



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:02 pm BST

PDB ID : 3PUQ  
Title : CEKDM7A from C.Elegans, complex with alpha-KG  
Authors : Yang, Y.; Wang, P.; Xu, W.; Xu, Y.  
Deposited on : 2010-12-06  
Resolution : 2.25 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.

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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 : 1.8.5 (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

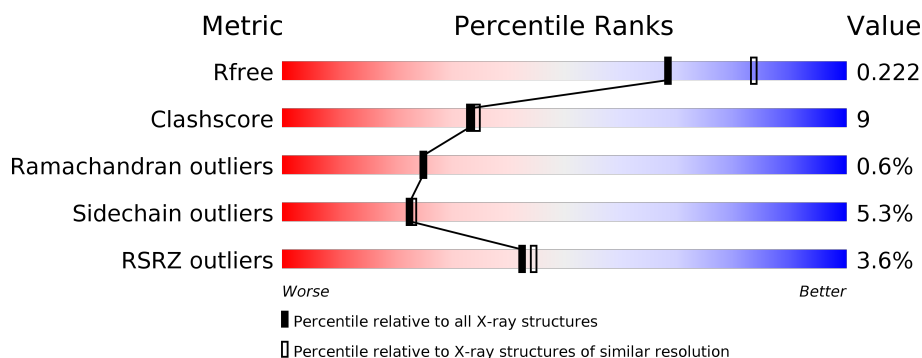
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	528	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	528	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8612 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 Lysine-specific demethylase 7 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3879	2480	651	721	27			
1	C	471	Total	C	N	O	S	0	0	0
			3872	2476	650	719	27			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	GLU	-	EXPRESSION TAG	UNP Q9GYI0
A	185	PHE	-	EXPRESSION TAG	UNP Q9GYI0
A	186	HIS	-	EXPRESSION TAG	UNP Q9GYI0
A	187	MET	-	EXPRESSION TAG	UNP Q9GYI0
C	184	GLU	-	EXPRESSION TAG	UNP Q9GYI0
C	185	PHE	-	EXPRESSION TAG	UNP Q9GYI0
C	186	HIS	-	EXPRESSION TAG	UNP Q9GYI0
C	187	MET	-	EXPRESSION TAG	UNP Q9GYI0

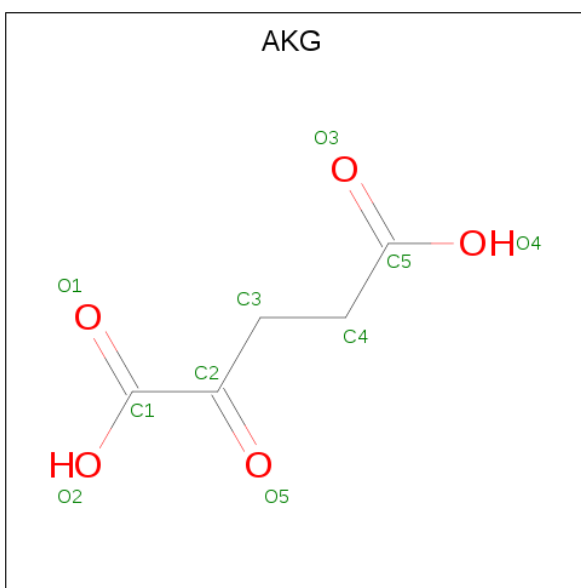
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

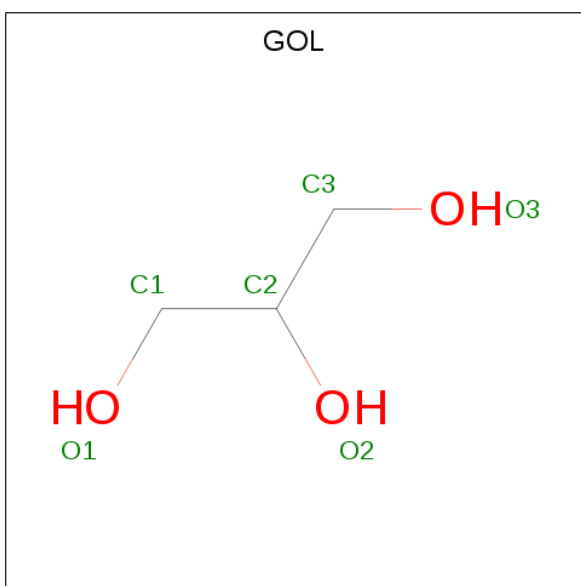
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula:  $C_5H_6O_5$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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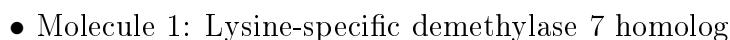
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	402	Total	O	0	0
			402	402		
6	C	421	Total	O	0	0
			421	421		



