



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:58 am GMT

PDB ID : 1IKA  
Title : STRUCTURE OF ISOCITRATE DEHYDROGENASE WITH ALPHA-KETOGLUTARATE AT 2.7 ANGSTROMS RESOLUTION: CONFORMATIONAL CHANGES INDUCED BY DECARBOXYLATION OF ISOCITRATE  
Authors : Stoddard, B.L.; Koshland Junior, D.E.  
Deposited on : 1993-06-15  
Resolution : 2.70 Å(reported)

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](mailto: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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

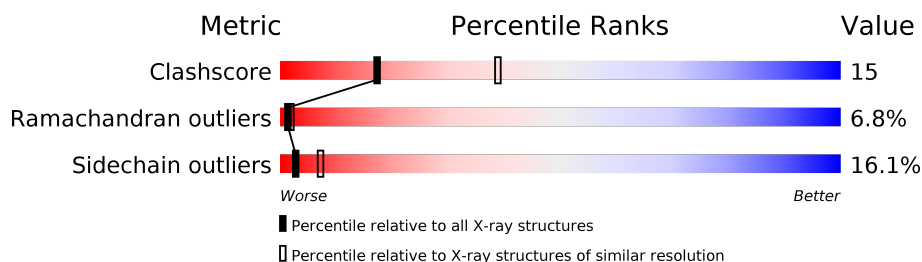
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	416	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3891 atoms, of which 684 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.

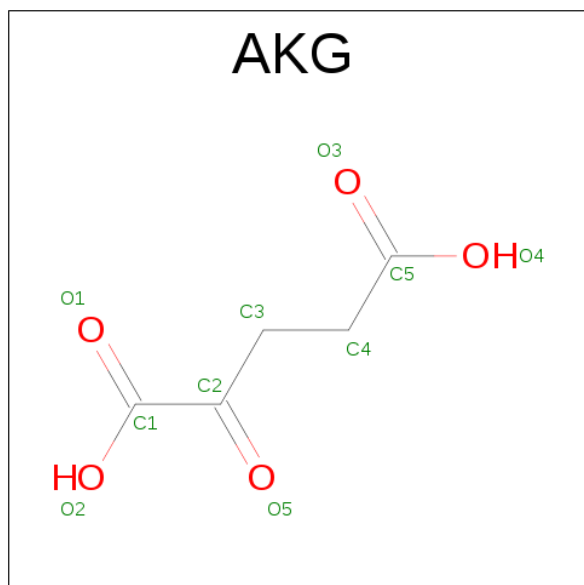
- Molecule 1 is a protein called ISOCITRATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	414	Total	C	H	N	O	S	87	0	0
			3880	2035	684	538	605	18			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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



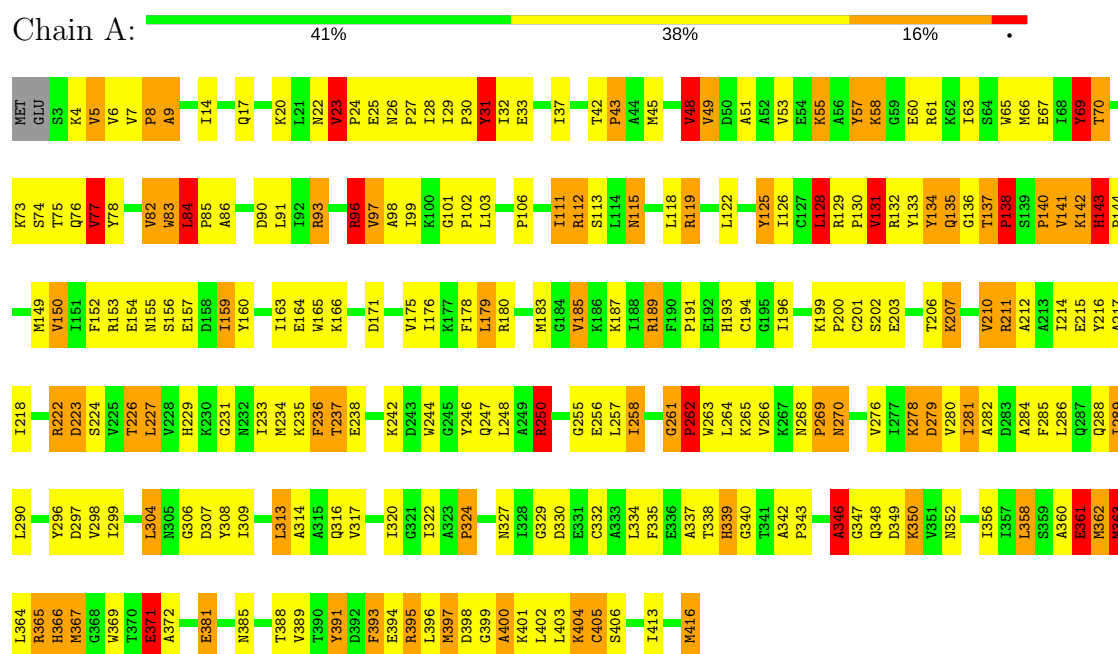
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

