	0/18/34/34	0/3/3/3
4	DGT	B	1414	5	-	0/18/34/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1414	DGT	C8-N7	-2.09	1.30	1.34
4	A	414	DGT	C6-N1	3.69	1.39	1.33
4	B	1414	DGT	C6-N1	3.69	1.39	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1414	DGT	C5-C6-N1	-8.22	111.78	123.48
4	A	414	DGT	C5-C6-N1	-7.59	112.67	123.48
4	B	1414	DGT	O1G-PG-O3G	-6.73	84.16	110.50
4	A	414	DGT	O1G-PG-O3G	-6.71	84.24	110.50
4	B	1414	DGT	O2G-PG-O3G	-6.70	84.27	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	414	DGT	1	0
4	B	1414	DGT	4	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, 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	341/341 (100%)	-0.23	0 100 100	22, 48, 77, 105	1 (0%)
1	B	341/341 (100%)	0.57	34 (9%) 8 4	63, 106, 157, 191	0
2	D	12/13 (92%)	-0.02	0 100 100	37, 54, 130, 139	0
2	H	9/13 (69%)	1.14	2 (22%) 1 1	113, 131, 190, 218	0
3	E	18/20 (90%)	0.01	1 (5%) 25 16	34, 64, 131, 160	0
3	J	11/20 (55%)	2.24	7 (63%) 0 0	103, 123, 212, 226	0
All	All	732/748 (97%)	0.21	44 (6%) 23 14	22, 76, 147, 226	1 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1329	LYS	6.7
3	J	1913	DT	6.5
1	B	1324	GLU	5.8
2	H	1805	DG	5.2
1	B	1115	VAL	4.9

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, 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(Å ²)	Q<0.9
2	DDG	D	814	21/22	0.87	0.28	-	59,73,76,76	0
2	DDG	H	1814	10/22	0.70	0.62	-	111,113,117,118	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ME6	E	906	20/21	0.97	0.15	-	43,47,57,60	0
3	ME6	J	1906	20/21	0.71	0.24	-	133,143,163,167	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. 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
4	DGT	B	1414	31/31	0.90	0.21	-0.44	113,117,129,134	0
4	DGT	A	414	31/31	0.98	0.14	-1.20	24,26,34,42	0
5	CA	A	416	1/1	0.98	0.13	-1.64	30,30,30,30	0
5	CA	B	1416	1/1	0.91	0.04	-4.64	50,50,50,50	0
5	CA	A	415	1/1	0.99	0.05	-	43,43,43,43	0
5	CA	B	1415	1/1	0.90	0.12	-	63,63,63,63	0
5	CA	A	417	1/1	0.94	0.08	-	52,52,52,52	0
5	CA	B	1417	1/1	0.94	0.12	-	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.