- Molecule 1: Lysine-specific demethylase 7 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.59Å 78.14Å 102.93Å 90.00° 92.07° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 38.60 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.25) 99.1 (38.60-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.09 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.188 , 0.224 0.183 , 0.222	Depositor DCC
$R_{free}$ test set	3574 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8612	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, AKG, FE2

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	1/3980 (0.0%)	0.54	0/5376
1	C	0.38	0/3973	0.53	0/5365
All	All	0.38	1/7953 (0.0%)	0.54	0/10741

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	CYS	CB-SG	-5.94	1.72	1.81

There are no bond angle outliers.

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	3879	0	3745	65	0
1	C	3872	0	3738	68	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	10	0	4	0	0
4	C	10	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	A	402	0	0	5	0
6	C	421	0	0	4	0
All	All	8612	0	7507	132	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 9.

All (132) 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:247:CYS:SG	1:C:249:THR:HG23	1.88	1.14
1:A:191:THR:HB	1:A:192:PRO:HD3	1.31	1.09
1:C:513:ILE:HD13	1:C:550:ARG:HH12	1.24	1.00
1:C:369:PRO:HG3	1:C:436:ILE:HG22	1.47	0.94
1:A:247:CYS:SG	1:A:249:THR:HG23	2.14	0.87
1:A:260:GLN:HE21	1:A:400:SER:H	1.24	0.85
1:A:369:PRO:HG3	1:A:436:ILE:HG22	1.61	0.83
1:C:513:ILE:HD13	1:C:550:ARG:NH1	1.92	0.83
1:C:260:GLN:HE21	1:C:400:SER:H	1.27	0.81
1:C:325:PRO:HG2	1:C:330:VAL:HG11	1.63	0.81
1:A:325:PRO:HG2	1:A:330:VAL:HG11	1.69	0.74
1:A:191:THR:HB	1:A:192:PRO:CD	2.12	0.74
1:A:376:GLU:OE2	1:A:411:ARG:HD2	1.87	0.73
1:C:702:ASN:O	1:C:705:ASN:HB2	1.88	0.73
1:A:430:ASN:HD22	1:A:433:MET:H	1.36	0.72
1:A:197:ARG:HG2	1:A:197:ARG:O	1.91	0.71
1:A:260:GLN:NE2	1:A:400:SER:H	1.89	0.69
1:C:297:PRO:O	1:C:300:LYS:HG3	1.90	0.69
1:A:664:MET:HG3	1:A:687:MET:HG3	1.74	0.69
1:C:319:GLU:OE1	1:C:550:ARG:NH1	2.25	0.69
1:C:643:ARG:HD2	1:C:701:GLN:CD	2.14	0.68
1:C:430:ASN:HD22	1:C:433:MET:H	1.40	0.67
1:A:191:THR:CB	1:A:192:PRO:HD3	2.19	0.66
1:C:369:PRO:HG3	1:C:436:ILE:CG2	2.25	0.66
1:C:569:VAL:HG21	4:C:4:AKG:H31	1.77	0.65
1:C:197:ARG:O	1:C:197:ARG:HG2	1.95	0.65
1:C:596:HIS:HE1	1:C:659:GLU:OE1	1.80	0.64
1:C:376:GLU:OE2	1:C:411:ARG:HD2	1.98	0.64
