



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:44 AM GMT

PDB ID : 2P5G
Title : Crystal structure of RB69 gp43 in complex with DNA with dAMP opposite
an abasic site analog in a 21mer template
Authors : Zahn, K.E.; Belrhali, H.; Wallace, S.S.; Doublié, S.
Deposited on : 2007-03-15
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

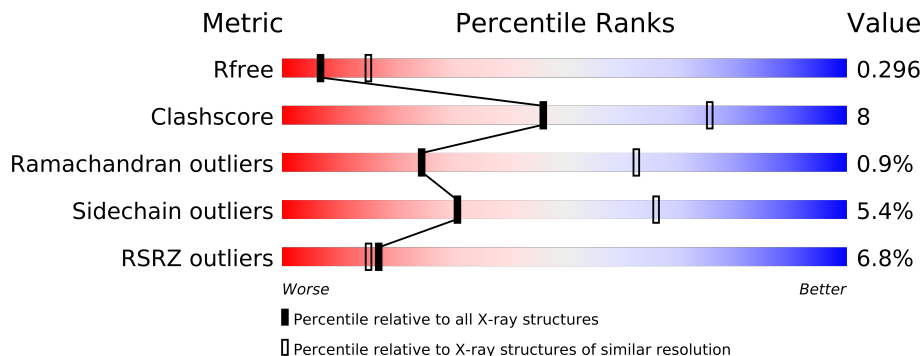
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	21	
1	G	21	
1	I	21	
1	K	21	
2	F	15	
2	H	15	
2	J	15	
2	L	15	
3	A	903	
3	B	903	
3	C	903	
3	D	903	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29179 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			
1	G	11	Total	C	N	O	P	0	0	0
			223	106	44	63	10			
1	I	20	Total	C	N	O	P	0	0	0
			395	188	72	116	19			
1	K	11	Total	C	N	O	P	0	0	0
			226	106	44	65	11			

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	H	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	J	15	Total	C	N	O	P	0	0	0
			308	147	60	87	14			
2	L	13	Total	C	N	O	P	0	0	0
			265	127	50	76	12			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	890	Total 7143	C 4588	N 1193	O 1331	S 8	Se 23	0	0	0
3	B	756	Total 6036	C 3877	N 998	O 1134	S 6	Se 21	0	0	0
3	C	885	Total 7113	C 4560	N 1180	O 1341	S 8	Se 24	0	0	0
3	D	875	Total 6148	C 3867	N 1039	O 1216	S 7	Se 19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	ENGINEERED	UNP Q38087
A	327	ALA	ASP	ENGINEERED	UNP Q38087
B	222	ALA	ASP	ENGINEERED	UNP Q38087
B	327	ALA	ASP	ENGINEERED	UNP Q38087
C	222	ALA	ASP	ENGINEERED	UNP Q38087
C	327	ALA	ASP	ENGINEERED	UNP Q38087
D	222	ALA	ASP	ENGINEERED	UNP Q38087
D	327	ALA	ASP	ENGINEERED	UNP Q38087

- Molecule 4 is water.

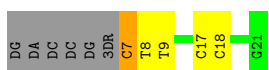
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total 125	O 125	0	0
4	B	86	Total 86	O 86	0	0
4	C	116	Total 116	O 116	0	0
4	D	24	Total 24	O 24	0	0
4	E	4	Total 4	O 4	0	0
4	F	7	Total 7	O 7	0	0
4	G	9	Total 9	O 9	0	0
4	H	9	Total 9	O 9	0	0
4	I	10	Total 10	O 10	0	0
4	J	10	Total 10	O 10	0	0
4	K	1	Total 1	O 1	0	0
4	L	2	Total 2	O 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 errors 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.

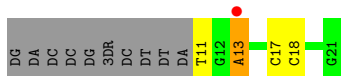
- Molecule 1: Template DNA

Chain E: 



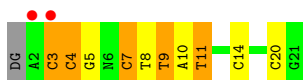
- Molecule 1: Template DNA

Chain G: 



- Molecule 1: Template DNA

Chain I: 



- Molecule 1: Template DNA

Chain K: 



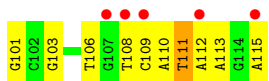
- Molecule 2: Primer DNA

Chain F: 



- Molecule 2: Primer DNA

Chain H: 



- Molecule 2: Primer DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	131.63Å 122.27Å 163.87Å 90.00° 96.45° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 49.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.4 (30.00-2.80) 96.1 (49.61-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.3.0011	Depositor
R, R_{free}	0.234 , 0.295 0.241 , 0.296	Depositor DCC
R_{free} test set	11753 reflections (10.65%)	DCC
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 249661 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29179	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