### 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.

Note EDS was not executed.

#### • Molecule 1: ISOCITRATE DEHYDROGENASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.10Å 105.10Å 150.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, $R_{free}$	0.185 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3891	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	1.29	10/3257 (0.3%)	2.30	175/4405 (4.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	VAL	CA-CB	8.46	1.72	1.54
1	A	23	VAL	CA-CB	6.92	1.69	1.54
1	A	97	VAL	CA-CB	6.27	1.68	1.54
1	A	119	ARG	CZ-NH2	6.13	1.41	1.33
1	A	244	TRP	CG-CD2	-6.03	1.33	1.43
1	A	125	TYR	CA-CB	5.84	1.66	1.53
1	A	250	ARG	CA-CB	5.82	1.66	1.53
1	A	361	GLU	CD-OE1	-5.24	1.19	1.25
1	A	391	TYR	CA-CB	5.20	1.65	1.53
1	A	101	GLY	CA-C	5.05	1.59	1.51

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH2	-13.39	113.60	120.30
1	A	96	ARG	NE-CZ-NH2	-11.06	114.77	120.30
1	A	250	ARG	NE-CZ-NH1	10.83	125.72	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	TYR	CB-CG-CD2	-10.80	114.52	121.00
1	A	112	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	222	ARG	NE-CZ-NH1	10.69	125.65	120.30
1	A	266	VAL	CG1-CB-CG2	-10.47	94.15	110.90
1	A	125	TYR	CA-CB-CG	10.24	132.86	113.40
1	A	112	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	A	363	MET	CA-CB-CG	9.95	130.22	113.30
1	A	257	LEU	CA-CB-CG	9.70	137.60	115.30
1	A	65	TRP	CD1-CG-CD2	9.69	114.05	106.30
1	A	397	MET	CA-CB-CG	9.43	129.33	113.30
1	A	346	ALA	CB-CA-C	-9.32	96.11	110.10
1	A	77	VAL	CG1-CB-CG2	-9.24	96.12	110.90
1	A	244	TRP	CD1-CG-CD2	9.16	113.63	106.30
1	A	231	GLY	O-C-N	8.98	137.08	122.70
1	A	134	TYR	CB-CG-CD2	8.83	126.30	121.00
1	A	163	ILE	N-CA-C	-8.59	87.81	111.00
1	A	214	ILE	CA-C-N	8.41	135.71	117.20
1	A	322	ILE	CA-C-N	8.39	135.66	117.20
1	A	369	TRP	CG-CD2-CE3	8.31	141.38	133.90
1	A	369	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	A	85	PRO	CA-C-N	-8.23	99.10	117.20
1	A	250	ARG	CA-CB-CG	8.13	131.28	113.40
1	A	369	TRP	CE2-CD2-CG	-8.12	100.80	107.30
1	A	346	ALA	CA-C-N	7.97	132.15	116.20
1	A	346	ALA	N-CA-C	7.95	132.46	111.00
1	A	365	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	65	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	A	8	PRO	N-CA-C	7.85	132.50	112.10
1	A	28	ILE	CA-C-N	-7.84	99.95	117.20
1	A	69	TYR	CB-CA-C	-7.75	94.91	110.40
1	A	403	LEU	CB-CG-CD1	-7.61	98.06	111.00
1	A	367	MET	CA-C-N	7.57	131.34	116.20
1	A	350	LYS	CA-CB-CG	7.55	130.00	113.40
1	A	112	ARG	CA-CB-CG	7.53	129.97	113.40
1	A	381	GLU	CA-CB-CG	7.40	129.69	113.40
1	A	244	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	404	LYS	C-N-CA	7.28	139.90	121.70
1	A	263	TRP	CA-CB-CG	7.26	127.50	113.70
1	A	28	ILE	O-C-N	7.19	134.20	122.70
1	A	365	ARG	CA-C-N	-7.17	101.43	117.20
1	A	119	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	393	PHE	CA-C-N	7.12	132.85	117.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	TRP	CE2-CD2-CG	-7.11	101.61	107.30
