



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:47 pm BST

PDB ID : 3AOW  
Title : Crystal structure of Pyrococcus horikoshii kynurenine aminotransferase in complex with AKG  
Authors : Okada, K.; Angkawidjaja, C.; Koga, Y.; Takano, K.; Kanaya, S.  
Deposited on : 2010-10-07  
Resolution : 1.56 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

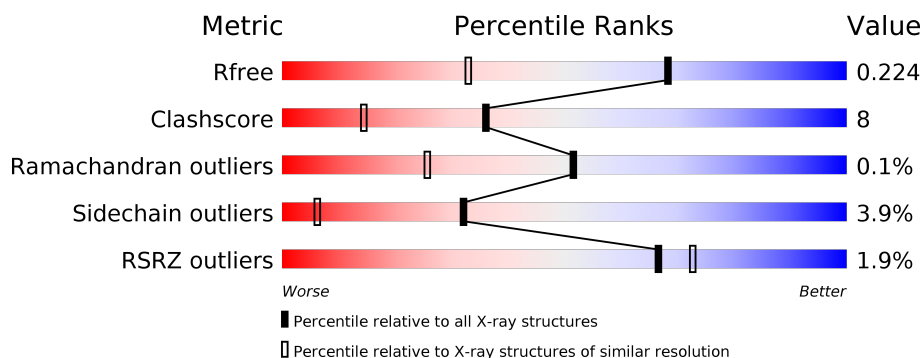
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.56 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))
$R_{free}$	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (1.56-1.56)

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 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  $\leq 5\%$ . 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	448	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>15%</div> <div>••</div> <div>10%</div> </div> </div>
1	C	448	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7382 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 Putative uncharacterized protein PH0207.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3247	2093	536	602	16			
1	C	404	Total	C	N	O	S	0	0	0
			3247	2093	536	602	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O57946
A	-18	GLY	-	EXPRESSION TAG	UNP O57946
A	-17	SER	-	EXPRESSION TAG	UNP O57946
A	-16	SER	-	EXPRESSION TAG	UNP O57946
A	-15	HIS	-	EXPRESSION TAG	UNP O57946
A	-14	HIS	-	EXPRESSION TAG	UNP O57946
A	-13	HIS	-	EXPRESSION TAG	UNP O57946
A	-12	HIS	-	EXPRESSION TAG	UNP O57946
A	-11	HIS	-	EXPRESSION TAG	UNP O57946
A	-10	HIS	-	EXPRESSION TAG	UNP O57946
A	-9	SER	-	EXPRESSION TAG	UNP O57946
A	-8	SER	-	EXPRESSION TAG	UNP O57946
A	-7	GLY	-	EXPRESSION TAG	UNP O57946
A	-6	LEU	-	EXPRESSION TAG	UNP O57946
A	-5	VAL	-	EXPRESSION TAG	UNP O57946
A	-4	PRO	-	EXPRESSION TAG	UNP O57946
A	-3	ARG	-	EXPRESSION TAG	UNP O57946
A	-2	GLY	-	EXPRESSION TAG	UNP O57946
A	-1	SER	-	EXPRESSION TAG	UNP O57946
A	0	HIS	-	EXPRESSION TAG	UNP O57946
C	-19	MET	-	EXPRESSION TAG	UNP O57946
C	-18	GLY	-	EXPRESSION TAG	UNP O57946
C	-17	SER	-	EXPRESSION TAG	UNP O57946
C	-16	SER	-	EXPRESSION TAG	UNP O57946
C	-15	HIS	-	EXPRESSION TAG	UNP O57946

*Continued on next page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP O57946
C	-13	HIS	-	EXPRESSION TAG	UNP O57946
C	-12	HIS	-	EXPRESSION TAG	UNP O57946
C	-11	HIS	-	EXPRESSION TAG	UNP O57946
C	-10	HIS	-	EXPRESSION TAG	UNP O57946
C	-9	SER	-	EXPRESSION TAG	UNP O57946
C	-8	SER	-	EXPRESSION TAG	UNP O57946
C	-7	GLY	-	EXPRESSION TAG	UNP O57946
C	-6	LEU	-	EXPRESSION TAG	UNP O57946
C	-5	VAL	-	EXPRESSION TAG	UNP O57946
C	-4	PRO	-	EXPRESSION TAG	UNP O57946
C	-3	ARG	-	EXPRESSION TAG	UNP O57946
C	-2	GLY	-	EXPRESSION TAG	UNP O57946
C	-1	SER	-	EXPRESSION TAG	UNP O57946
C	0	HIS	-	EXPRESSION TAG	UNP O57946

