



# Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 04:36 AM GMT

PDB ID : 3K5K  
Title : Discovery of a 2,4-Diamino-7-aminoalkoxy-quinazoline as a Potent Inhibitor of Histone Lysine Methyltransferase, G9a  
Authors : Dong,A.; Wasney,G.A.; Liu,F.; Chen,X.; Allali-Hassani,A.; Senisterra,G.; Chau,I.; Bountra,C.; Weigelt,J.; Edwards,A.M.; Arrowsmith,C.H.; Frye,S.V.; Bochkarev,A.; Brown,P.J.; Jin,J.; Vedadi,M.  
Deposited on : 2009-10-07  
Resolution : 1.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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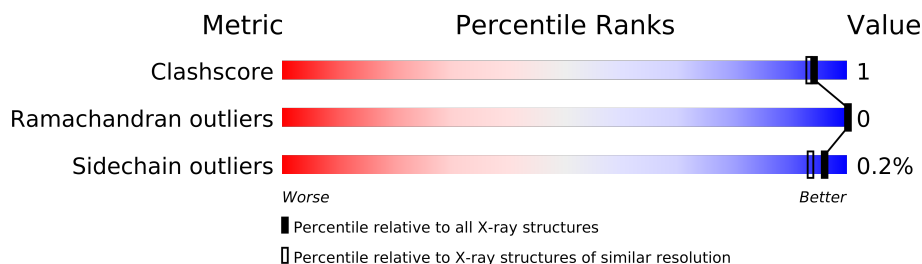
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : **FAILED**  
Percentile statistics : 21963  
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 1.70 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	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)

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  $\geq 3$ , 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4816 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 protein called Histone-lysine N-methyltransferase, H3 lysine-9 specific 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	11	3	0
			2126	1329	370	404	23			
1	B	269	Total	C	N	O	S	6	1	0
			2095	1307	362	403	23			

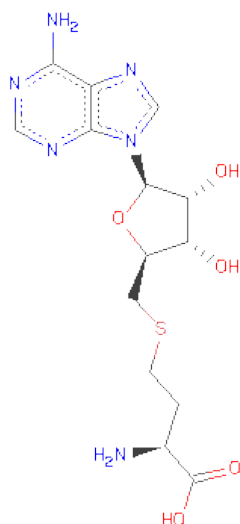
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	911	GLY	-	EXPRESSION TAG	UNP Q96KQ7
A	912	SER	-	EXPRESSION TAG	UNP Q96KQ7
B	911	GLY	-	EXPRESSION TAG	UNP Q96KQ7
B	912	SER	-	EXPRESSION TAG	UNP Q96KQ7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

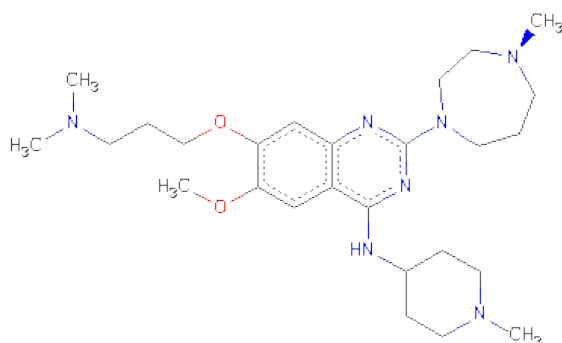
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Zn	0	0
			4	4		
2	A	4	Total	Zn	0	0
			4	4		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is 7-[3-(DIMETHYLAMINO)PROPOXY]-6-METHOXY-2-(4-METHYL-1,4-DIAZEPAN-1-YL)-N-(1-METHYLPIPERIDIN-4-YL)QUINAZOLIN-4-AMINE (three-letter code: DXQ) (formula: C<sub>26</sub>H<sub>43</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	26	7	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			35	26	7	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Cl	0	0
			2	2		
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	X	0	0
			1	1		
6	A	1	Total	X	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	236	Total	O	0	0
			236	236		
7	B	223	Total	O	0	0
			223	223		

### 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.

Note EDS failed to run properly.

- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain A: 



- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-9 specific 3

Chain B: 



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.67Å 78.07Å 72.51Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	29.58 – 1.70	Depositor
% Data completeness (in resolution range)	97.0 (29.58-1.70)	Depositor
$R_{merge}$	0.04	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0102, COOT 0.5.2	Depositor
R, $R_{free}$	0.209 , 0.264	Depositor
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.103	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67674 reflections	Xtriage
Total number of atoms	4816	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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 21.86 % 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 6.4178e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities 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: UNX, ZN, SAH, DXQ, CL

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	0/2171	0.60	0/2946
1	B	0.54	0/2140	0.60	0/2906
All	All	0.54	0/4311	0.60	0/5852

There are no bond length outliers.

There are no bond angle outliers.

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	A	2126	0	1928	7	0
1	B	2095	0	1895	3	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
4	A	35	0	43	1	0
4	B	35	0	43	2	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	236	0	0	1	0
7	B	223	0	0	2	0
All	All	4816	0	3947	12	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 1.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:919:GLU:HG3	1:B:940:GLY:HA3	1.75	0.68
1:B:919:GLU:CD	1:B:1053:ARG:HH22	2.15	0.49
1:A:1060:GLN:HG2	7:A:208:HOH:O	2.13	0.48
4:B:2001:DXQ:HAP	7:B:344:HOH:O	2.13	0.47
1:A:962:MET:HE3	1:A:1133:PHE:CE1	2.53	0.44
1:A:1025:ARG:O	1:A:1030:ARG:HD2	2.19	0.43
1:A:962:MET:HE3	1:A:1133:PHE:HE1	1.84	0.43
1:A:1086:LEU:O	4:A:2000:DXQ:HAJ	2.20	0.41
1:A:1113:HIS:HB2	1:A:1154:TYR:CG	2.56	0.41
1:B:1080:ARG:HD2	1:B:1100:ASP:OD2	2.21	0.40
1:A:1071:LEU:HD23	1:A:1099:ILE:HG12	2.03	0.40
4:B:2001:DXQ:HABB	7:B:310:HOH:O	2.22	0.40

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	271/283 (96%)	261 (96%)	10 (4%)	0	100	100
1	B	266/283 (94%)	253 (95%)	13 (5%)	0	100	100
All	All	537/566 (95%)	514 (96%)	23 (4%)	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	220/253 (87%)	219 (100%)	1 (0%)	94	89
1	B	221/253 (87%)	221 (100%)	0	100	100
All	All	441/506 (87%)	440 (100%)	1 (0%)	96	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	991	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	972	GLN
1	A	1060	GLN
1	B	1091	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

Of 18 ligands modelled in this entry, 2 are unknown and 12 are monoatomic - leaving 4 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
3	SAH	A	1198	-	28,28,28	1.21	2 (7%)	40,40,40	1.89	10 (25%)
4	DXQ	A	2000	-	38,38,38	1.17	5 (13%)	52,52,52	2.71	15 (28%)
3	SAH	B	1198	-	28,28,28	1.20	4 (14%)	40,40,40	1.88	9 (22%)
4	DXQ	B	2001	-	38,38,38	1.26	2 (5%)	52,52,52	2.73	16 (30%)

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	SAH	A	1198	-	-	0/15/31/31	0/1/3/3
4	DXQ	A	2000	-	-	0/17/38/38	0/1/4/4
3	SAH	B	1198	-	-	0/15/31/31	0/1/3/3
4	DXQ	B	2001	-	-	0/17/38/38	0/1/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	DXQ	C6-C5	-4.20	1.39	1.45
4	A	2000	DXQ	C6-C5	-3.63	1.40	1.45
3	A	1198	SAH	C5-C4	3.34	1.48	1.40
3	B	1198	SAH	C5-C4	3.16	1.47	1.40
4	B	2001	DXQ	CAO-NBI	2.88	1.49	1.46
3	A	1198	SAH	C4-N9	-2.69	1.33	1.37
3	B	1198	SAH	C4-N9	-2.46	1.34	1.37
4	A	2000	DXQ	CAF-CAZ	2.36	1.40	1.36
3	B	1198	SAH	C5'-SD	-2.29	1.76	1.81
4	A	2000	DXQ	CAO-NBI	2.12	1.48	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1198	SAH	C2-N3	2.12	1.36	1.32
4	A	2000	DXQ	CAG-CAY	2.09	1.40	1.36
4	A	2000	DXQ	CAS-NBI	2.03	1.48	1.46

