



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:28 PM GMT

PDB ID : 3KV6
Title : Structure of KIAA1718, human Jumonji demethylase, in complex with alpha-ketoglutarate
Authors : Horton, J.R.; Upadhyay, A.K.; Qi, H.H.; Zhang, X.; Shi, Y.; Cheng, X.
Deposited on : 2009-11-29
Resolution : 2.89 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

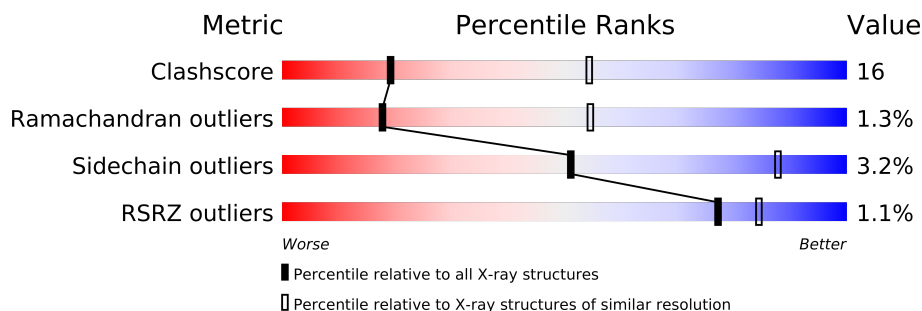
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.89 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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	488	
1	D	488	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	OXY	A	492	-	X
4	OXY	D	492	-	X
5	AKG	A	702	-	X
5	AKG	D	701	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7389 atoms, of which 0 are hydrogen and 0 are deuterium.

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 JmjC domain-containing histone demethylation protein 1D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	3	0
			3580	2305	609	640	26			
1	D	448	Total	C	N	O	S	0	2	0
			3614	2327	608	653	26			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

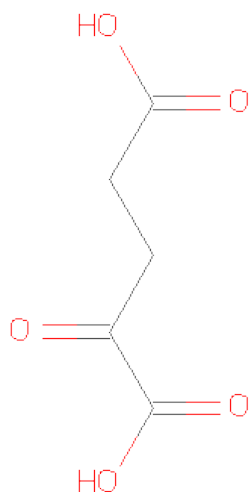
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			2	2		

- Molecule 5 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	82	Total 82	O 82	0	0
6	D	83	Total 83	O 83	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.40Å 125.20Å 206.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.54 – 2.89 34.55 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.3 (34.54-2.89) 93.1 (34.55-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.215 , 0.253 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 4.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 36619 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7389	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0/3684	0.62	0/5007
1	D	0.40	0/3720	0.63	0/5056
All	All	0.39	0/7404	0.62	0/10063

