Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 01:53 AM EDT

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 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:

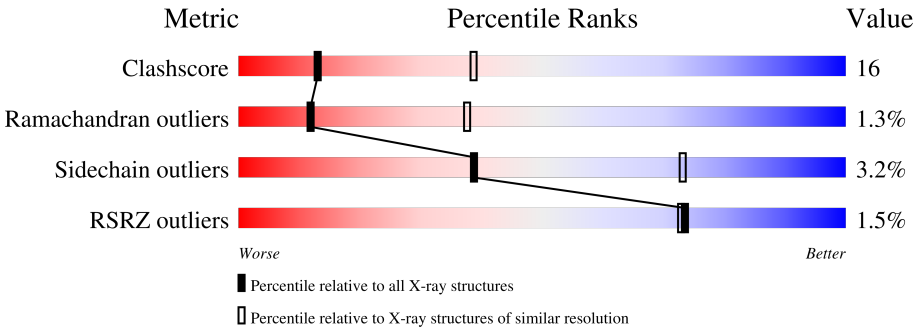
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	488	% 60% 29% • 8%
1	D	488	% 60% 31% • 8%

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	OXY	D	492	-	-	-	X
5	AKG	D	701	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7389 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 JmjC domain-containing histone demethylation protein 1D.

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

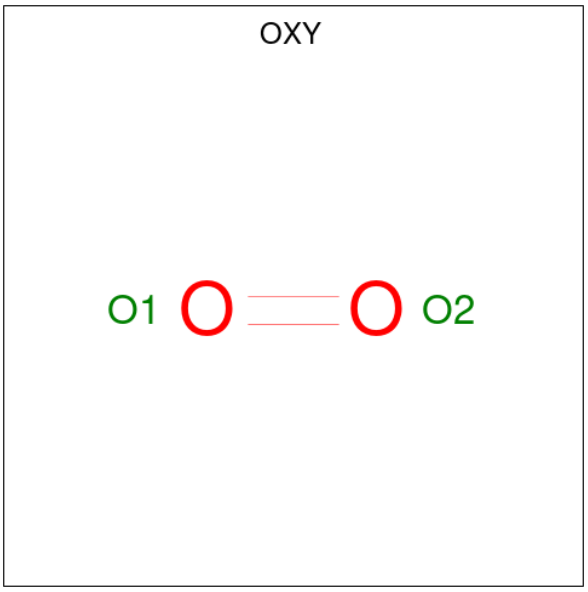
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

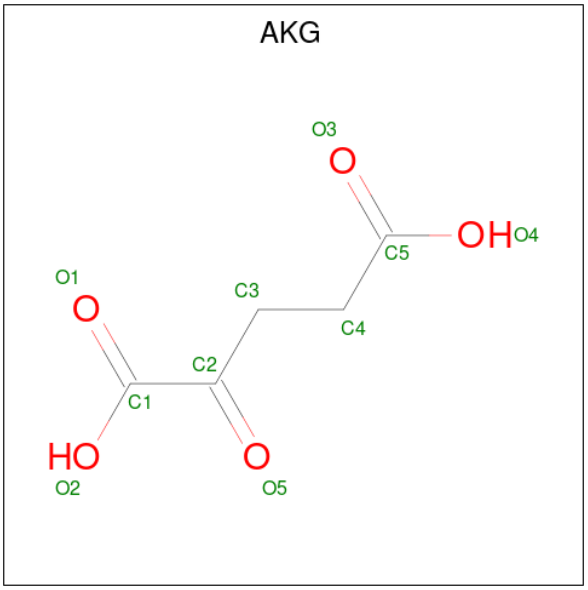
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Fe 1	0	0
3	D	1	Total 1	Fe 1	0	0

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



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

- 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 10 5 5	0	0
5	D	1	Total C O 10 5 5	0	0

- Molecule 6 is water.

