



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:21 PM UTC

PDB ID : 3PUQ / pdb_00003puq
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

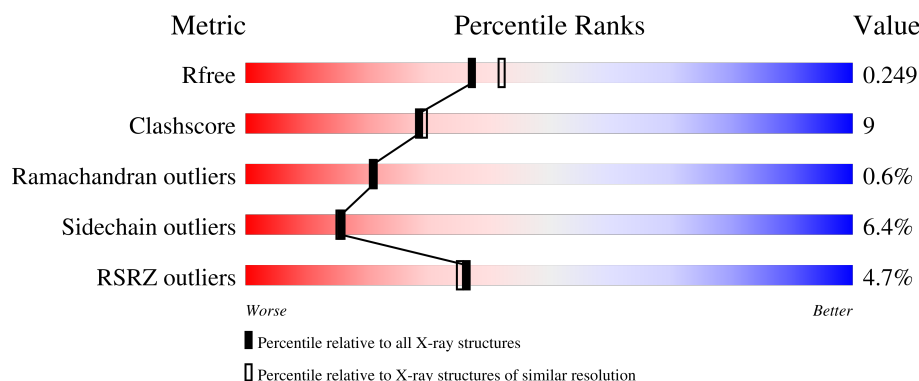
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

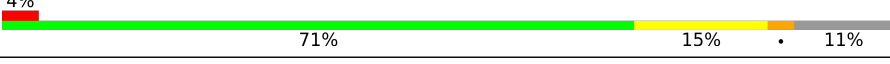
The reported resolution of this entry is 2.25 Å.

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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 of 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 $\leq 5\%$. 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	
1	C	528	

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	AKG	C	4	-	X	-	-

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

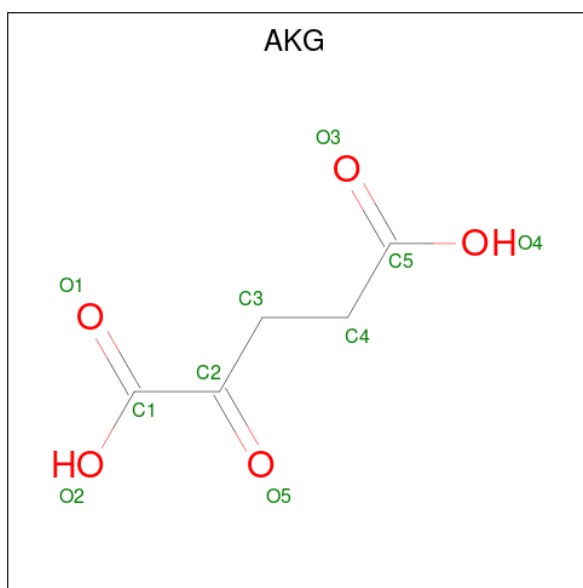
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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 (CCD ID: ZN) (formula: Zn).

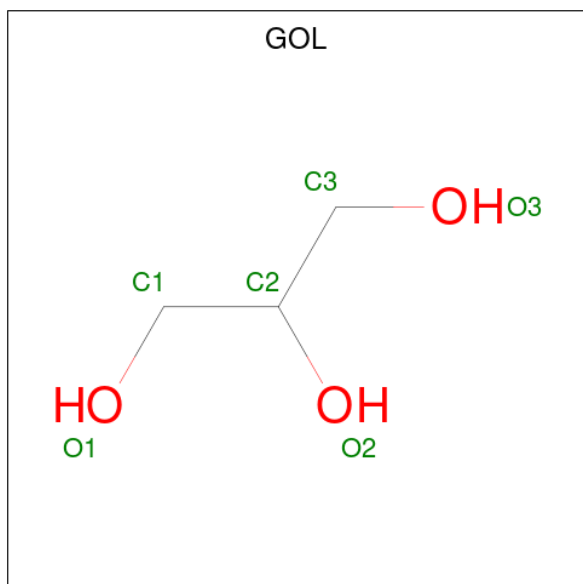
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 2-OXOGLUTARIC ACID (CCD ID: 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 (CCD ID: 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		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.59Å 78.14Å 102.93Å 90.00° 92.07° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.25) 99.4 (50.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.188 , 0.224 (Not available) , 0.249	Depositor DCC
R_{free} test set	3574 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ZN, FE2, GOL, 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	0.47	0/3980	0.82	4/5376 (0.1%)
1	C	0.47	0/3973	0.81	0/5365
All	All	0.47	0/7953	0.82	4/10741 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	611	PHE	N-CA-C	5.99	119.31	109.85
1	A	374	ASP	N-CA-C	5.93	116.06	108.24
1	A	288	ALA	CA-C-N	5.30	124.96	119.56
1	A	288	ALA	C-N-CA	5.30	124.96	119.56

