



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 14, 2017 – 09:29 PM EDT

PDB ID : 2GWE
Title : Crystal structure of D(G4T4G4) with six quadruplexes in the asymmetric unit.
Authors : Lee, M.P.H.; Haider, S.; Parkinson, G.N.; Neidle, S.
Deposited on : unknown
Resolution : 2.20 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
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

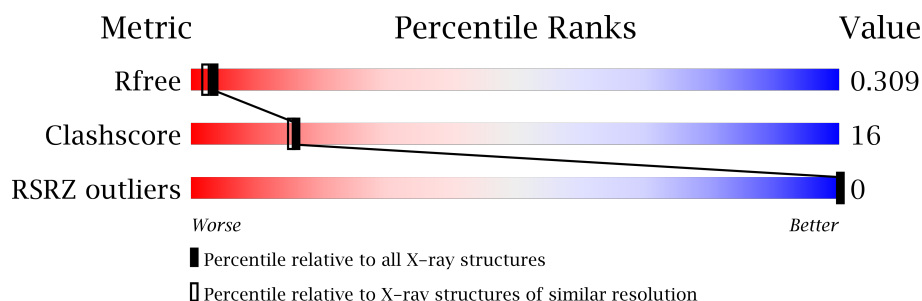
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.






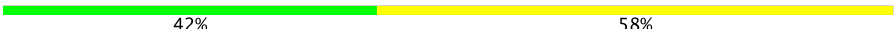
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	12	<div> <div>25%</div> <div>75%</div> </div>
1	B	12	<div> <div>25%</div> <div>75%</div> </div>
1	C	12	<div> <div>33%</div> <div>67%</div> </div>
1	D	12	<div> <div>42%</div> <div>58%</div> </div>
1	E	12	<div> <div>25%</div> <div>75%</div> </div>
1	F	12	<div> <div>17%</div> <div>83%</div> </div>
1	G	12	<div> <div>17%</div> <div>83%</div> </div>
1	H	12	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	12	 17% 83%
1	J	12	 25% 75%
1	K	12	 50% 50%
1	L	12	 42% 58%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3229 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 DNA chain called 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	B	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	C	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	D	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	E	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	F	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	G	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	H	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	I	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	J	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	K	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			
1	L	12	Total	C	N	O	P	0	0	0
			253	120	48	74	11			

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	4	Total	K	0	0
			4	4		
2	J	3	Total	K	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total K 1 1	0	0
2	K	3	Total K 3 3	0	0
2	E	3	Total K 3 3	0	0
2	H	1	Total K 1 1	0	0
2	B	1	Total K 1 1	0	0
2	I	2	Total K 2 2	0	0
2	C	4	Total K 4 4	0	0
2	A	4	Total K 4 4	0	0
2	L	2	Total K 2 2	0	0
2	F	2	Total K 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	14	Total O 14 14	0	0
3	C	13	Total O 13 13	0	0
3	D	12	Total O 12 12	0	0
3	E	15	Total O 15 15	0	0
3	F	14	Total O 14 14	0	0
3	G	13	Total O 13 13	0	0
3	H	15	Total O 15 15	0	0
3	I	12	Total O 12 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	13	Total 13	O 13	0	0
3	K	12	Total 12	O 12	0	0
3	L	12	Total 12	O 12	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: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain A: 



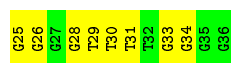
- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain B: 



- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain C: 



- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain D: 



- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain E: 




- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain F: 

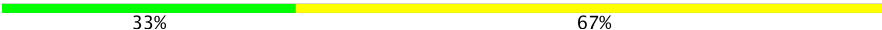
G61 G62 G63 G64 T65 T66 T67 T68 G69 G70 G71 G72

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain G:  17% 83%

G73 G74 G75 G76 T77 T78 T79 T80 G81 G82 G83 G84

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain H:  33% 67%

G85 G88 T89 T90 T91 T92 G93 G94 G95 G96

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain I:  17% 83%

G97 G98 G99 G100 T101 T102 T103 G106 G107 G108

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain J:  25% 75%

G109 G110 G111 G112 T113 T114 T115 T116 G117 G118 G119 G120

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain K:  50% 50%

G121 G124 T125 G129 G130 G131 G132

- Molecule 1: 5'-D(*GP*GP*GP*GP*TP*TP*TP*TP*GP*GP*GP*G)-3'

Chain L:  42% 58%

G133 G136 T137 T138 T139 T140 G141 G142 G143 G144

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.65Å 78.88Å 97.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20 17.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	83.4 (8.00-2.20) 93.9 (17.00-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.49 (at 2.21Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.233 , 0.318 0.224 , 0.309	Depositor DCC
R_{free} test set	1734 reflections (9.93%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3229	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.73 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1023e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/284	0.75	0/440
1	B	0.22	0/284	0.73	0/440
1	C	0.21	0/284	0.72	0/440
1	D	0.22	0/284	0.74	0/440
1	E	0.22	0/284	0.74	0/440
1	F	0.22	0/284	0.71	0/440
1	G	0.21	0/284	0.71	0/440
1	H	0.22	0/284	0.70	0/440
1	I	0.22	0/284	0.72	0/440
1	J	0.22	0/284	0.72	0/440
1	K	0.21	0/284	0.73	0/440
1	L	0.22	0/284	0.72	0/440
All	All	0.22	0/3408	0.72	0/5280

