

# Full wwPDB X-ray Structure Validation Report (i)

#### May 13, 2020 – 05:37 pm BST

PDB ID 2IUW

Title Crystal structure of human ABH3 in complex with iron ion and 2- oxoglutarate Authors Sundheim, O.; Vagbo, C.B.; Bjoras, M.; deSousa, M.M.L.; Talstad, V.; Aas,

P.A.; Drablos, F.; Krokan, H.E.; Tainer, J.A.; Slupphaug, G.

Deposited on 2006-06-07

1.50 Å(reported) Resolution

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at

https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity 4.02b-467

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13 EDS 2.11

Percentile statistics 20191225.v01 (using entries in the PDB archive December 25th 2019)

> Refmac 5.8.0158

7.0.044 (Gargrove) CCP4

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

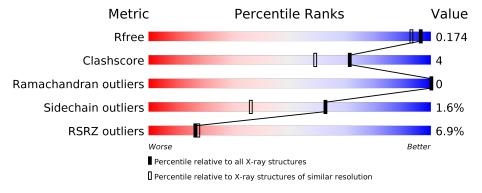
Validation Pipeline (wwPDB-VP) 2.11

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$ 

The reported resolution of this entry is 1.50 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$\begin{array}{c} {\rm Similar \; resolution} \\ (\#{\rm Entries, \; resolution \; range(\AA)}) \end{array}$
$R_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 respectively. 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 <=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	
			6%	
1	Α	238	75%	9% • 14%



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1959 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.

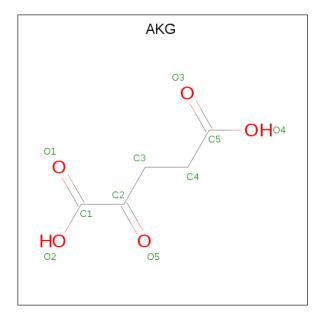
• Molecule 1 is a protein called ALKYLATED REPAIR PROTEIN ALKB HOMOLOG 3.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	Λ	205	Total	С	N	О	S	0	1	0
1	A	203	1703	1079	305	311	8	0	1	0

• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Fe	0	0

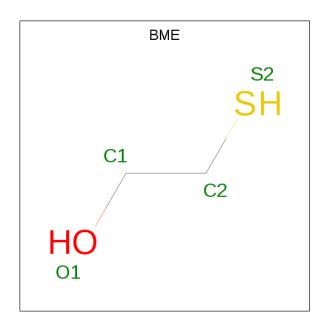
• Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C<sub>5</sub>H<sub>6</sub>O<sub>5</sub>).



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

• Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	Α	1	Total C O S	0	0	
1	71	1	4 2 1 1	0		
1	Λ.	1	Total C O S	0	0	
4	Α	1	$\begin{vmatrix} 4 & 2 & 1 & 1 \end{vmatrix}$	0		
4	Λ	1	Total C O S	0	0	
4	A	1	$\begin{vmatrix} 4 & 2 & 1 & 1 \end{vmatrix}$	0	U	
1	Λ	1	Total C O S	0	0	
4	A	1	$\begin{vmatrix} 4 & 2 & 1 & 1 \end{vmatrix}$		U	

• Molecule 5 is water.

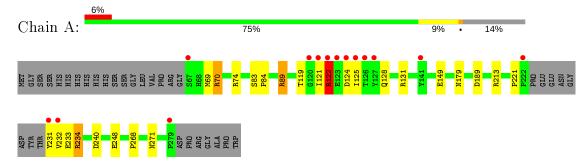
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	227	Total O 227 227	0	0



# 3 Residue-property plots (i)

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: ALKYLATED REPAIR PROTEIN ALKB HOMOLOG 3





# 4 Data and refinement statistics (i)

Property	Value	Source	
Space group	I 41	Depositor	
Cell constants	119.95Å 119.95Å 40.55Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor	
Resolution (Å)	45.00 - 1.50	Depositor	
rtesolution (A)	37.93 - 1.50	EDS	
% Data completeness	94.7 (45.00-1.50)	Depositor	
(in resolution range)	96.3 (37.93-1.50)	EDS	
$R_{merge}$	0.10	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.10 (at 1.50Å)	Xtriage	
Refinement program	SHELXL-97	Depositor	
D D.	0.141 , 0.191	Depositor	
$R, R_{free}$	0.131 , $0.174$	DCC	
$R_{free}$ test set	2302 reflections $(5.00\%)$	wwPDB-VP	
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage	
Anisotropy	0.190	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.35, 69.3	EDS	
L-test for twinning <sup>2</sup>	$< L >=0.49, < L^2>=0.32$	Xtriage	
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage	
$F_o, F_c$ correlation	0.97	EDS	
Total number of atoms	1959	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.49% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: AKG, LED, FE, BME

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	Boı	nd lengths	$\mathbf{B}_{0}$	ond angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z >5
1	A	0.59	1/1748 (0.1%)	1.33	$16/2377 \ (0.7\%)$