1:C:260:GLN:NE2	1:C:400:SER:H	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:LYS:NZ	1:C:195:SER:HB2	2.12	0.62
1:A:193:LYS:HD3	1:A:196:ASP:OD2	2.00	0.61
1:A:669:ARG:O	1:A:670:LEU:HD23	1.99	0.61
1:A:470:TYR:O	1:A:471:LEU:HB2	2.02	0.60
1:C:430:ASN:ND2	1:C:433:MET:H	2.00	0.60
1:C:507:ILE:HG13	1:C:553:ILE:HG22	1.84	0.60
1:A:630:GLU:O	1:A:634:GLU:HG3	2.02	0.59
1:C:513:ILE:HG21	1:C:550:ARG:NH1	2.17	0.59
1:C:563:ALA:H	1:C:587:ASN:ND2	2.00	0.59
1:C:320:ASN:H	1:C:320:ASN:HD22	1.50	0.59
1:A:325:PRO:HB2	1:A:330:VAL:HG12	1.84	0.58
1:A:247:CYS:HB3	1:A:249:THR:H	1.68	0.58
1:A:430:ASN:ND2	1:A:433:MET:H	2.02	0.58
1:C:283:ARG:HH22	1:C:418:LEU:HD22	1.68	0.58
1:A:244:CYS:SG	1:A:247:CYS:HB2	2.43	0.58
1:C:648:ASN:H	1:C:648:ASN:HD22	1.49	0.58
1:C:664:MET:HG3	1:C:687:MET:HG3	1.87	0.57
1:A:247:CYS:SG	1:A:249:THR:CG2	2.92	0.56
1:A:669:ARG:C	1:A:670:LEU:HD23	2.25	0.56
1:C:513:ILE:HG21	1:C:550:ARG:HH11	1.69	0.56
1:A:494:PHE:CD1	1:A:540:PHE:HB3	2.40	0.55
1:C:648:ASN:HD22	1:C:648:ASN:N	2.03	0.55
1:C:325:PRO:HB2	1:C:330:VAL:HG12	1.88	0.55
1:A:648:ASN:HD22	1:A:648:ASN:H	1.53	0.55
1:A:643:ARG:HD2	1:A:701:GLN:CD	2.26	0.55
1:A:563:ALA:H	1:A:587:ASN:ND2	2.04	0.55
1:C:423:LEU:HD22	4:C:4:AKG:H41	1.89	0.54
1:C:201:CYS:SG	1:C:203:LYS:HB2	2.47	0.54
1:A:426:GLU:HG3	1:A:478:LYS:O	2.08	0.54
1:C:625:ARG:HD2	1:C:626:ASN:OD1	2.07	0.54
1:A:625:ARG:HD2	1:A:626:ASN:OD1	2.07	0.54
1:A:456:VAL:HA	6:A:1720:HOH:O	2.08	0.54
1:C:194:GLU:OE1	1:C:195:SER:N	2.42	0.53
1:C:283:ARG:NH2	1:C:418:LEU:HD22	2.23	0.53
1:C:193:LYS:HZ2	1:C:195:SER:HB2	1.74	0.52
1:A:201:CYS:SG	1:A:203:LYS:HB2	2.50	0.51
1:C:563:ALA:H	1:C:587:ASN:HD22	1.59	0.51
1:C:619:LEU:HD23	1:C:619:LEU:C	2.32	0.50
1:A:553:ILE:N	1:A:553:ILE:HD12	2.26	0.49
1:C:641:ASP:OD1	1:C:643:ARG:HD3	2.12	0.49
1:A:191:THR:CB	1:A:192:PRO:CD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LEU:HD12	1:A:484:LEU:N	2.27	0.48
1:A:593:ARG:HD2	6:A:1728:HOH:O	2.13	0.48
1:A:641:ASP:OD1	1:A:643:ARG:HD3	2.13	0.48
1:C:372:GLY:HA2	6:C:1438:HOH:O	2.13	0.48
1:C:678:LEU:HD23	1:C:679:PRO:HD2	1.95	0.48
1:A:515:TYR:O	1:A:567:HIS:HA	2.14	0.48
1:C:386:TYR:HE2	1:C:425:LEU:HD13	1.78	0.48
1:C:690:VAL:O	1:C:694:ILE:HG12	2.14	0.47
1:C:647:LYS:O	1:C:651:THR:HG23	2.13	0.47
1:A:345:LYS:HG3	6:A:1556:HOH:O	2.14	0.47
1:A:690:VAL:O	1:A:694:ILE:HG12	2.14	0.47
1:C:193:LYS:HZ1	1:C:195:SER:HB2	1.79	0.47
1:A:503:VAL:CG1	1:A:581:ASN:ND2	2.78	0.47