- PLP
- 
- The diagram shows the chemical structure of PLP (Pyridoxal Phosphate). It consists of a central pyridine ring. At the 2-position of the ring, there is a hydroxyl group (-OH) labeled O3. At the 3-position, there is a carboxylate group (-COO-) labeled C4A and O4A. At the 4-position, there is a phosphate group (-PO3^2-) labeled C5A, O4P, O3P, and O1P. The pyridine ring is labeled with N1, C2, C3, C4, C5, and C6. The phosphate group is labeled with P. The hydroxyl group is labeled with O3. The carboxylate group is labeled with C4A and O4A. The phosphate group is labeled with C5A, O4P, O3P, and O1P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	C	1	Total 15	C 8	N 1	O 5	P 1	0	0

- 



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	422	Total	O	0	0
			422	422		
4	C	416	Total	O	0	0
			416	416		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.77Å 70.98Å 136.72Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	26.81 – 1.56 26.81 – 1.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (26.81-1.56) 99.5 (26.81-1.56)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.177 , 0.224 0.179 , 0.224	Depositor DCC
$R_{free}$ test set	5780 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, PLP

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	1.25	3/3313 (0.1%)	1.18	14/4463 (0.3%)
1	C	1.25	3/3313 (0.1%)	1.16	6/4463 (0.1%)
All	All	1.25	6/6626 (0.1%)	1.17	20/8926 (0.2%)

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	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	TYR	CE2-CZ	-5.87	1.30	1.38
1	C	390	TYR	CG-CD2	5.70	1.46	1.39
1	A	330	LYS	CE-NZ	5.66	1.63	1.49
1	A	358	PHE	CD2-CE2	5.57	1.50	1.39
1	A	184	GLU	CB-CG	5.12	1.61	1.52
1	C	94	TYR	CD2-CE2	-5.11	1.31	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	173	LEU	CB-CG-CD2	-5.98	100.84	111.00
1	A	409	ASP	CB-CG-OD2	5.96	123.66	118.30
1	C	98	LYS	CD-CE-NZ	-5.88	98.19	111.70
1	A	267	PHE	CB-CG-CD1	-5.87	116.69	120.80

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	A	107	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	161	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	C	190	LEU	CB-CG-CD1	-5.51	101.63	111.00
1	A	98	LYS	CD-CE-NZ	-5.50	99.06	111.70
1	C	332	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	175	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	417	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	191	LYS	CD-CE-NZ	-5.39	99.30	111.70
1	C	358	PHE	CB-CG-CD2	-5.35	117.06	120.80
1	A	298	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	230	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	243	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	104	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	138	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	LEU	Peptide
1	A	405	TYR	Peptide
1	A	406	VAL	Peptide

## 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	3247	0	3306	60	0
1	C	3247	0	3306	55	0
2	A	15	0	6	1	0
2	C	15	0	6	2	0
3	A	10	0	4	1	0
3	C	10	0	4	2	0
4	A	422	0	0	19	0
4	C	416	0	0	18	0
All	All	7382	0	6632	105	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 8.