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3580	0	3440	112	0
1	D	3614	0	3475	120	0
2	A	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	10	0	4	1	0
5	D	10	0	4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	82	0	0	4	0
6	D	83	0	0	2	0
All	All	7389	0	6923	232	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (232) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:LYS:HD2	1:A:234:LYS:H	1.24	1.00
1:D:460:ARG:N	1:D:460:ARG:HD3	1.83	0.93
1:A:75:VAL:HG11	1:A:199:ARG:HH11	1.37	0.89
1:D:70:GLU:H	1:D:73[B]:HIS:HD2	1.22	0.88
1:A:185:TYR:O	1:A:234:LYS:HD3	1.78	0.84
1:D:408:LYS:HA	1:D:464:LEU:HD11	1.61	0.81
1:D:398:PHE:HB3	1:D:401:ALA:HB3	1.66	0.78
1:D:99:ASN:ND2	1:D:102:ARG:H	1.84	0.76
1:A:234:LYS:H	1:A:234:LYS:CD	1.93	0.75
1:A:234:LYS:HD2	1:A:234:LYS:N	2.01	0.75
1:A:416:GLU:O	1:A:420:ASP:HB2	1.88	0.74
1:D:159:PRO:HG2	1:D:303:LEU:HD13	1.69	0.74
1:D:460:ARG:HG2	1:D:463:HIS:HB3	1.68	0.73
1:D:148:GLN:OE1	1:D:247:LYS:HE3	1.88	0.73
1:A:297:GLY:HA3	1:A:362:CYS:HB2	1.71	0.72
1:D:299:LYS:HE2	1:D:362:CYS:SG	2.30	0.71
1:D:392:ASP:C	1:D:394:PHE:H	1.94	0.71
1:A:304:ILE:HD12	1:A:332:VAL:HG21	1.72	0.70
1:A:99:ASN:HD21	1:A:102:ARG:HG2	1.56	0.70
1:D:467:GLU:O	1:D:471:VAL:HG23	1.92	0.70
1:D:349:PRO:HG2	1:D:352:TRP:CD1	2.29	0.68
1:D:467:GLU:HA	1:D:470:LYS:HG2	1.76	0.67
1:D:99:ASN:HD21	1:D:102:ARG:H	1.42	0.67
1:A:75:VAL:HG11	1:A:199:ARG:NH1	2.07	0.66
1:A:398:PHE:HB3	1:A:401:ALA:HB3	1.78	0.66
1:A:249:SER:HB3	1:A:252:GLU:HB2	1.79	0.65
1:D:254:TYR:CD2	1:D:406:VAL:HG22	2.33	0.64
1:D:81:HIS:H	1:D:92:SER:HB3	1.61	0.63
1:D:110:ASP:O	1:D:112:SER:N	2.32	0.63
1:D:138:ILE:HG22	1:D:159:PRO:HB2	1.79	0.63
1:A:318:SER:HA	1:A:323:GLN:NE2	2.13	0.63
1:D:142:HIS:HB3	6:D:496:HOH:O	2.00	0.62
1:D:464:LEU:O	1:D:468:LEU:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:211:VAL:O	1:D:215:MET:HB2	2.01	0.61
1:D:408:LYS:HE3	1:D:460:ARG:HH12	1.64	0.61
1:A:100:TRP:CE3	1:A:100:TRP:HA	2.35	0.61
1:D:72:HIS:HD2	1:D:221:LYS:NZ	1.98	0.61
1:A:304:ILE:HB	1:A:353:ILE:HB	1.83	0.60
1:A:137:ILE:HG13	1:A:138:ILE:N	2.17	0.60
1:D:80:TYR:HA	1:D:92:SER:HB3	1.82	0.59
1:A:213:TYR:CE2	1:A:223:LEU:HB2	2.37	0.59
1:A:99:ASN:HB2	1:A:105:TYR:HA	1.82	0.59
1:A:349:PRO:HG2	1:A:352:TRP:CD1	2.37	0.59
1:A:417:LEU:HD12	1:A:424:PRO:HG3	1.85	0.59
1:A:112:SER:O	1:A:113:LYS:HB2	2.01	0.59
1:D:392:ASP:O	1:D:394:PHE:N	2.37	0.58
1:A:306:PRO:HG3	1:A:352:TRP:HA	1.85	0.58
1:A:159:PRO:HG2	1:A:303:LEU:HD13	1.85	0.57
1:D:287:GLY:O	1:D:350:THR:HG23	2.04	0.57
1:A:142[A]:HIS:HD2	1:A:144:SER:OG	1.88	0.57
1:A:267[A]:GLN:HG3	1:A:268:LYS:HG2	1.87	0.56
1:A:304:ILE:HD13	1:A:335:CYS:HA	1.86	0.56