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	${ m Observed}( m \AA)$	$\operatorname{Ideal}( ext{\AA})$
1	A	221	PRO	C-N	5.66	1.45	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	A	131	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	A	131	ARG	NH1-CZ-NH2	11.88	132.47	119.40
1	A	231	TYR	CA-CB-CG	11.40	135.06	113.40
1	A	131	ARG	NE-CZ-NH1	-11.27	114.67	120.30
1	A	221	PRO	O-C-N	10.25	140.57	121.10
1	A	189	ASP	CB-CG-OD2	8.12	125.61	118.30
1	A	122	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	89	ARG	NE-CZ-NH2	7.66	124.13	120.30
1	A	234	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	A	74	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	122	ARG	CD-NE-CZ	7.06	133.49	123.60
1	A	221	PRO	CA-C-N	-6.05	100.17	117.10
1	A	70	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	213	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	231	TYR	CB-CG-CD2	5.23	124.14	121.00
1	A	240	ASP	CB-CG-OD2	5.21	122.99	118.30

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	1703	0	1649	12	0
2	A	3	0	0	0	0
3	A	10	0	4	0	0
4	A	16	0	21	1	0
5	A	227	0	0	2	0
All	All	1959	0	1674	12	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 4.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance}  ({\rm \AA}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
1:A:268:PRO:HG2	4:A:802:BME:H11	1.62	0.82
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.63	0.63
1:A:70:ARG:HG3	1:A:232:VAL:HG11	1.83	0.60
1:A:179:ASN:HD22	1:A:271:ASN:HD22	1.53	0.54
1:A:83:SER:HB2	1:A:84:PRO:HA	1.93	0.49
1:A:119:THR:HG23	1:A:128:GLN:NE2	2.28	0.48
1:A:233:GLU:HG3	1:A:234:ARG:HG2	1.95	0.48
1:A:149:GLU:HA	5:A:2089:HOH:O	2.17	0.44
1:A:89:ARG:HD2	1:A:248:GLU:OE1	2.17	0.44
1:A:124:ASP:N	1:A:124:ASP:OD1	2.50	0.43
1:A:122:ARG:HD2	5:A:2143:HOH:O	2.18	0.41
1:A:69:MET:HE2	1:A:69:MET:HB2	2.01	0.40

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	201/238 (84%)	201 (100%)	0	0	100 100		

There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

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.

Me	ol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1		A	189/215 (88%)	186 (98%)	3 (2%)	62 36		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain Res		$\mathbf{Type}$	
1	A	121	ILE	
1	A	122	ARG	
1	A	125	ILE	

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	128	GLN
1	A	168	ASN
1	A	271	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 C		Chain Res		Link	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LED	A	177	1	6,8,9	1.27	1 (16%)	5,9,11	1.29	1 (20%)

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	LED	A	177	1	-	3/6/8/10	-

#### All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	Z	${f Observed(\AA)}$	$\operatorname{Ideal}( ext{\AA})$
1	A	177	LED	CG-CD2	2.74	1.55	1.50

#### All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	177	LED	OE-CD2-CG	-2.49	119.63	125.32

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	177	LED	OE-CD2-CG-CB
1	A	177	LED	CA-CB-CG-CD1
1	A	177	LED	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.



### 5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	Tune	Chain	Res	Link	Bond lengths				Bond angles		
MIOI	Type	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
4	BME	A	801	1	3,3,3	0.57	0	1,2,2	0.89	0	
3	AKG	A	700	2	3,9,9	1.01	0	4,11,11	2.89	2 (50%)	
4	BME	A	800	1	3,3,3	0.64	0	1,2,2	0.25	0	
4	BME	A	802	1	3,3,3	0.71	0	1,2,2	0.37	0	
4	BME	A	901	-	3,3,3	0.69	0	1,2,2	1.01	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	BME	A	801	1	-	1/1/1/1	_
3	AKG	A	700	2	-	0/3/9/9	_
4	BME	A	800	1	-	0/1/1/1	-
4	BME	A	802	1	-	1/1/1/1	_
4	BME	A	901	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms Z		$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
3	A	700	AKG	O5-C2-C3	5.06	129.01	120.38
3	A	700	AKG	C3-C2-C1	-2.36	115.44	121.32

There are no chirality outliers.



All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	BME	O1-C1-C2-S2
4	A	802	BME	O1-C1-C2-S2
4	A	901	BME	O1-C1-C2-S2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	802	BME	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,  $95^{th}$  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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(A^2)$	Q < 0.9
1	A	$204/238 \ (85\%)$	-0.23	14 (6%) 1	6 17	10, 16, 44, 106	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	ILE	11.9
1	A	231	TYR	11.4
1	A	124	ASP	6.7
1	A	123	GLU	5.5
1	A	279	PRO	5.5
1	A	122	ARG	4.2
1	A	222	PRO	3.6
1	A	141	TYR	3.6
1	A	232	VAL	3.2
1	A	127	TYR	3.1
1	A	126	THR	2.7
1	A	121	ILE	2.5
1	A	120	GLY	2.3
1	A	67	SER	2.2

### 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	LED	A	177	9/10	0.99	0.08	8,9,14,30	1



### 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
4	BME	A	801	4/4	0.80	0.24	71,75,76,92	0
4	BME	A	901	4/4	0.86	0.12	40,41,61,64	0
4	BME	A	802	4/4	0.91	0.20	53,65,69,71	0
3	AKG	A	700	10/10	0.96	0.10	12,22,26,39	0
4	BME	A	800	4/4	0.97	0.09	36,60,64,76	0
2	FE	A	502	1/1	0.98	0.12	48,48,48,48	0
2	FE	A	500	1/1	1.00	0.05	20,20,20,20	0
2	FE	A	501	1/1	1.00	0.13	35,35,35,35	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