1	A	5	VAL	CA-C-N	-7.11	101.56	117.20
1	A	93	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	194	CYS	CA-CB-SG	7.09	126.76	114.00
1	A	160	TYR	CB-CG-CD2	-7.05	116.77	121.00
1	A	128	LEU	CA-CB-CG	6.95	131.28	115.30
1	A	133	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	A	211	ARG	CA-CB-CG	6.88	128.54	113.40
1	A	69	TYR	CB-CG-CD1	-6.86	116.88	121.00
1	A	129	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	262	PRO	CA-C-N	6.76	132.08	117.20
1	A	210	VAL	CG1-CB-CG2	-6.70	100.17	110.90
1	A	165	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	49	VAL	CG1-CB-CG2	-6.63	100.29	110.90
1	A	405	CYS	N-CA-C	6.62	128.88	111.00
1	A	348	GLN	CA-CB-CG	6.59	127.91	113.40
1	A	317	VAL	CA-CB-CG1	-6.57	101.05	110.90
1	A	257	LEU	CB-CA-C	-6.54	97.78	110.20
1	A	33	GLU	CA-CB-CG	6.53	127.77	113.40
1	A	236	PHE	O-C-N	-6.52	112.28	122.70
1	A	227	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	216	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	A	246	TYR	CA-CB-CG	6.49	125.72	113.40
1	A	231	GLY	CA-C-N	-6.46	103.00	117.20
1	A	266	VAL	CA-CB-CG1	6.45	120.58	110.90
1	A	372	ALA	CB-CA-C	-6.44	100.44	110.10
1	A	83	TRP	CD1-CG-CD2	6.43	111.44	106.30
1	A	244	TRP	CE2-CD2-CE3	6.41	126.39	118.70
1	A	313	LEU	CB-CG-CD2	-6.41	100.11	111.00
1	A	416	MET	CA-CB-CG	6.41	124.20	113.30
1	A	322	ILE	O-C-N	-6.40	112.46	122.70
1	A	57	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	A	395	ARG	CA-CB-CG	6.31	127.28	113.40
1	A	82	VAL	CA-CB-CG1	-6.28	101.48	110.90
1	A	365	ARG	O-C-N	6.28	132.74	122.70
1	A	399	GLY	N-CA-C	6.24	128.70	113.10
1	A	9	ALA	N-CA-C	6.22	127.79	111.00
1	A	266	VAL	N-CA-C	6.21	127.77	111.00
1	A	84	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	264	LEU	CA-C-N	6.15	130.72	117.20
1	A	266	VAL	N-CA-CB	-6.10	98.09	111.50
1	A	119	ARG	CG-CD-NE	6.07	124.54	111.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	VAL	CG1-CB-CG2	-6.04	101.23	110.90
1	A	371	GLU	CA-CB-CG	6.04	126.68	113.40
1	A	189	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	214	ILE	O-C-N	-6.03	113.05	122.70
1	A	97	VAL	CA-CB-CG1	6.02	119.93	110.90
1	A	185	VAL	CA-C-N	-6.01	103.97	117.20
1	A	332	CYS	N-CA-C	6.00	127.21	111.00
1	A	154	GLU	CA-CB-CG	5.98	126.55	113.40
1	A	406	SER	N-CA-CB	-5.93	101.61	110.50
1	A	223	ASP	N-CA-C	5.92	126.99	111.00
1	A	400	ALA	CB-CA-C	-5.91	101.23	110.10
1	A	264	LEU	O-C-N	-5.89	113.27	122.70
1	A	222	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	132	ARG	CA-CB-CG	5.85	126.28	113.40
1	A	76	GLN	C-N-CA	5.84	136.30	121.70
1	A	207	LYS	CB-CG-CD	-5.83	96.45	111.60
1	A	138	PRO	N-CA-C	5.82	127.24	112.10
1	A	141	VAL	CG1-CB-CG2	-5.82	101.60	110.90
1	A	263	TRP	CA-C-N	5.81	129.99	117.20
1	A	131	VAL	CA-CB-CG1	-5.78	102.23	110.90
1	A	366	HIS	N-CA-CB	-5.78	100.20	110.60
1	A	135	GLN	N-CA-C	5.77	126.58	111.00
1	A	165	TRP	CD1-CG-CD2	5.75	110.90	106.30
1	A	393	PHE	CA-C-O	-5.71	108.12	120.10