All (105) 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:C:85:GLU:HG2	4:C:780:HOH:O	1.46	1.12
1:A:320:LYS:HE2	4:A:782:HOH:O	1.62	0.97
1:A:142:ASN:HD21	1:C:36:LYS:H	1.08	0.97
1:A:169:ILE:CD1	1:A:190:LEU:HD11	1.95	0.96
1:C:170:GLN:NE2	1:C:392:HIS:H	1.67	0.93
1:A:170:GLN:NE2	1:A:392:HIS:H	1.68	0.92
1:A:36:LYS:H	1:C:142:ASN:HD21	1.10	0.92
1:C:106:THR:HG23	4:C:544:HOH:O	1.73	0.88
1:C:412:MET:HG2	4:C:574:HOH:O	1.78	0.81
1:A:170:GLN:HE22	1:A:392:HIS:H	1.29	0.79
1:A:56:SER:HB2	4:A:547:HOH:O	1.83	0.78
1:C:224:GLU:HG2	4:C:786:HOH:O	1.81	0.78
1:A:82:GLU:HG3	1:A:86:LYS:HE3	1.65	0.78
1:A:106:THR:HG23	4:A:605:HOH:O	1.83	0.77
1:A:169:ILE:HD11	1:A:190:LEU:HD11	1.64	0.76
1:A:36:LYS:NZ	1:A:36:LYS:HB2	2.02	0.75
1:C:100:PHE:H	1:C:306:GLN:HE22	1.35	0.74
1:C:342:GLU:HG2	4:C:535:HOH:O	1.88	0.73
1:A:100:PHE:H	1:A:306:GLN:HE22	1.37	0.72
1:A:406:VAL:HG22	4:A:620:HOH:O	1.90	0.71
1:A:43:ALA:HB2	1:C:288:ARG:NH2	2.07	0.70
1:C:170:GLN:HE22	1:C:392:HIS:H	1.35	0.70
1:C:77:ARG:NH1	4:C:722:HOH:O	2.26	0.68
1:C:100:PHE:H	1:C:306:GLN:NE2	1.92	0.66
1:C:364:PRO:HB3	4:C:836:HOH:O	1.97	0.65
1:A:142:ASN:HD21	1:C:36:LYS:N	1.89	0.65
1:A:142:ASN:ND2	1:C:36:LYS:H	1.90	0.62
1:A:100:PHE:H	1:A:306:GLN:NE2	1.96	0.62
1:C:407:ASP:C	1:C:407:ASP:OD2	2.37	0.62
1:A:44:SER:HB3	1:A:47:ARG:HB3	1.81	0.61
1:A:170:GLN:HE21	1:A:391:ALA:HB3	1.66	0.61
1:A:73:LYS:HE3	4:A:519:HOH:O	2.00	0.60
1:A:288:ARG:NH2	1:C:43:ALA:HB2	2.17	0.58
1:C:375:ARG:HG3	4:C:584:HOH:O	2.03	0.58
1:A:36:LYS:HZ3	1:A:36:LYS:HB2	1.67	0.58
1:C:407:ASP:OD2	1:C:409:ASP:OD2	2.22	0.58
1:C:170:GLN:HE21	1:C:391:ALA:HB3	1.70	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ASP:HB3	4:C:502:HOH:O	2.05	0.57
1:A:138:ARG:HG2	1:A:164:TYR:OH	2.06	0.56
1:C:108:MET:HB3	1:C:119:GLN:HE22	1.70	0.56
1:C:75:ILE:HD11	4:C:573:HOH:O	2.07	0.54
1:A:375:ARG:HG3	4:A:609:HOH:O	2.07	0.54
1:C:138:ARG:HG2	1:C:164:TYR:OH	2.08	0.54
1:C:250:LYS:HD3	1:C:255:LEU:HD21	1.90	0.54
1:A:407:ASP:C	1:A:407:ASP:OD1	2.47	0.53
1:A:138:ARG:NH2	1:C:164:TYR:OH	2.41	0.52
1:C:181:GLU:HG2	4:C:620:HOH:O	2.09	0.52
1:A:408:GLU:HB2	4:A:761:HOH:O	2.08	0.52
1:C:75:ILE:CD1	4:C:573:HOH:O	2.56	0.52
1:C:148:VAL:HB	1:C:200:VAL:HG22	1.92	0.52
1:A:170:GLN:NE2	1:A:392:HIS:N	2.48	0.51
1:A:352:LYS:NZ	4:A:1073:HOH:O	2.24	0.51