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	E	0.71	0/339	1.37	2/521 (0.4%)
1	G	0.77	0/250	1.53	3/384 (0.8%)
1	I	0.75	1/429 (0.2%)	1.43	8/657 (1.2%)
1	K	0.70	0/253	1.46	5/388 (1.3%)
2	F	0.71	0/346	1.58	7/533 (1.3%)
2	H	0.71	0/346	1.39	3/533 (0.6%)
2	J	0.75	0/346	1.45	4/533 (0.8%)
2	L	0.69	0/297	1.25	1/457 (0.2%)
3	A	0.40	0/7294	0.54	0/9830
3	B	0.37	0/6163	0.52	0/8319
3	C	0.39	0/7262	0.52	0/9788
3	D	0.33	0/6255	0.47	0/8520
All	All	0.42	1/29580 (0.0%)	0.67	33/40463 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	11	DT	C3'-O3'	-5.08	1.37	1.44

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	105	DC	O4'-C1'-N1	12.32	116.62	108.00
2	J	114	DG	O4'-C1'-N9	11.08	115.76	108.00
2	H	111	DT	O4'-C1'-N1	10.57	115.40	108.00
1	K	20	DC	O4'-C1'-N1	9.93	114.95	108.00
1	G	13	DA	O4'-C1'-N9	9.26	114.48	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	303	0	170	2	0
1	G	223	0	124	2	0
1	I	395	0	222	5	0
1	K	226	0	123	4	0
2	F	308	0	170	2	0
2	H	308	0	170	9	0
2	J	308	0	170	4	0
2	L	265	0	148	5	0
3	A	7143	0	6923	111	0
3	B	6036	0	5779	116	0
3	C	7113	0	6872	122	0
3	D	6148	0	5083	74	0
4	A	125	0	0	2	0
4	B	86	0	0	5	0
4	C	116	0	0	3	0
4	D	24	0	0	1	0
4	E	4	0	0	0	0
4	F	7	0	0	1	0
4	G	9	0	0	0	0
4	H	9	0	0	1	0
4	I	10	0	0	1	0
4	J	10	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
All	All	29179	0	25954	445	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 445 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:728:MSE:HG2	4:B:983:HOH:O	1.47	1.11
3:A:85:MSE:CE	3:A:87:ASP:HB3	1.82	1.08
3:A:85:MSE:HE3	3:A:87:ASP:HB3	1.10	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:85:MSE:HE3	3:A:87:ASP:CB	1.95	0.95
3:A:422:GLN:HG3	3:A:678:GLN:O	1.66	0.94

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	
3	A	886/903 (98%)	828 (94%)	51 (6%)	7 (1%)	27	65
3	B	750/903 (83%)	683 (91%)	61 (8%)	6 (1%)	27	65
3	C	879/903 (97%)	816 (93%)	58 (7%)	5 (1%)	33	72
3	D	865/903 (96%)	750 (87%)	101 (12%)	14 (2%)	14	44
All	All	3380/3612 (94%)	3077 (91%)	271 (8%)	32 (1%)	25	63

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	622	THR
3	D	622	THR
3	D	796	PHE
3	A	521	ASP
3	A	622	THR

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	
3	A	752/775 (97%)	723 (96%)	29 (4%)	43	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	632/775 (82%)	590 (93%)	42 (7%)	24	56
3	C	752/775 (97%)	710 (94%)	42 (6%)	30	64
3	D	518/775 (67%)	489 (94%)	29 (6%)	30	64
All	All	2654/3100 (86%)	2512 (95%)	142 (5%)	31	66

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	779	ILE
3	C	238	THR
3	D	639	SER
3	B	871	LEU
3	C	73	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	153	ASN
3	C	386	HIS
3	D	742	GLN
3	C	245	HIS
3	C	539	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	3DR	I	6	1	9,11,12	0.63	0	11,14,17	0.74	0

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	3DR	I	6	1	-	0/4/15/16	0/1/1/1

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.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	E	15/21 (71%)	-0.36	0 100 100	50, 71, 97, 100	0
1	G	11/21 (52%)	0.85	1 (9%) 9 8	68, 102, 119, 121	0
1	I	20/21 (95%)	-0.05	2 (10%) 8 6	42, 56, 136, 139	0
1	K	11/21 (52%)	-0.03	0 100 100	49, 104, 111, 112	0
2	F	15/15 (100%)	-0.08	0 100 100	64, 85, 111, 114	0
2	H	15/15 (100%)	1.32	5 (33%) 1 1	88, 116, 121, 124	0
2	J	15/15 (100%)	-0.36	0 100 100	39, 65, 82, 90	0
2	L	13/15 (86%)	0.26	0 100 100	115, 119, 124, 124	0
3	A	890/903 (98%)	0.22	26 (2%) 49 50	39, 55, 101, 124	0
3	B	756/903 (83%)	0.42	38 (5%) 28 28	42, 66, 109, 115	0
3	C	885/903 (98%)	0.33	26 (2%) 49 50	35, 62, 99, 126	0
3	D	875/903 (96%)	0.85	142 (16%) 2 2	98, 118, 133, 141	0
All	All	3521/3756 (93%)	0.44	240 (6%) 17 15	35, 69, 127, 141	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	259	SER	8.5
3	D	491	ALA	7.9
3	B	257	TYR	7.6
3	C	535	ALA	6.8
3	B	259	SER	6.3

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	3DR	I	6	11/12	0.16	-1.34	94,99,110,110	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.