



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:06 AM GMT

PDB ID : 3KV6
Title : Structure of KIAA1718, human Jumonji demethylase, in complex with alpha-ketoglutarate
Authors : Horton, J.R.; Upadhyay, A.K.; Qi, H.H.; Zhang, X.; Shi, Y.; Cheng, X.
Deposited on : 2009-11-29
Resolution : 2.89 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

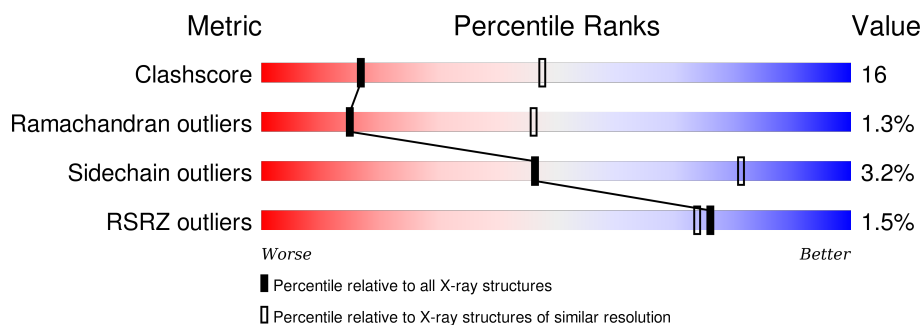
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	488	
1	D	488	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	OXY	A	492	-	-	-	X
4	OXY	D	492	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AKG	A	702	-	-	-	X
5	AKG	D	701	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7389 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 JmjC domain-containing histone demethylation protein 1D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	3	0
			3580	2305	609	640	26			
1	D	448	Total	C	N	O	S	0	2	0
			3614	2327	608	653	26			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

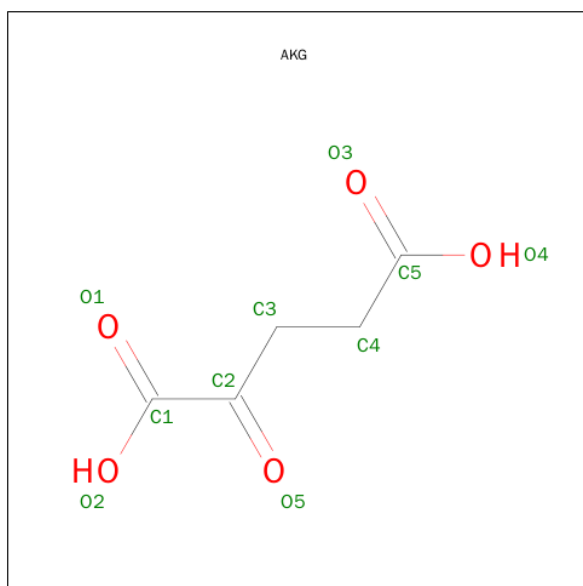
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			2	2		

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).




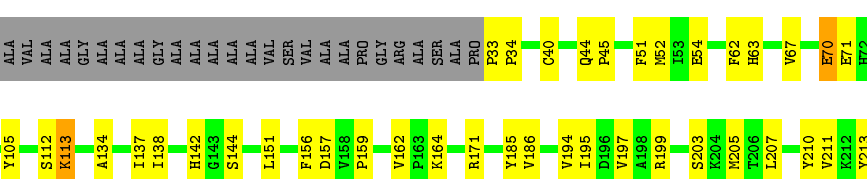
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	5	5		
5	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total 82	O 82	0	0
6	D	83	Total 83	O 83	0	0

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.

- Chain A: 



Residue	Conservation (%)
Y427	60%
L428	60%
V429	60%
Q430	60%
G431	60%
V432	60%
K433	60%
K434	60%
L435	60%
K436	60%
T437	60%
A438	60%
L439	60%
K440	60%
L441	60%
W442	60%
M443	60%
L447	60%
V448	60%
S449	60%
A450	60%
H451	60%
A452	60%
I455	60%
A456	60%
R460	60%
P461	60%
H463	60%
L464	60%
I465	60%
K466	60%
E467	60%
L468	60%
S469	60%
K470	60%
V471	60%
H479	60%
GLY	60%
LYS	60%
PRO	60%
VAL	60%
LYS	60%
SER	60%
GLN	60%
GLY	60%
ILE	60%
L223	60%
H224	60%
V225	60%
K234	60%
E237	60%
L238	60%
V239	60%
E240	60%
V241	60%
T244	60%
A245	60%
S249	60%
K250	60%
E252	60%
N253	60%
Y254	60%
W255	60%
P256	60%
D257	60%
D258	60%
S259	60%
V260	60%
P261	60%
P262	60%
P265	60%
V266	60%
K267	60%
K268	60%
Q275	60%
D276	60%
S277	60%
V278	60%
F285	60%
T288	60%
S289	60%
V290	60%
W291	60%
W296	60%
G297	60%
K298	60%
L303	60%
L304	60%
K305	60%
P306	60%
R313	60%
Y314	60%
E315	60%
S318	60%
Q323	60%
K331	60%
V332	60%
D333	60%
K334	60%
G335	60%
V336	60%
P349	60%
V352	60%
L353	60%
Q360	60%
D361	60%
K362	60%
M363	60%
G367	60%
L370	60%
H371	60%
N372	60%
L375	60%
L379	60%
M384	60%
E385	60%
F386	60%
P387	60%
F388	60%
F399	60%
E400	60%
A401	60%
L402	60%
V406	60%
A407	60%
L410	60%
T413	60%
L414	60%
K415	60%
E416	60%
L417	60%
D420	60%
K421	60%
P424	60%
K425	60%
T426	60%
R98	60%
N99	60%
V100	60%
H101	60%
R102	60%
Y105	60%
S112	60%
K113	60%
A134	60%
I137	60%
I138	60%
H142	60%
G143	60%
S144	60%
L151	60%
F156	60%
D157	60%
V158	60%
P159	60%
V162	60%
P163	60%
K164	60%
R171	60%
Y165	60%
V166	60%
V194	60%
I195	60%
D196	60%
V197	60%
A198	60%
R199	60%
S203	60%
K204	60%
N205	60%
T206	60%
L207	60%
V210	60%
V211	60%
K212	60%
Y213	60%
P214	60%
N215	60%
N216	60%
P217	60%
N218	60%
R219	60%
Q40	29%
Q44	29%
P45	29%
P51	29%
H52	29%
I53	29%
E54	29%
T62	29%
H63	29%
V67	29%
E70	29%
E71	29%