1:C:210:ALA:HA	1:C:360:TRP:HB2	1.93	0.50
1:A:374:GLU:O	1:A:378:LYS:HG3	2.11	0.50
1:C:408:GLU:HG2	1:C:409:ASP:N	2.26	0.50
1:C:389:PHE:HE1	4:C:608:HOH:O	1.93	0.49
1:A:77:ARG:NH1	4:A:680:HOH:O	2.44	0.49
3:A:430:AKG:O5	4:A:1445:HOH:O	2.20	0.49
1:C:154:TYR:CG	2:C:429:PLP:H2A3	2.48	0.49
1:A:108:MET:HB3	1:A:119:GLN:HE22	1.78	0.48
1:A:295:GLN:OE1	4:A:550:HOH:O	2.20	0.48
1:C:73:LYS:HE3	4:C:522:HOH:O	2.12	0.48
1:C:138:ARG:NH2	1:C:297:THR:HG22	2.30	0.47
1:C:114:ARG:HG2	1:C:115:TYR:CE1	2.50	0.47
3:C:430:AKG:H32	4:C:1451:HOH:O	2.13	0.46
1:A:36:LYS:HZ2	1:A:36:LYS:HB2	1.79	0.46
1:C:56:SER:HB2	4:C:550:HOH:O	2.15	0.46
1:C:170:GLN:NE2	1:C:392:HIS:N	2.50	0.46
1:A:36:LYS:H	1:C:142:ASN:ND2	1.94	0.46
1:A:36:LYS:N	1:C:142:ASN:HD21	1.93	0.46
1:A:408:GLU:CB	4:A:761:HOH:O	2.64	0.46
1:C:378:LYS:O	1:C:378:LYS:HG3	2.15	0.45
1:A:25:SER:N	4:A:1441:HOH:O	2.50	0.45
1:A:138:ARG:HG2	1:A:164:TYR:CZ	2.51	0.45
1:A:406:VAL:CG2	4:A:620:HOH:O	2.56	0.45
4:A:576:HOH:O	1:C:26:MET:HE3	2.16	0.45
1:A:43:ALA:CB	1:C:288:ARG:NH2	2.78	0.45
1:A:114:ARG:HG2	1:A:115:TYR:CE1	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ILE:HD12	1:A:190:LEU:HD11	1.89	0.44
1:A:119:GLN:NE2	4:A:508:HOH:O	2.50	0.44
1:A:154:TYR:CG	2:A:429:PLP:H2A3	2.53	0.44
1:A:320:LYS:CE	4:A:782:HOH:O	2.42	0.44
1:A:179:LYS:NZ	4:A:644:HOH:O	2.51	0.44
1:A:26:MET:HG3	1:C:259:GLY:HA3	2.00	0.44
1:A:148:VAL:HB	1:A:200:VAL:HG22	2.00	0.43
1:A:176:GLU:CD	1:A:215:ASN:HD22	2.22	0.43
3:C:430:AKG:O5	4:C:516:HOH:O	2.21	0.43
1:A:412:MET:HG2	4:A:522:HOH:O	2.19	0.43
1:A:81:VAL:O	1:A:85:GLU:HG3	2.19	0.43
1:C:269:LYS:NZ	2:C:429:PLP:C5A	2.81	0.43
1:A:210:ALA:HA	1:A:360:TRP:HB2	2.01	0.42
1:A:302:ASN:HA	1:C:276:ARG:HG2	2.00	0.42
1:A:150:GLU:HB3	1:A:173:LEU:HD21	2.01	0.42
1:C:409:ASP:N	1:C:409:ASP:OD2	2.53	0.42
1:A:408:GLU:O	1:A:410:LYS:N	2.53	0.41
1:A:82:GLU:CG	1:A:86:LYS:HE3	2.45	0.41
1:A:286:ILE:HG13	1:C:30:VAL:HG21	2.01	0.41
1:C:138:ARG:CG	1:C:164:TYR:OH	2.68	0.41
1:C:138:ARG:HG2	1:C:164:TYR:CZ	2.56	0.41
1:C:424:GLU:HA	1:C:427:LYS:HE2	2.02	0.41
1:C:76:ILE:O	1:C:80:LEU:HG	2.20	0.41
1:C:408:GLU:HB3	4:C:685:HOH:O	2.21	0.41
1:A:44:SER:O	1:A:48:GLU:HG2	2.21	0.41
1:C:288:ARG:O	1:C:288:ARG:HG3	2.20	0.41
1:A:375:ARG:NE	1:A:425:GLU:OE2	2.47	0.41