1:D:412:GLU:O	1:D:416:GLU:HG3	2.05	0.56
1:D:435:LEU:O	1:D:439:LEU:HD13	2.05	0.56
1:D:468:LEU:O	1:D:472:ILE:HG13	2.05	0.56
1:A:414:LEU:HD11	1:A:432:VAL:HG21	1.87	0.56
1:A:100:TRP:HA	1:A:100:TRP:HE3	1.70	0.56
1:A:461:PRO:O	1:A:465:ILE:HG13	2.06	0.56
1:D:410:LEU:HD13	1:D:432:VAL:HG22	1.86	0.56
1:D:254:TYR:HD2	1:D:406:VAL:HG22	1.69	0.55
1:A:151:LEU:HD12	1:A:244:ILE:HD11	1.87	0.55
1:D:392:ASP:C	1:D:394:PHE:N	2.59	0.55
1:A:254:TYR:CD2	1:A:406:VAL:HG22	2.43	0.54
1:A:399:PHE:O	1:A:402:ILE:HG22	2.08	0.54
1:A:290:VAL:HG23	1:A:367:GLY:O	2.08	0.54
1:D:356:VAL:HG21	5:D:701:AKG:H41	1.90	0.54
1:D:315:GLU:HB2	1:D:384:MET:CE	2.38	0.54
1:A:435:LEU:O	1:A:439:LEU:HD13	2.07	0.53
1:A:379:LEU:HD13	1:A:438:ALA:HB2	1.90	0.53
1:A:197:VAL:HG11	1:A:278:TYR:H	1.74	0.53
1:D:207:LEU:O	1:D:211:VAL:HG23	2.08	0.53
1:D:408:LYS:CE	1:D:460:ARG:HH12	2.21	0.53
1:D:110:ASP:OD1	1:D:112:SER:CB	2.57	0.53
1:A:290:VAL:HG22	1:A:291:TRP:N	2.24	0.53
1:D:98:ARG:HD2	1:D:106:THR:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:70:GLU:H	1:D:73[B]:HIS:CD2	2.13	0.52
1:A:99:ASN:HD22	1:A:101:HIS:H	1.57	0.52
1:D:410:LEU:HD13	1:D:432:VAL:CG2	2.39	0.52
1:D:290:VAL:HG23	1:D:367:GLY:O	2.10	0.52
1:D:54:GLU:HB2	1:D:61:TRP:CE2	2.45	0.52
1:D:402:ILE:HA	1:D:405:PHE:HD1	1.74	0.52
1:D:292[A]:TYR:HE2	1:D:299:LYS:HG3	1.73	0.52
1:A:313:ARG:HD3	1:A:331:LYS:O	2.09	0.52
1:A:413:THR:O	1:A:417:LEU:HG	2.10	0.52
1:D:81:HIS:N	1:D:92:SER:HB3	2.24	0.51
1:A:241:VAL:HG22	6:A:561:HOH:O	2.11	0.51
1:D:459:VAL:HG23	1:D:460:ARG:N	2.25	0.51
1:D:292[A]:TYR:OH	1:D:299:LYS:HE3	2.09	0.51
1:A:194:VAL:HG21	1:A:205:MET:SD	2.50	0.51
1:D:427:TYR:CG	1:D:428:LEU:N	2.78	0.51
1:D:360:GLN:O	1:D:361:ASP:C	2.49	0.51
1:D:460:ARG:H	1:D:460:ARG:HD3	1.70	0.51
1:D:456:PRO:HB2	1:D:459:VAL:HG13	1.94	0.50
1:D:446:GLU:H	1:D:446:GLU:CD	2.15	0.50
1:A:285:PHE:HA	1:A:385:GLU:OE1	2.11	0.50
1:A:185:TYR:CE2	1:A:238:LEU:HD11	2.45	0.50
1:D:404:TRP:CD1	1:D:456:PRO:HD3	2.47	0.50
1:A:99:ASN:HD21	1:A:102:ARG:CG	2.22	0.49
1:A:162:VAL:HG12	1:A:164:LYS:O	2.12	0.49
1:A:171:ARG:NH2	1:A:237:GLU:O	2.45	0.49
1:D:315:GLU:HB2	1:D:384:MET:HE1	1.95	0.49
1:D:134:ALA:O	1:D:138:ILE:HG12	2.13	0.49
1:D:254:TYR:O	1:D:256:PRO:HD3	2.11	0.49
1:A:52:MET:HA	1:A:62:PHE:O	2.13	0.49
1:A:219:ARG:NH2	1:A:361:ASP:OD2	2.46	0.49
1:A:262:PRO:HD2	1:A:398:PHE:CE2	2.48	0.48
1:A:288:THR:HG22	1:A:370:LEU:CD2	2.42	0.48
1:D:137:ILE:HD13	1:D:336:TYR:CD2	2.48	0.48
1:D:72:HIS:HD2	1:D:221:LYS:HZ2	1.61	0.48
1:A:215:MET:HA	1:A:215:MET:CE	2.43	0.48
1:D:110:ASP:OD1	1:D:112:SER:HB2	2.13	0.48
1:D:122:PHE:HD2	1:D:123:ILE:HD12	1.79	0.48
1:D:408:LYS:HA	1:D:464:LEU:CD1	2.39	0.48
1:D:103:HIS:O	1:D:199:ARG:HG2	2.14	0.48