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	69	0
1	C	3872	0	3738	67	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
4	A	10	0	4	0	0
4	C	10	0	4	3	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	A	402	0	0	6	0
6	C	421	0	0	4	0
All	All	8612	0	7507	135	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 (135) 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:C:643:ARG:HD2	1:C:701:GLN:CD	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:193:LYS:HZ2	1:C:195:SER:HB2	1.64	0.63
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:C	1:A:670:LEU:HD23	2.25	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:643:ARG:HD2	1:A:701:GLN:CD	2.26	0.59
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:HD22	1:C:320:ASN:H	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:HD22	1:C:648:ASN:H	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: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:H	1:A:648:ASN:HD22	1.53	0.55
1:A:563:ALA:H	1:A:587:ASN:ND2	2.04	0.55
1:C:448:MET:HE2	1:C:619:LEU:HD21	1.87	0.55
1:C:619:LEU:HD23	1:C:619:LEU:C	2.32	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:A:361:MET:HE3	6:A:1037:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:669:ARG:C	1:C:670:LEU:HD23	2.36	0.50
1:A:553:ILE:HD12	1:A:553:ILE:N	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
1:A:320:ASN:C	1:A:320:ASN:HD22	2.20	0.49
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:A:204:PHE:O	1:A:205:THR:C	2.58	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: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:378:VAL:HG22	1:A:433:MET:HE1	1.97	0.46
1:A:647:LYS:O	1:A:651:THR:HG23	2.16	0.45
1:C:273:LYS:NZ	6:C:1221:HOH:O	2.49	0.45
1:C:512:LYS:NZ	4:C:4:AKG:O4	2.50	0.45
1:C:605:ILE:O	1:C:605:ILE:HG13	2.16	0.45
1:C:425:LEU:HD12	1:C:425:LEU:C	2.42	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:C:283:ARG:HG2	6:C:1190:HOH:O	2.17	0.44
1:A:508:LEU:HD12	1:A:508:LEU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:454:PRO:O	1:A:455:ASP:C	2.63	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:664:MET:HA	1:A:664:MET:HE2	2.01	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:A:364:LEU:HD23	1:A:364:LEU:HA	1.88	0.40
1:C:686:ILE:O	1:C:690:VAL:HG23	2.21	0.40
1:A:193:LYS:HZ3	1:A:193:LYS:HG3	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: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 [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	466/528 (88%)	454 (97%)	9 (2%)	3 (1%)	21	21
1	C	465/528 (88%)	451 (97%)	11 (2%)	3 (1%)	21	21
All	All	931/1056 (88%)	905 (97%)	20 (2%)	6 (1%)	21	21

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%)	399 (94%)	24 (6%)	18	19
1	C	422/475 (89%)	392 (93%)	30 (7%)	13	12
All	All	845/950 (89%)	791 (94%)	54 (6%)	16	15

All (54) 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	282	ILE
1	A	287	VAL
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	379	VAL
1	A	411	ARG
1	A	418	LEU
1	A	456	VAL
1	A	498	PHE
1	A	551	VAL
1	A	585	LEU
1	A	611	PHE
1	A	619	LEU
1	A	628	LEU
1	A	629	LEU
1	A	643	ARG
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	282	ILE
1	C	320	ASN
1	C	379	VAL
1	C	403	LEU
1	C	407	ARG
1	C	411	ARG
1	C	418	LEU
1	C	425	LEU
1	C	456	VAL
1	C	470	TYR
1	C	484	LEU
1	C	498	PHE
1	C	543	ILE
1	C	551	VAL
1	C	573	VAL
1	C	585	LEU
1	C	628	LEU
1	C	629	LEU
1	C	643	ARG
1	C	648	ASN
1	C	664	MET
1	C	670	LEU