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	402/448 (90%)	387 (96%)	14 (4%)	1 (0%)	47	23
1	C	402/448 (90%)	388 (96%)	14 (4%)	0	100	100
All	All	804/896 (90%)	775 (96%)	28 (4%)	1 (0%)	51	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	GLU

### 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	349/388 (90%)	334 (96%)	15 (4%)	29	5
1	C	349/388 (90%)	337 (97%)	12 (3%)	37	9
All	All	698/776 (90%)	671 (96%)	27 (4%)	32	6

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	27	LEU
1	A	37	LYS
1	A	42	ARG
1	A	50	LEU
1	A	52	LEU
1	A	114	ARG
1	A	120	ASP
1	A	138	ARG
1	A	257	ASN
1	A	346	GLU
1	A	405	TYR
1	A	406	VAL
1	A	408	GLU
1	A	409	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	27	LEU
1	C	37	LYS
1	C	47	ARG
1	C	55	THR
1	C	57	ASP
1	C	114	ARG
1	C	120	ASP
1	C	181	GLU
1	C	196	LYS
1	C	405	TYR
1	C	406	VAL
1	C	407	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	142	ASN
1	A	170	GLN
1	A	306	GLN
1	C	119	GLN
1	C	142	ASN
1	C	170	GLN
1	C	306	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

4 ligands are 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$
3	AKG	A	430	-	3,9,9	2.01	1 (33%)	4,11,11	4.32	3 (75%)
2	PLP	A	429	1	15,15,16	1.42	1 (6%)	20,22,23	1.48	4 (20%)
3	AKG	C	430	-	3,9,9	0.92	0	4,11,11	3.11	2 (50%)
2	PLP	C	429	1	15,15,16	1.48	3 (20%)	20,22,23	1.66	5 (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	430	-	-	1/3/9/9	-
2	PLP	A	429	1	-	0/6/6/8	0/1/1/1
3	AKG	C	430	-	-	0/3/9/9	-
2	PLP	C	429	1	-	0/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	429	PLP	C3-C2	3.61	1.44	1.40
2	C	429	PLP	C2A-C2	2.88	1.55	1.50
3	A	430	AKG	O5-C2	2.86	1.26	1.22
2	C	429	PLP	C6-N1	2.52	1.39	1.34
2	C	429	PLP	C3-C2	2.11	1.43	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	430	AKG	C3-C4-C5	-6.41	101.92	112.67
3	C	430	AKG	C3-C4-C5	-5.34	103.72	112.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	430	AKG	C4-C3-C2	-4.33	103.81	113.14
2	C	429	PLP	C2A-C2-C3	3.38	125.07	120.89
3	A	430	AKG	O5-C2-C3	-3.34	114.68	120.38
2	A	429	PLP	C4A-C4-C5	-3.13	117.72	120.94
2	C	429	PLP	C6-C5-C4	2.79	120.36	118.16
3	C	430	AKG	C4-C3-C2	-2.75	107.20	113.14
2	A	429	PLP	C3-C2-N1	-2.69	117.30	120.77
2	A	429	PLP	C6-N1-C2	2.43	123.68	119.17
2	C	429	PLP	O4P-C5A-C5	2.37	113.88	109.35
2	C	429	PLP	C5-C6-N1	-2.35	119.91	123.82
2	C	429	PLP	C3-C2-N1	-2.29	117.81	120.77
2	A	429	PLP	C5-C6-N1	-2.09	120.34	123.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	430	AKG	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	430	AKG	1	0
2	A	429	PLP	1	0
3	C	430	AKG	2	0
2	C	429	PLP	2	0

## 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/448 (90%)	-0.32	8 (1%) 65 71	14, 21, 44, 60	0
1	C	404/448 (90%)	-0.31	7 (1%) 70 75	14, 21, 43, 58	0
All	All	808/896 (90%)	-0.31	15 (1%) 66 73	14, 21, 44, 60	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	THR	4.8
1	A	428	ALA	4.2
1	C	55	THR	3.9
1	A	409	ASP	3.6
1	A	405	TYR	3.4
1	C	428	ALA	2.9
1	C	405	TYR	2.6
1	C	407	ASP	2.5
1	A	43	ALA	2.4
1	C	409	ASP	2.4
1	C	365	ASP	2.4
1	C	43	ALA	2.3
1	A	51	LYS	2.3
1	A	365	ASP	2.1
1	A	406	VAL	2.0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	AKG	A	430	10/10	0.71	0.36	37,41,45,47	0
3	AKG	C	430	10/10	0.71	0.33	35,38,46,47	0
2	PLP	A	429	15/16	0.98	0.07	13,15,17,18	0
2	PLP	C	429	15/16	0.98	0.07	14,15,17,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.