1	A	317	VAL	CA-CB-CG2	5.70	119.45	110.90
1	A	155	ASN	CA-CB-CG	5.67	125.87	113.40
1	A	330	ASP	N-CA-C	-5.66	95.71	111.00
1	A	263	TRP	CD1-CG-CD2	5.66	110.83	106.30
1	A	65	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	244	TRP	CG-CD1-NE1	-5.63	104.47	110.10
1	A	263	TRP	CE2-CD2-CG	-5.60	102.82	107.30
1	A	70	THR	CA-CB-CG2	5.58	120.21	112.40
1	A	149	MET	CA-CB-CG	5.51	122.67	113.30
1	A	278	LYS	CA-CB-CG	5.50	125.50	113.40
1	A	55	LYS	CA-C-N	5.47	129.24	117.20
1	A	244	TRP	CB-CG-CD2	-5.46	119.50	126.60
1	A	74	SER	CA-C-N	-5.46	105.19	117.20
1	A	31	TYR	N-CA-CB	-5.46	100.78	110.60
1	A	86	ALA	N-CA-CB	-5.46	102.46	110.10
1	A	329	GLY	CA-C-N	-5.45	105.21	117.20
1	A	361	GLU	CG-CD-OE2	5.44	129.18	118.30
1	A	115	ASN	O-C-N	-5.42	114.02	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	PRO	CA-CB-CG	-5.42	93.71	104.00
1	A	159	ILE	CA-C-N	5.41	129.10	117.20
1	A	48	VAL	N-CA-CB	-5.38	99.65	111.50
1	A	103	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	236	PHE	CA-C-N	5.38	129.03	117.20
1	A	77	VAL	O-C-N	-5.37	114.11	122.70
1	A	53	VAL	CA-CB-CG2	5.36	118.94	110.90
1	A	75	THR	N-CA-C	-5.36	96.53	111.00
1	A	226	THR	CA-C-N	-5.33	105.48	117.20
1	A	83	TRP	CG-CD2-CE3	5.30	138.67	133.90
1	A	289	ILE	CA-CB-CG1	5.29	121.04	111.00
1	A	42	THR	N-CA-CB	-5.26	100.30	110.30
1	A	223	ASP	CB-CA-C	-5.25	99.91	110.40
1	A	308	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	A	367	MET	O-C-N	-5.23	114.30	123.20
1	A	159	ILE	CA-C-O	-5.23	109.11	120.10
1	A	362	MET	CB-CG-SD	-5.22	96.74	112.40
1	A	193	HIS	CA-CB-CG	5.21	122.46	113.60
1	A	236	PHE	N-CA-C	-5.21	96.93	111.00
1	A	58	LYS	CB-CG-CD	-5.19	98.10	111.60
1	A	308	TYR	CB-CG-CD1	5.19	124.11	121.00
1	A	51	ALA	CB-CA-C	-5.19	102.32	110.10
1	A	74	SER	CA-C-O	5.18	130.99	120.10
1	A	401	LYS	N-CA-C	-5.17	97.05	111.00
1	A	166	LYS	CB-CG-CD	5.17	125.03	111.60
1	A	402	LEU	O-C-N	5.17	130.96	122.70
1	A	246	TYR	CD1-CE1-CZ	5.16	124.44	119.80
1	A	346	ALA	CA-C-O	-5.16	109.27	120.10
1	A	43	PRO	CA-N-CD	-5.16	104.28	111.50
1	A	256	GLU	CA-C-N	5.14	128.51	117.20
1	A	132	ARG	O-C-N	-5.13	114.49	122.70
1	A	352	ASN	CB-CG-ND2	5.12	128.98	116.70
1	A	111	ILE	CA-C-N	5.11	128.45	117.20
1	A	53	VAL	CA-CB-CG1	-5.08	103.27	110.90
1	A	338	THR	CA-CB-CG2	-5.08	105.29	112.40
1	A	279	ASP	O-C-N	-5.07	114.58	122.70
1	A	5	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	A	242	LYS	CB-CG-CD	-5.05	98.46	111.60
1	A	203	GLU	CA-CB-CG	-5.04	102.32	113.40
1	A	96	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	362	MET	O-C-N	5.03	130.74	122.70
1	A	276	VAL	CA-CB-CG2	-5.02	103.37	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	VAL	CA-C-N	-5.02	106.17	117.20
1	A	7	VAL	CA-CB-CG1	-5.01	103.39	110.90
1	A	143	HIS	CA-CB-CG	5.00	122.11	113.60
1	A	119	ARG	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	ARG	Peptide
1	A	125	TYR	Sidechain
1	A	134	TYR	Sidechain
1	A	261	GLY	Peptide
1	A	296	TYR	Sidechain
1	A	31	TYR	Sidechain
1	A	69	TYR	Sidechain