1:D:413:THR:O	1:D:417:LEU:HG	2.14	0.48
1:D:229:GLU:HA	1:D:268:LYS:O	2.14	0.47
1:D:256:PRO:HG2	1:D:405:PHE:CE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:241:VAL:HG12	1:D:291:TRP:HZ2	1.78	0.47
1:A:63:HIS:O	1:A:67:VAL:HG22	2.15	0.47
1:A:251:VAL:HG23	6:A:504:HOH:O	2.14	0.47
1:A:112:SER:O	1:A:113:LYS:CB	2.62	0.47
1:D:239:VAL:HG12	1:D:240:GLU:N	2.30	0.47
1:D:240:GLU:HA	1:D:240:GLU:OE1	2.14	0.47
1:D:194:VAL:HG12	1:D:195:ILE:N	2.30	0.47
1:A:290:VAL:CG2	1:A:291:TRP:N	2.78	0.47
1:D:219:ARG:NH1	1:D:274:VAL:HB	2.29	0.47
1:D:281:PHE:CD1	1:D:355:ALA:HB2	2.49	0.46
1:A:443:MET:O	1:A:448:VAL:HB	2.15	0.46
1:D:185:TYR:HB3	1:D:235:MET:HB2	1.97	0.46
1:A:427:TYR:CG	1:A:428:LEU:N	2.84	0.46
1:A:448:VAL:O	1:A:452:ALA:HB2	2.15	0.46
1:D:275:GLN:O	1:D:276:ASP:HB2	2.16	0.46
1:D:99:ASN:HD22	1:D:101:HIS:H	1.63	0.46
1:A:194:VAL:HG12	1:A:195:ILE:N	2.31	0.46
1:D:101:HIS:HD2	6:D:513:HOH:O	1.99	0.46
1:A:70:GLU:O	1:A:73[B]:HIS:HB2	2.16	0.46
1:A:134:ALA:HA	1:A:336:TYR:HB3	1.98	0.46
1:D:460:ARG:HG2	1:D:460:ARG:O	2.16	0.46
1:A:250:TRP:CD2	1:A:406:VAL:HG21	2.51	0.46
1:A:288:THR:HG22	1:A:370:LEU:HG	1.97	0.46
1:D:281:PHE:HA	1:D:354:HIS:O	2.16	0.46
1:A:44:GLN:OE1	1:A:45:PRO:HD2	2.16	0.46
1:A:75:VAL:CG1	1:A:199:ARG:HH11	2.20	0.45
1:D:311:LEU:O	1:D:384:MET:HE1	2.15	0.45
1:A:464:LEU:O	1:A:468:LEU:HB2	2.16	0.45
1:D:460:ARG:HA	1:D:461:PRO:HD2	1.70	0.45
1:A:296:TRP:HB3	6:A:503:HOH:O	2.16	0.45
1:A:467:GLU:O	1:A:471:VAL:HG23	2.16	0.45
1:A:244:ILE:HG23	1:A:245:ALA:N	2.32	0.45
1:D:410:LEU:CD1	1:D:432:VAL:HG22	2.45	0.45
1:A:407:ALA:HB2	1:A:435:LEU:HD21	1.98	0.45
1:A:275:GLN:O	1:A:276:ASP:HB2	2.16	0.45
1:A:447:LEU:O	1:A:449:SER:N	2.50	0.45
1:D:317:TRP:O	1:D:320:SER:HB3	2.17	0.45
1:D:165:LEU:HD21	1:D:293:HIS:CE1	2.52	0.45
1:D:292[A]:TYR:CE2	1:D:299:LYS:HG3	2.53	0.44
1:A:315:GLU:HB2	1:A:384:MET:HE2	2.00	0.44
1:A:75:VAL:CG1	1:A:199:ARG:NH1	2.78	0.44
1:A:442:TRP:O	1:A:448:VAL:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:443:MET:CE	1:A:461:PRO:HB2	2.48	0.44
1:D:302:TYR:HB2	1:D:355:ALA:HB3	2.00	0.44
1:A:396:PHE:HA	1:A:397:PRO:HD2	1.71	0.44
1:D:127:ARG:HH11	1:D:127:ARG:HG2	1.82	0.44
1:D:440:LYS:HG2	1:D:465:ILE:HG21	1.98	0.44
1:D:102:ARG:CZ	1:D:113:LYS:HB3	2.48	0.44
1:D:172:LEU:HB3	1:D:173:PRO:HD2	2.00	0.44
1:A:255:TRP:HA	1:A:256:PRO:HD3	1.85	0.44
1:D:239:VAL:CG1	1:D:240:GLU:N	2.81	0.43
1:A:54:GLU:O	1:A:80:TYR:HB3	2.18	0.43
1:D:230:PHE:HB2	1:D:233:THR:OG1	2.19	0.43
1:D:407:ALA:HB3	1:D:464:LEU:HD21	1.99	0.43
1:D:265:PHE:HA	1:D:267:GLN:HE22	1.83	0.43
1:A:372:ASN:O	1:A:375:ILE:HG13	2.18	0.43
1:A:99:ASN:ND2	1:A:102:ARG:HG2	2.26	0.43
1:A:241:VAL:HG12	1:A:291:TRP:HZ2	1.82	0.43