1:C:494:PHE:CD1	1:C:540:PHE:HB3	2.50	0.47
1:A:650:TRP:CZ3	1:A:697:GLN:HG2	2.51	0.46
1:C:432:GLU:O	1:C:436:ILE:HG12	2.14	0.46
1:A:386:TYR:CE2	1:A:425:LEU:CD1	2.97	0.46
1:C:237:ASN:HA	1:C:240:GLN:OE1	2.16	0.46
1:A:647:LYS:O	1:A:651:THR:HG23	2.16	0.45
1:C:669:ARG:C	1:C:670:LEU:HD23	2.36	0.45
1:C:273:LYS:NZ	6:C:1221:HOH:O	2.49	0.45
1:C:605:ILE:HG13	1:C:605:ILE:O	2.16	0.45
1:A:283:ARG:HH22	1:A:418:LEU:HD22	1.82	0.44
1:A:204:PHE:O	1:A:205:THR:O	2.35	0.44
1:A:320:ASN:C	1:A:320:ASN:HD22	2.20	0.44
1:C:283:ARG:HG2	6:C:1190:HOH:O	2.17	0.44
1:A:508:LEU:HA	1:A:508:LEU:HD12	1.87	0.44
1:C:441:ARG:HA	1:C:444:GLN:HE21	1.83	0.44
1:C:470:TYR:O	1:C:471:LEU:HB2	2.18	0.44
1:A:478:LYS:HE3	6:A:1584:HOH:O	2.17	0.43
1:C:585:LEU:HD12	1:C:585:LEU:HA	1.70	0.43
1:A:319:GLU:OE1	1:A:550:ARG:NH1	2.50	0.43
1:C:677:ILE:HD12	1:C:677:ILE:N	2.34	0.43
1:A:204:PHE:O	1:A:205:THR:C	2.58	0.43
1:C:247:CYS:SG	1:C:249:THR:CG2	2.82	0.43
1:C:515:TYR:O	1:C:567:HIS:HA	2.19	0.42
1:A:283:ARG:NH2	1:A:418:LEU:HD22	2.33	0.42
1:C:368:MET:HG3	1:C:506:HIS:CD2	2.54	0.42
1:C:361:MET:HE3	1:C:366:MET:HE3	2.00	0.42
1:C:426:GLU:HG3	1:C:478:LYS:O	2.20	0.42
1:C:484:LEU:HD12	1:C:484:LEU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:SER:HA	1:A:534:PRO:HD3	1.92	0.42
1:A:402:LYS:HE2	6:A:1159:HOH:O	2.19	0.42
1:A:191:THR:HA	1:A:250:TRP:CH2	2.56	0.41
1:A:507:ILE:HG13	1:A:553:ILE:HG22	2.03	0.41
1:A:256:SER:OG	1:A:258:LEU:HB2	2.20	0.41
1:A:509:LYS:HE2	1:A:509:LYS:HB2	1.85	0.41
1:A:677:ILE:HD12	1:A:677:ILE:N	2.36	0.41
1:C:553:ILE:N	1:C:553:ILE:HD12	2.36	0.41
1:A:372:GLY:O	1:C:273:LYS:HE3	2.21	0.40
1:C:361:MET:HE3	1:C:366:MET:CE	2.51	0.40
1:A:364:LEU:HA	1:A:364:LEU:HD23	1.88	0.40
1:C:686:ILE:O	1:C:690:VAL:HG23	2.21	0.40
1:A:193:LYS:HG3	1:A:193:LYS:HZ3	1.73	0.40
1:A:247:CYS:CB	1:A:249:THR:HG23	2.52	0.40
1:A:648:ASN:HD22	1:A:648:ASN:N	2.18	0.40
1:C:370:LYS:CG	6:C:1712:HOH:O	2.69	0.40
1:C:448:MET:HB3	1:C:448:MET:HE2	2.00	0.40
1:C:471:LEU:HA	1:C:472:PRO:HD3	1.90	0.40
1:A:262:GLU:HA	1:A:265:LEU:HG	2.04	0.40
1:A:387:GLU:HA	1:A:387:GLU:OE1	2.21	0.40
1:A:551:VAL:HG23	1:A:553:ILE:HD11	2.02	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	466/528 (88%)	454 (97%)	9 (2%)	3 (1%)	25	25
1	C	465/528 (88%)	451 (97%)	11 (2%)	3 (1%)	25	25
All	All	931/1056 (88%)	905 (97%)	20 (2%)	6 (1%)	25	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	194	GLU
1	C	455	ASP
1	A	455	ASP
1	A	194	GLU
1	A	471	LEU
1	C	471	LEU