## 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	3196	684	3222	97	0
2	A	1	0	0	0	0
3	A	10	0	4	1	0
All	All	3207	684	3226	97	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 15.

All (97) 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:343:PRO:HA	1:A:346:ALA:HB2	1.32	1.11
1:A:207:LYS:HG2	1:A:248:LEU:HB2	1.56	0.85
1:A:97:VAL:HG11	1:A:367:MET:SD	2.23	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:O	1:A:206:THR:HG23	1.87	0.74
1:A:131:VAL:HG11	1:A:314:ALA:HA	1.68	0.74
1:A:30:PRO:HG2	1:A:98:ALA:HB2	1.68	0.74
1:A:343:PRO:HA	1:A:346:ALA:CB	2.15	0.72
1:A:307:ASP:OD1	3:A:418:AKG:O2	2.08	0.71
1:A:211:ARG:HA	1:A:248:LEU:HD11	1.74	0.70
1:A:179:LEU:HA	1:A:183:MET:HB2	1.75	0.69
1:A:247:GLN:HA	1:A:250:ARG:HB2	1.74	0.68
1:A:324:PRO:HB3	1:A:358:LEU:HB3	1.76	0.67
1:A:227:LEU:O	1:A:279:ASP:HA	1.94	0.67
1:A:128:LEU:HD12	1:A:130:PRO:HD3	1.76	0.65
1:A:335:PHE:CD2	1:A:363:MET:HG2	2.31	0.65
1:A:360:ALA:O	1:A:363:MET:HB2	1.98	0.64
1:A:138:PRO:HG2	1:A:393:PHE:CD1	2.32	0.64
1:A:229:HIS:O	1:A:281:ILE:HA	1.99	0.63
1:A:413:ILE:HA	1:A:416:MET:SD	2.40	0.61
1:A:84:LEU:HD13	1:A:111:ILE:HG23	1.81	0.61
1:A:14:ILE:HD12	1:A:97:VAL:HG12	1.82	0.60
1:A:201:CYS:HB3	1:A:237:THR:HA	1.82	0.59
1:A:138:PRO:HG2	1:A:393:PHE:HD1	1.68	0.59
1:A:226:THR:O	1:A:299:ILE:HA	2.02	0.58
1:A:115:ASN:O	1:A:119:ARG:HG3	2.04	0.58
1:A:142:LYS:O	1:A:144:PRO:HD3	2.05	0.56
1:A:335:PHE:CG	1:A:363:MET:HG2	2.40	0.56
1:A:77:VAL:HG12	1:A:78:TYR:CD1	2.40	0.56
1:A:49:VAL:HG12	1:A:63:ILE:HD12	1.88	0.54
1:A:93:ARG:HH21	1:A:122:LEU:HD23	1.73	0.54
1:A:141:VAL:HG23	1:A:144:PRO:HB3	1.90	0.53
1:A:309:ILE:O	1:A:313:LEU:HB2	2.08	0.53
1:A:284:ALA:O	1:A:288:GLN:HG2	2.09	0.53
1:A:57:TYR:O	1:A:60:GLU:HG2	2.08	0.53
1:A:29:ILE:HD12	1:A:63:ILE:HD13	1.91	0.53
1:A:45:MET:O	1:A:48:VAL:HG12	2.08	0.53
1:A:201:CYS:CB	1:A:237:THR:HA	2.38	0.52
1:A:37:ILE:HD11	1:A:340:GLY:O	2.08	0.52
1:A:363:MET:O	1:A:366:HIS:HB3	2.09	0.52
1:A:389:VAL:HG22	1:A:400:ALA:HB2	1.92	0.52
1:A:176:ILE:HG12	1:A:196:ILE:HD12	1.91	0.51
1:A:153:ARG:HG3	1:A:306:GLY:HA3	1.94	0.50
1:A:218:ILE:HG21	1:A:269:PRO:HD2	1.94	0.50
1:A:255:GLY:HA2	1:A:265:LYS:O	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:TYR:HA	1:A:99:ILE:O	2.13	0.49
1:A:138:PRO:HD3	1:A:397:MET:HB2	1.94	0.48