1:D:240:GLU:CD	1:D:246:LYS:NZ	2.71	0.43
1:A:207:LEU:O	1:A:211:VAL:HG23	2.19	0.43
1:A:410:LEU:HD13	1:A:432:VAL:HG22	2.01	0.43
1:D:295:LEU:HD23	1:D:363:MET:HE1	2.01	0.43
1:A:213:TYR:CZ	1:A:223:LEU:HB2	2.54	0.43
1:A:239:VAL:CG1	1:A:240:GLU:N	2.81	0.43
1:A:296:TRP:CZ2	1:A:363:MET:HB2	2.54	0.42
1:A:210:TYR:CZ	1:A:225:VAL:HG23	2.54	0.42
1:D:35:PRO:HB2	1:D:36:PRO:HD2	2.00	0.42
1:A:33:PRO:N	1:A:34:PRO:HD3	2.34	0.42
1:A:253:ASN:O	1:A:254:TYR:CD1	2.72	0.42
1:A:455:ILE:HA	1:A:456:PRO:HD3	1.91	0.42
1:A:460:ARG:HB2	1:A:463:HIS:HB3	2.01	0.42
1:A:97:ARG:NH1	1:A:100:TRP:CE3	2.87	0.42
1:A:265:PHE:HA	1:A:267[B]:GLN:OE1	2.20	0.42
1:A:360:GLN:O	1:A:361:ASP:C	2.58	0.42
1:A:433:LYS:HB2	1:A:433:LYS:HE3	1.86	0.42
1:D:113:LYS:HA	1:D:114:PRO:HD3	1.79	0.42
1:D:141:MET:HE1	1:D:146:LEU:HA	2.02	0.42
1:A:197:VAL:HG11	1:A:278:TYR:N	2.35	0.42
1:D:35:PRO:HB2	1:D:36:PRO:CD	2.50	0.42
1:D:213:TYR:CE2	1:D:223:LEU:HB2	2.54	0.42
1:A:441:LEU:O	1:A:447:LEU:HD12	2.20	0.42
1:D:141:MET:CE	1:D:146:LEU:HA	2.49	0.42
1:A:186:VAL:O	1:A:234:LYS:HE2	2.18	0.42
1:D:467:GLU:HA	1:D:470:LYS:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:ARG:HG3	1:D:107:GLU:O	2.20	0.41
1:D:210:TYR:O	1:D:213:TYR:HB3	2.19	0.41
1:A:99:ASN:ND2	1:A:102:ARG:N	2.69	0.41
1:A:426:THR:O	1:A:430:GLN:HG3	2.21	0.41
1:A:151:LEU:HD22	1:A:156:PHE:HB2	2.02	0.41
1:A:219:ARG:NH2	1:A:361:ASP:CG	2.73	0.41
1:A:333:ASP:HB2	6:A:502:HOH:O	2.19	0.41
1:D:467:GLU:CA	1:D:470:LYS:HG2	2.48	0.41
1:D:110:ASP:OD1	1:D:112:SER:HB3	2.21	0.41
1:D:179:VAL:HG12	1:D:272:MET:SD	2.61	0.41
1:D:255:TRP:HA	1:D:256:PRO:HD3	1.90	0.41
1:D:246:LYS:HB2	1:D:246:LYS:HE3	1.90	0.41
1:D:160:ILE:O	1:D:346:LEU:HD12	2.20	0.41
1:D:121:THR:O	1:D:125:GLU:HG3	2.21	0.41
1:D:177:PHE:CE1	1:D:181:ASP:HB3	2.55	0.41
1:D:137:ILE:HD13	1:D:336:TYR:CE2	2.56	0.41
1:A:51:PHE:CG	1:A:71:GLU:HG2	2.55	0.41
1:D:461:PRO:O	1:D:465:ILE:HG13	2.21	0.40
1:A:99:ASN:ND2	1:A:102:ARG:H	2.19	0.40
1:D:72:HIS:CE1	1:D:223:LEU:HD11	2.56	0.40
1:A:215:MET:O	1:A:217:PRO:HD3	2.20	0.40
1:D:240:GLU:CD	1:D:246:LYS:HZ3	2.24	0.40
1:D:438:ALA:O	1:D:441:LEU:HB3	2.21	0.40
1:D:442:TRP:HB3	1:D:451:HIS:CG	2.56	0.40
1:D:174:SER:C	1:D:176:THR:H	2.25	0.40
1:A:436:HIS:HE1	1:A:465:ILE:O	2.04	0.40
1:A:75:VAL:O	1:A:75:VAL:HG22	2.20	0.40
1:A:254:TYR:HD2	1:A:406:VAL:HG22	1.85	0.40
1:D:127:ARG:NH1	1:D:127:ARG:HG2	2.36	0.40
1:A:299:LYS:HE3	5:A:702:AKG:O4	2.22	0.40
1:D:304:ILE:HB	1:D:353:ILE:HB	2.03	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	448/488 (92%)	404 (90%)	39 (9%)	5 (1%)	21	60
1	D	448/488 (92%)	401 (90%)	40 (9%)	7 (2%)	14	47
All	All	896/976 (92%)	805 (90%)	79 (9%)	12 (1%)	18	54