### 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	423/475 (89%)	402 (95%)	21 (5%)	24	26
1	C	422/475 (89%)	398 (94%)	24 (6%)	20	20
All	All	845/950 (89%)	800 (95%)	45 (5%)	22	23

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	LYS
1	A	195	SER
1	A	196	ASP
1	A	197	ARG
1	A	247	CYS
1	A	249	THR
1	A	258	LEU
1	A	283	ARG
1	A	320	ASN
1	A	379	VAL
1	A	418	LEU
1	A	456	VAL
1	A	470	TYR
1	A	498	PHE
1	A	551	VAL
1	A	585	LEU
1	A	611	PHE

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Mol	Chain	Res	Type
1	A	628	LEU
1	A	629	LEU
1	A	648	ASN
1	A	664	MET
1	C	193	LYS
1	C	194	GLU
1	C	196	ASP
1	C	197	ARG
1	C	249	THR
1	C	258	LEU
1	C	320	ASN
1	C	379	VAL
1	C	407	ARG
1	C	411	ARG
1	C	418	LEU
1	C	425	LEU
1	C	430	ASN
1	C	456	VAL
1	C	470	TYR
1	C	484	LEU
1	C	498	PHE
1	C	585	LEU
1	C	628	LEU
1	C	629	LEU
1	C	648	ASN
1	C	664	MET
1	C	678	LEU
1	C	705	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	320	ASN
1	A	395	ASN
1	A	421	ASN
1	A	430	ASN
1	A	475	GLN
1	A	587	ASN
1	A	596	HIS
1	A	648	ASN
1	A	705	ASN

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Mol	Chain	Res	Type
1	C	252	HIS
1	C	260	GLN
1	C	320	ASN
1	C	395	ASN
1	C	421	ASN
1	C	430	ASN
1	C	444	GLN
1	C	587	ASN
1	C	596	HIS
1	C	648	ASN

### 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 ⓘ

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	AKG	C	4	2	3,9,9	0.47	0	4,11,11	2.58	3 (75%)
4	AKG	A	4	2	3,9,9	0.43	0	4,11,11	2.05	1 (25%)
5	GOL	A	5	-	5,5,5	0.43	0	5,5,5	0.36	0
5	GOL	C	5	-	5,5,5	0.38	0	5,5,5	0.53	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	AKG	C	4	2	-	3/3/9/9	-
4	AKG	A	4	2	-	1/3/9/9	-
5	GOL	A	5	-	-	4/4/4/4	-
5	GOL	C	5	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	AKG	C3-C4-C5	3.45	118.45	112.67
4	C	4	AKG	C3-C4-C5	3.42	118.41	112.67
4	C	4	AKG	C4-C3-C2	3.09	119.82	113.14
4	C	4	AKG	O5-C2-C3	-2.29	116.46	120.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5	GOL	O1-C1-C2-C3
5	C	5	GOL	O1-C1-C2-C3
4	C	4	AKG	O5-C2-C3-C4
5	A	5	GOL	C1-C2-C3-O3
5	A	5	GOL	O1-C1-C2-O2
5	C	5	GOL	O1-C1-C2-O2
4	C	4	AKG	C1-C2-C3-C4
4	C	4	AKG	C2-C3-C4-C5
5	A	5	GOL	O2-C2-C3-O3
4	A	4	AKG	O5-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	AKG	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	472/528 (89%)	-0.04	15 (3%)	47	50	16, 33, 60, 100	0
1	C	471/528 (89%)	-0.04	19 (4%)	38	40	18, 33, 58, 94	0
All	All	943/1056 (89%)	-0.04	34 (3%)	42	44	16, 33, 60, 100	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	606	ARG	8.1
1	C	456	VAL	7.9
1	C	606	ARG	7.8
1	A	456	VAL	7.5
1	A	470	TYR	5.4
1	A	197	ARG	5.1
1	C	470	TYR	5.1
1	C	197	ARG	4.2
1	C	608	GLU	3.9
1	A	607	SER	3.7
1	A	239	PHE	3.7
1	C	607	SER	3.6
1	C	455	ASP	3.5
1	A	195	SER	3.5
1	A	608	GLU	3.4
1	C	706	LYS	3.3
1	C	609	GLU	3.3
1	C	670	LEU	3.3
1	C	675	ASN	3.2
1	A	609	GLU	3.0
1	C	674	LYS	3.0
1	C	239	PHE	3.0
1	A	191	THR	2.7
1	A	610	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	455	ASP	2.6
1	A	674	LYS	2.6
1	C	193	LYS	2.5
1	C	705	ASN	2.5
1	C	611	PHE	2.5
1	C	300	LYS	2.2
1	A	703	ALA	2.1
1	A	706	LYS	2.0
1	C	192	PRO	2.0
1	C	195	SER	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( $\text{\AA}^2$ )	Q<0.9
5	GOL	C	5	6/6	0.90	0.34	28,44,47,52	0
5	GOL	A	5	6/6	0.92	0.27	29,40,46,49	0
4	AKG	C	4	10/10	0.95	0.16	22,26,33,36	0
4	AKG	A	4	10/10	0.98	0.15	21,26,31,32	0
3	ZN	C	3	1/1	0.99	0.06	38,38,38,38	0
3	ZN	A	2	1/1	0.99	0.06	45,45,45,45	0
3	ZN	C	2	1/1	0.99	0.07	46,46,46,46	0
2	FE2	A	1	1/1	1.00	0.16	17,17,17,17	0
3	ZN	A	3	1/1	1.00	0.07	34,34,34,34	0
2	FE2	C	1	1/1	1.00	0.15	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.