1:A:313:LEU:O	1:A:316:GLN:HG2	2.12	0.48
1:A:126:ILE:O	1:A:327:ASN:HA	2.14	0.47
1:A:394:GLU:HA	1:A:397:MET:HB3	1.97	0.47
1:A:269:PRO:HG2	1:A:270:ASN:OD1	2.14	0.47
1:A:393:PHE:O	1:A:397:MET:HB3	2.14	0.47
1:A:199:LYS:NZ	1:A:238:GLU:HG2	2.30	0.46
1:A:247:GLN:HG3	1:A:250:ARG:HD2	1.96	0.46
1:A:289:ILE:HD12	1:A:313:LEU:HD13	1.97	0.46
1:A:77:VAL:HG12	1:A:78:TYR:HD1	1.79	0.46
1:A:350:LYS:HD2	1:A:404:LYS:HE2	1.97	0.46
1:A:206:THR:O	1:A:210:VAL:HG23	2.16	0.46
1:A:157:GLU:HB3	1:A:200:PRO:O	2.16	0.45
1:A:175:VAL:O	1:A:178:PHE:HB3	2.17	0.45
1:A:360:ALA:O	1:A:364:LEU:HG	2.16	0.45
1:A:66:MET:CE	1:A:91:LEU:HD22	2.47	0.45
1:A:358:LEU:O	1:A:362:MET:HG3	2.17	0.45
1:A:159:ILE:HG21	1:A:304:LEU:HD13	1.99	0.44
1:A:23:VAL:HA	1:A:24:PRO:HD3	1.64	0.44
1:A:30:PRO:HD2	1:A:97:VAL:O	2.17	0.44
1:A:32:ILE:HG23	1:A:69:TYR:HA	2.00	0.44
1:A:25:GLU:O	1:A:61:ARG:HA	2.17	0.44
1:A:285:PHE:HA	1:A:288:GLN:HG2	1.99	0.44
1:A:6:VAL:O	1:A:66:MET:HG3	2.18	0.44
1:A:57:TYR:OH	1:A:371:GLU:HG2	2.18	0.43
1:A:66:MET:HE1	1:A:91:LEU:HD22	2.01	0.43
1:A:217:ALA:HA	1:A:222:ARG:HB2	2.00	0.43
1:A:224:SER:HB2	1:A:297:ASP:HB3	2.01	0.43
1:A:247:GLN:HA	1:A:250:ARG:HD2	1.99	0.43
1:A:175:VAL:O	1:A:179:LEU:HD22	2.18	0.42
1:A:236:PHE:O	1:A:238:GLU:N	2.52	0.42
1:A:289:ILE:HD13	1:A:289:ILE:HG21	1.92	0.42
1:A:142:LYS:HG3	1:A:143:HIS:N	2.34	0.42
1:A:126:ILE:HD11	1:A:212:ALA:CB	2.49	0.42
1:A:234:MET:HE2	1:A:238:GLU:HG3	2.01	0.42
1:A:24:PRO:HD2	1:A:27:PRO:HB3	2.01	0.42
1:A:143:HIS:H	1:A:143:HIS:CD2	2.38	0.42
1:A:102:PRO:HG3	1:A:339:HIS:HD1	1.84	0.42
1:A:152:PHE:CE1	1:A:298:VAL:HG13	2.55	0.42
1:A:211:ARG:HB2	1:A:211:ARG:HE	1.78	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:HE2	1:A:58:LYS:HB3	1.80	0.42
1:A:49:VAL:HG21	1:A:360:ALA:HB1	2.02	0.41
1:A:171:ASP:O	1:A:175:VAL:HG23	2.20	0.41
1:A:361:GLU:O	1:A:365:ARG:HG2	2.20	0.41
1:A:258:ILE:HD13	1:A:265:LYS:HE2	2.01	0.41
1:A:137:THR:HG22	1:A:138:PRO:HD2	2.03	0.41
1:A:138:PRO:O	1:A:140:PRO:HD3	2.21	0.41
1:A:31:TYR:HB2	1:A:99:ILE:HG23	2.03	0.40
1:A:83:TRP:CE3	1:A:106:PRO:HD3	2.56	0.40
1:A:164:GLU:HG3	1:A:164:GLU:O	2.21	0.40
1:A:337:ALA:HB1	1:A:339:HIS:CE1	2.57	0.40
1:A:159:ILE:HD12	1:A:159:ILE:HA	1.86	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	412/416 (99%)	319 (77%)	65 (16%)	28 (7%)	<a href="#">1</a> <a href="#">2</a>