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	DXQ	CAG-C5-C6	-8.90	120.20	124.98
4	A	2000	DXQ	CAG-C5-C6	-8.86	120.22	124.98
4	B	2001	DXQ	C6-NAV-CBE	7.51	133.20	123.84
4	A	2000	DXQ	C6-NAV-CBE	7.29	132.92	123.84
3	B	1198	SAH	N3-C2-N1	-7.06	122.80	128.71
3	A	1198	SAH	N3-C2-N1	-6.95	122.90	128.71
4	A	2000	DXQ	C6-C5-C4	6.80	119.51	115.63
4	B	2001	DXQ	C6-C5-C4	6.72	119.46	115.63
4	A	2000	DXQ	CAQ-NBH-CAP	6.55	118.67	109.54
4	B	2001	DXQ	CAQ-NBH-CAP	5.62	117.38	109.54
3	B	1198	SAH	N3-C4-N9	5.41	135.19	125.43
3	A	1198	SAH	N3-C4-N9	4.76	134.02	125.43
4	A	2000	DXQ	C5-C4-N3	-4.66	118.56	122.86
4	B	2001	DXQ	C5-C6-NAV	-4.17	115.56	120.38
4	B	2001	DXQ	C5-C4-N3	-4.10	119.08	122.86
4	B	2001	DXQ	CAS-NBI-CAO	3.90	122.99	116.53
4	A	2000	DXQ	N3-C2-N1	-3.86	119.63	126.29
4	A	2000	DXQ	CAR-CAS-NBI	-3.60	106.79	113.43
4	B	2001	DXQ	N3-C2-N1	-3.58	120.12	126.29
4	A	2000	DXQ	C5-C6-NAV	-3.48	116.36	120.38
4	B	2001	DXQ	CAI-CAN-NBG	-3.43	109.35	115.30
4	B	2001	DXQ	CAR-CAS-NBI	-3.42	107.11	113.43
4	A	2000	DXQ	CAK-CBE-NAV	3.26	115.63	110.55
4	A	2000	DXQ	N3-C2-NBI	3.23	120.81	117.11
4	B	2001	DXQ	OAW-CAY-CAG	-3.17	121.26	125.25
4	B	2001	DXQ	N1-C2-NBI	3.00	120.52	117.11
4	A	2000	DXQ	CAS-NBI-CAO	2.92	121.36	116.53
4	A	2000	DXQ	OAW-CAY-CAG	-2.83	121.68	125.25
3	A	1198	SAH	C4-C5-N7	-2.80	107.13	109.52
3	B	1198	SAH	OXT-C-O	-2.78	117.78	124.07
3	B	1198	SAH	C8-N9-C4	2.78	109.02	106.90
3	A	1198	SAH	C5-C4-N3	-2.73	119.76	125.70
4	B	2001	DXQ	CAL-CBE-NAV	2.71	114.77	110.55
3	B	1198	SAH	C5-C4-N3	-2.71	119.80	125.70
4	B	2001	DXQ	NAV-C6-N1	2.70	125.42	118.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	DXQ	CAK-CBE-NAV	2.69	114.74	110.55
3	A	1198	SAH	C2-N1-C6	2.63	123.53	118.77
3	A	1198	SAH	O4'-C1'-N9	2.51	110.77	108.44
4	B	2001	DXQ	OAW-CAY-CAZ	2.43	118.95	115.42
4	A	2000	DXQ	NAV-C6-N1	2.33	124.48	118.58
3	B	1198	SAH	OXT-C-CA	2.22	121.87	116.88
4	A	2000	DXQ	N1-C2-NBI	2.15	119.55	117.11
4	A	2000	DXQ	C2-N1-C6	2.14	121.49	117.65
3	B	1198	SAH	C2-N3-C4	2.13	120.07	114.01
3	A	1198	SAH	O4'-C1'-C2'	-2.12	103.53	106.77
3	A	1198	SAH	OXT-C-O	-2.11	119.30	124.07
3	A	1198	SAH	C2-N3-C4	2.11	120.01	114.01
3	B	1198	SAH	N6-C6-N1	2.10	123.49	119.36
3	B	1198	SAH	C2-N1-C6	2.07	122.51	118.77
3	A	1198	SAH	C3'-C2'-C1'	2.03	104.08	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.