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 [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	253	0	138	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	253	0	138	9	0
1	C	253	0	138	7	0
1	D	253	0	138	5	0
1	E	253	0	138	6	0
1	F	253	0	138	5	0
1	G	253	0	138	8	0
1	H	253	0	138	7	0
1	I	253	0	138	9	0
1	J	253	0	138	8	0
1	K	253	0	138	5	0
1	L	253	0	138	6	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	C	4	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
2	G	4	0	0	0	0
2	H	1	0	0	0	0
2	I	2	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
3	A	18	0	0	1	0
3	B	14	0	0	1	0
3	C	13	0	0	0	0
3	D	12	0	0	0	0
3	E	15	0	0	0	0
3	F	14	0	0	0	0
3	G	13	0	0	0	0
3	H	15	0	0	0	0
3	I	12	0	0	1	0
3	J	13	0	0	0	0
3	K	12	0	0	0	0
3	L	12	0	0	0	0
All	All	3229	0	1656	76	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 16.

The worst 5 of 76 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:F:64:DG:H1'	1:F:65:DT:H5'	1.60	0.84
1:G:76:DG:H1'	1:G:77:DT:H5'	1.69	0.74
1:C:28:DG:H1'	1:C:29:DT:H5'	1.69	0.73
1:G:76:DG:H2''	1:G:77:DT:O5'	2.00	0.62
1:H:95:DG:H1'	1:H:96:DG:H5'	1.81	0.61

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](#)

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 30 ligands modelled in this entry, 30 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	12/12 (100%)	0.40	0 100 100	9, 12, 16, 16	0
1	B	12/12 (100%)	0.22	0 100 100	10, 12, 16, 17	0
1	C	12/12 (100%)	0.78	0 100 100	11, 15, 19, 21	0
1	D	12/12 (100%)	0.85	0 100 100	14, 16, 20, 23	0
1	E	12/12 (100%)	0.23	0 100 100	7, 12, 14, 16	0
1	F	12/12 (100%)	0.26	0 100 100	9, 12, 16, 16	0
1	G	12/12 (100%)	0.41	0 100 100	11, 16, 20, 23	0
1	H	12/12 (100%)	0.42	0 100 100	10, 15, 18, 20	0
1	I	12/12 (100%)	0.69	0 100 100	10, 15, 18, 23	0
1	J	12/12 (100%)	0.64	0 100 100	11, 14, 18, 19	0
1	K	12/12 (100%)	0.33	0 100 100	7, 13, 21, 21	0
1	L	12/12 (100%)	0.38	0 100 100	10, 15, 21, 21	0
All	All	144/144 (100%)	0.47	0 100 100	7, 14, 20, 23	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	K	K	172	1/1	0.99	0.23	1.82	12,12,12,12	0
2	K	G	167	1/1	0.98	0.21	1.22	7,7,7,7	0
2	K	C	147	1/1	0.99	0.23	0.71	14,14,14,14	0
2	K	F	152	1/1	0.97	0.18	0.47	6,6,6,6	0
2	K	A	164	1/1	0.99	0.16	-0.03	12,12,12,12	0
2	K	A	161	1/1	0.98	0.18	-0.22	14,14,14,14	0
2	K	C	145	1/1	0.93	0.18	-0.74	14,14,14,14	0
2	K	G	166	1/1	0.98	0.16	-0.90	11,11,11,11	0
2	K	L	173	1/1	0.97	0.15	-0.90	13,13,13,13	0
2	K	E	151	1/1	0.99	0.14	-1.04	8,8,8,8	0
2	K	E	154	1/1	0.98	0.14	-1.12	12,12,12,12	0
2	K	K	171	1/1	0.97	0.15	-1.13	11,11,11,11	0
2	K	L	174	1/1	0.98	0.14	-1.25	11,11,11,11	0
2	K	A	162	1/1	0.99	0.15	-1.46	4,4,4,4	0
2	K	J	157	1/1	0.96	0.17	-1.64	8,8,8,8	0
2	K	G	169	1/1	0.94	0.14	-1.66	10,10,10,10	0
2	K	H	165	1/1	0.99	0.12	-1.71	9,9,9,9	0
2	K	C	146	1/1	0.97	0.16	-1.98	12,12,12,12	0
2	K	E	153	1/1	0.99	0.14	-2.11	5,5,5,5	0
2	K	K	170	1/1	0.99	0.10	-2.12	8,8,8,8	0
2	K	A	163	1/1	1.00	0.14	-2.15	6,6,6,6	0
2	K	B	160	1/1	0.98	0.11	-2.29	15,15,15,15	0
2	K	F	150	1/1	0.98	0.11	-2.67	12,12,12,12	0
2	K	G	168	1/1	0.99	0.14	-2.81	7,7,7,7	0
2	K	C	148	1/1	0.99	0.12	-3.07	9,9,9,9	0
2	K	D	149	1/1	0.95	0.11	-3.56	10,10,10,10	0
2	K	I	156	1/1	0.99	0.11	-3.92	8,8,8,8	0
2	K	J	155	1/1	0.93	0.09	-4.51	9,9,9,9	0
2	K	I	159	1/1	0.93	0.13	-4.76	11,11,11,11	0
2	K	J	158	1/1	0.93	0.11	-5.35	6,6,6,6	0

6.5 Other polymers

There are no such residues in this entry.