- [illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 125.20Å 206.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 2.89 34.55 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.54-2.89) 93.1 (34.55-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.253 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 36619 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7389	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: AKG, ZN, FE2, OXY

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	0.39	0/3684	0.62	0/5007
1	D	0.40	0/3720	0.63	0/5056
All	All	0.39	0/7404	0.62	0/10063

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

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	3580	0	3440	112	0
1	D	3614	0	3475	120	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	4	1	0
5	D	10	0	4	1	0
6	A	82	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	83	0	0	2	0
All	All	7389	0	6923	232	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 232 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:234:LYS:HD2	1:A:234:LYS:H	1.24	1.00
1:D:460:ARG:N	1:D:460:ARG:HD3	1.83	0.93
1:A:75:VAL:HG11	1:A:199:ARG:HH11	1.37	0.89
1:D:70:GLU:H	1:D:73[B]:HIS:HD2	1.22	0.88
1:A:185:TYR:O	1:A:234:LYS:HD3	1.78	0.84

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	448/488 (92%)	404 (90%)	39 (9%)	5 (1%)	17	51
1	D	448/488 (92%)	401 (90%)	40 (9%)	7 (2%)	12	40
All	All	896/976 (92%)	805 (90%)	79 (9%)	12 (1%)	15	46

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	111	GLY
1	A	100	TRP
1	A	397	PRO

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Mol	Chain	Res	Type
1	D	448	VAL
1	A	40	CYS

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	388/424 (92%)	377 (97%)	11 (3%)	51	84
1	D	396/424 (93%)	382 (96%)	14 (4%)	43	78
All	All	784/848 (92%)	759 (97%)	25 (3%)	46	81

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	87	VAL
1	D	120	ARG
1	D	450	GLU
1	D	92	SER
1	D	152	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	99	ASN
1	D	101	HIS
1	D	253	ASN
1	D	72	HIS
1	D	224	ASN

5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 6 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	$\# Z > 2$
4	OXY	A	492	-	1,1,1	1.36	0	0,0,0	0.00	-
5	AKG	A	702	3	3,9,9	0.97	0	4,11,11	1.18	0
4	OXY	D	492	-	1,1,1	1.36	0	0,0,0	0.00	-
5	AKG	D	701	3	3,9,9	0.80	0	4,11,11	1.09	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
4	OXY	A	492	-	-	0/0/0/0	0/0/0/0
5	AKG	A	702	3	-	0/3/9/9	0/0/0/0
4	OXY	D	492	-	-	0/0/0/0	0/0/0/0
5	AKG	D	701	3	-	0/3/9/9	0/0/0/0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	702	AKG	1	0
5	D	701	AKG	1	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	447/488 (91%)	-0.33	6 (1%) 79 78	13, 32, 55, 84	0
1	D	448/488 (91%)	-0.34	7 (1%) 74 72	13, 31, 55, 84	0
All	All	895/976 (91%)	-0.33	13 (1%) 76 74	13, 32, 55, 84	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	PRO	3.9
1	D	457	ASP	3.4
1	A	260	VAL	2.9
1	D	429	VAL	2.8
1	D	424	PRO	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

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
5	AKG	A	702	10/10	0.86	0.41	12.32	97,97,99,99	0
4	OXY	A	492	2/2	0.93	0.50	11.42	61,61,61,61	0
4	OXY	D	492	2/2	0.71	0.66	9.86	72,72,72,73	0
5	AKG	D	701	10/10	0.79	0.43	4.34	102,103,103,103	0
2	ZN	D	489	1/1	1.00	0.06	-1.45	30,30,30,30	0
2	ZN	A	490	1/1	0.99	0.06	-1.59	26,26,26,26	0
2	ZN	D	490	1/1	1.00	0.05	-2.07	27,27,27,27	0
2	ZN	A	489	1/1	1.00	0.07	-7.77	21,21,21,21	0
3	FE2	A	491	1/1	0.94	0.12	-	65,65,65,65	0
3	FE2	D	491	1/1	0.99	0.14	-	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.