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	111	GLY
1	A	100	TRP
1	A	397	PRO
1	D	448	VAL
1	A	40	CYS
1	D	393	LEU
1	A	113	LYS
1	A	448	VAL
1	D	112	SER
1	D	397	PRO
1	D	421	GLY
1	D	461	PRO

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	388/424 (92%)	377 (97%)	11 (3%)	56	90
1	D	396/424 (93%)	382 (96%)	14 (4%)	48	85
All	All	784/848 (92%)	759 (97%)	25 (3%)	51	88

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	GLU
1	A	100	TRP
1	A	157	ASP
1	A	203	SER
1	A	219	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	LYS
1	A	252	GLU
1	A	268	LYS
1	A	362	CYS
1	A	450	GLU
1	A	469	SER
1	D	87	VAL
1	D	92	SER
1	D	120	ARG
1	D	152	GLU
1	D	157	ASP
1	D	219	ARG
1	D	234	LYS
1	D	257	ASP
1	D	271	LEU
1	D	397	PRO
1	D	419	GLU
1	D	428	LEU
1	D	450	GLU
1	D	460	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	409	ASN
1	A	458	ASN
1	D	49	ASN
1	D	72	HIS
1	D	99	ASN
1	D	101	HIS
1	D	200	GLN
1	D	224	ASN
1	D	253	ASN
1	D	267	GLN
1	D	430	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	OXY	A	492	-	1,1,1	1.32	0	0,0,0	0.00	-
5	AKG	A	702	3	9,9,9	1.06	0	11,11,11	1.44	3 (27%)
4	OXY	D	492	-	1,1,1	1.33	0	0,0,0	0.00	-
5	AKG	D	701	3	9,9,9	0.97	0	11,11,11	1.60	3 (27%)