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Mol	Chain	Res	Type
1	C	678	LEU
1	C	705	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	260	GLN
1	A	298	ASN
1	A	320	ASN
1	A	351	ASN
1	A	395	ASN
1	A	421	ASN
1	A	430	ASN
1	A	475	GLN
1	A	581	ASN
1	A	587	ASN
1	A	596	HIS
1	A	648	ASN
1	A	705	ASN
1	C	237	ASN
1	C	252	HIS
1	C	260	GLN
1	C	320	ASN
1	C	351	ASN
1	C	395	ASN
1	C	421	ASN
1	C	430	ASN
1	C	444	GLN
1	C	581	ASN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	AKG	A	4	2	9,9,9	1.30	1 (11%)	11,11,11	1.63	3 (27%)
5	GOL	C	5	-	5,5,5	0.39	0	5,5,5	0.57	0
4	AKG	C	4	2	9,9,9	1.30	1 (11%)	11,11,11	2.13	6 (54%)
5	GOL	A	5	-	5,5,5	0.43	0	5,5,5	0.39	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	A	4	2	-	2/9/9/9	-
5	GOL	C	5	-	-	2/4/4/4	-
4	AKG	C	4	2	-	6/9/9/9	-
5	GOL	A	5	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4	AKG	C2-C1	-2.33	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4	AKG	C2-C1	-2.11	1.50	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4	AKG	C4-C3-C2	3.68	119.82	112.91
4	C	4	AKG	C3-C2-C1	3.24	121.36	115.86
4	A	4	AKG	O2-C1-O1	-2.53	117.87	123.90
4	C	4	AKG	O2-C1-C2	2.47	120.44	113.59
4	A	4	AKG	C4-C3-C2	2.33	117.29	112.91
4	C	4	AKG	O2-C1-O1	-2.26	118.53	123.90
4	C	4	AKG	O5-C2-C3	-2.20	116.46	121.17
4	C	4	AKG	O4-C5-O3	-2.13	117.85	123.33
4	A	4	AKG	O4-C5-C4	2.06	120.51	114.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	4	AKG	O2-C1-C2-C3
5	A	5	GOL	O1-C1-C2-C3
5	C	5	GOL	O1-C1-C2-C3
5	A	5	GOL	O1-C1-C2-O2
5	C	5	GOL	O1-C1-C2-O2
4	C	4	AKG	C2-C3-C4-C5
4	C	4	AKG	O5-C2-C3-C4
4	C	4	AKG	O1-C1-C2-C3
5	A	5	GOL	C1-C2-C3-O3
4	A	4	AKG	C1-C2-C3-C4
5	A	5	GOL	O2-C2-C3-O3
4	C	4	AKG	C3-C4-C5-O4
4	C	4	AKG	C3-C4-C5-O3
4	A	4	AKG	C3-C4-C5-O4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	4	AKG	3	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 ⓘ

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	472/528 (89%)	0.12	23 (4%) 35 34	16, 33, 60, 100	0
1	C	471/528 (89%)	0.12	21 (4%) 38 37	18, 33, 58, 94	0
All	All	943/1056 (89%)	0.12	44 (4%) 36 35	16, 33, 60, 100	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	456	VAL	7.1
1	C	470	TYR	6.2
1	C	611	PHE	5.6
1	A	195	SER	5.3
1	A	197	ARG	5.0
1	A	456	VAL	5.0
1	A	470	TYR	5.0
1	C	197	ARG	4.9
1	A	611	PHE	4.3
1	C	192	PRO	4.2
1	A	371	PRO	3.7
1	A	608	GLU	3.6
1	C	239	PHE	3.4
1	C	706	LYS	3.3
1	A	239	PHE	3.2
1	A	606	ARG	3.2
1	C	608	GLU	3.1
1	C	195	SER	3.0
1	C	196	ASP	3.0
1	C	606	ARG	2.9
1	C	705	ASN	2.9
1	C	371	PRO	2.8
1	C	612	TYR	2.8
1	A	196	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	676	ALA	2.6
1	A	706	LYS	2.6
1	A	612	TYR	2.6
1	A	191	THR	2.5
1	A	676	ALA	2.5
1	A	609	GLU	2.4
1	A	610	LYS	2.4
1	C	455	ASP	2.4
1	A	192	PRO	2.4
1	A	204	PHE	2.4
1	C	374	ASP	2.3
1	C	675	ASN	2.2
1	A	372	GLY	2.2
1	C	609	GLU	2.2
1	A	280	HIS	2.2
1	C	193	LYS	2.2
1	C	194	GLU	2.2
1	A	193	LYS	2.1
1	A	287	VAL	2.1
1	A	247	CYS	2.1

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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
5	GOL	C	5	6/6	0.82	0.15	28,44,47,52	0
5	GOL	A	5	6/6	0.90	0.12	29,40,46,49	0
4	AKG	C	4	10/10	0.95	0.09	22,26,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	A	4	10/10	0.97	0.06	21,26,31,32	0
3	ZN	C	2	1/1	0.99	0.03	46,46,46,46	0
3	ZN	C	3	1/1	0.99	0.03	38,38,38,38	0
3	ZN	A	2	1/1	0.99	0.03	45,45,45,45	0
2	FE2	C	1	1/1	1.00	0.03	17,17,17,17	0
2	FE2	A	1	1/1	1.00	0.04	17,17,17,17	0
3	ZN	A	3	1/1	1.00	0.01	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.