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	9	ALA
1	A	96	ARG
1	A	135	GLN
1	A	138	PRO
1	A	320	ILE
1	A	346	ALA
1	A	405	CYS
1	A	20	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	77	VAL
1	A	113	SER
1	A	215	GLU
1	A	237	THR
1	A	262	PRO
1	A	269	PRO
1	A	282	ALA
1	A	347	GLY
1	A	4	LYS
1	A	187	LYS
1	A	270	ASN
1	A	395	ARG
1	A	73	LYS
1	A	136	GLY
1	A	258	ILE
1	A	8	PRO
1	A	191	PRO
1	A	342	ALA
1	A	261	GLY

### 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	336/338 (99%)	282 (84%)	54 (16%)	<b>3</b> <b>7</b>

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	ASN
1	A	23	VAL
1	A	26	ASN
1	A	31	TYR
1	A	43	PRO
1	A	48	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	55	LYS
1	A	67	GLU
1	A	69	TYR
1	A	70	THR
1	A	82	VAL
1	A	84	LEU
1	A	90	ASP
1	A	96	ARG
1	A	118	LEU
1	A	128	LEU
1	A	131	VAL
1	A	137	THR
1	A	140	PRO
1	A	142	LYS
1	A	143	HIS
1	A	150	VAL
1	A	156	SER
1	A	179	LEU
1	A	180	ARG
1	A	185	VAL
1	A	189	ARG
1	A	223	ASP
1	A	233	ILE
1	A	235	LYS
1	A	250	ARG
1	A	262	PRO
1	A	268	ASN
1	A	278	LYS
1	A	281	ILE
1	A	286	LEU
1	A	290	LEU
1	A	304	LEU
1	A	324	PRO
1	A	334	LEU
1	A	339	HIS
1	A	349	ASP
1	A	356	ILE
1	A	358	LEU
1	A	361	GLU
1	A	363	MET
1	A	371	GLU
1	A	381	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	385	ASN
1	A	388	THR
1	A	391	TYR
1	A	396	LEU
1	A	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS

### 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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	AKG	A	418	2	3,9,9	5.65	2 (66%)	4,11,11	2.30	1 (25%)

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	AKG	A	418	2	-	0/3/9/9	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	418	AKG	O5-C2	-7.16	1.10	1.22
3	A	418	AKG	C3-C2	-6.67	1.40	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	418	AKG	C3-C4-C5	-4.05	105.74	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	418	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.