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	OXY	A	492	-	-	0/0/0/0	0/0/0/0
5	AKG	A	702	3	-	0/9/9/9	0/0/0/0
4	OXY	D	492	-	-	0/0/0/0	0/0/0/0
5	AKG	D	701	3	-	0/9/9/9	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	AKG	O2-C1-C2	3.04	121.06	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	701	AKG	O2-C1-O1	-2.75	117.11	123.62
5	A	702	AKG	O2-C1-C2	2.38	119.62	114.37
5	A	702	AKG	O2-C1-O1	-2.31	118.15	123.62
5	A	702	AKG	O4-C5-O3	-2.16	117.81	123.30
5	D	701	AKG	O4-C5-O3	-2.12	117.89	123.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	447/488 (91%)	-0.36	5 (1%) 77 84	13, 32, 55, 84	0
1	D	448/488 (91%)	-0.37	4 (0%) 81 88	13, 31, 55, 84	0
All	All	895/976 (91%)	-0.36	9 (1%) 77 86	13, 32, 55, 84	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	PRO	4.3
1	D	457	ASP	3.4
1	D	424	PRO	2.9
1	A	260	VAL	2.7
1	D	429	VAL	2.6
1	A	421	GLY	2.6
1	A	262	PRO	2.6
1	A	258	ASP	2.3
1	D	422	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	OXY	D	492	2/2	0.65	13.90	72,72,72,73	0
4	OXY	A	492	2/2	0.47	12.88	61,61,61,61	0
5	AKG	A	702	10/10	0.35	10.28	97,97,99,99	0
5	AKG	D	701	10/10	0.39	5.69	102,103,103,103	0
3	FE2	D	491	1/1	0.14	-0.75	69,69,69,69	0
2	ZN	D	489	1/1	0.07	-1.32	30,30,30,30	0
2	ZN	A	490	1/1	0.07	-1.54	26,26,26,26	0
2	ZN	D	490	1/1	0.06	-1.83	27,27,27,27	0
2	ZN	A	489	1/1	0.07	-3.88	21,21,21,21	0
3	FE2	A	491	1/1	0.10	-5.85	65,65,65,65	0

6.5 Other polymers ⓘ

There are no such residues in this entry.