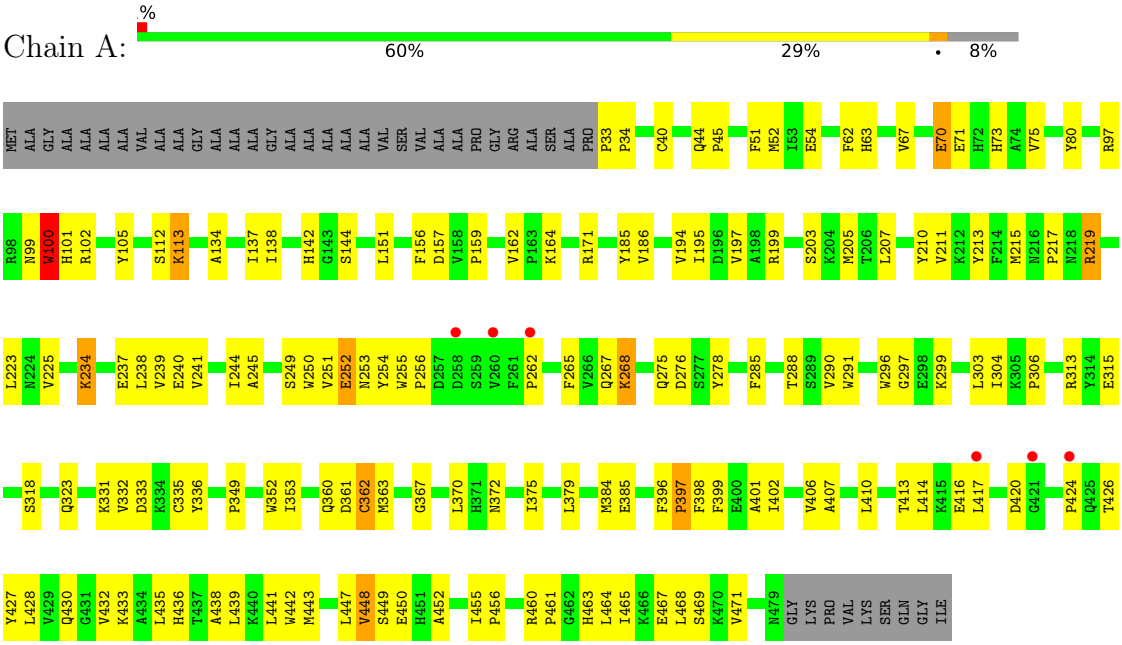
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	82	Total O 82 82	0	0
6	D	83	Total O 83 83	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

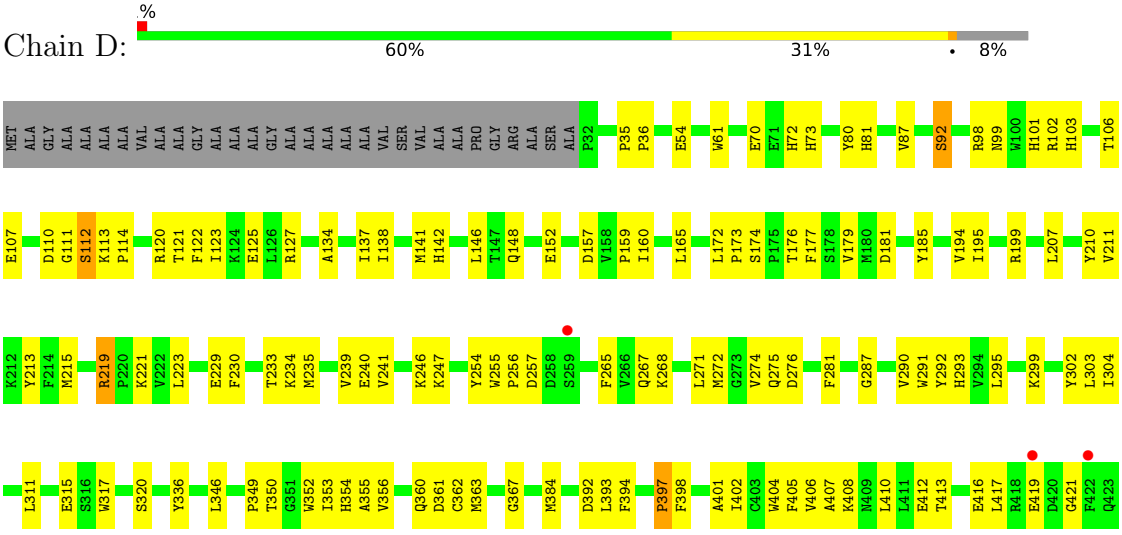
• Molecule 1: JmjC domain-containing histone demethylation protein 1D

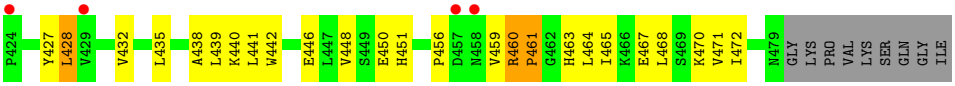
Chain A:



• Molecule 1: JmjC domain-containing histone demethylation protein 1D

Chain D:




P424
Y427
L428
V429
V432
L435
A438
L439
K440
L441
W442
E446
L447
V448
S449
E450
H451
P456
D457
N458
V459
R460
P461
G462
H463
L464
I465
K466
E467
L468
S469
K470
V471
I472
N479
GLY
LYS
PRO
VAL
LYS
SER
GLN
GLY
ILE

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.61 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.253 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	36.7	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	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 14.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FE2, OXY, ZN, 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	0.39	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 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	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
6	A	82	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	83	0	0	2	0
All	All	7389	0	6923	232	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 16.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:H	1:A:234:LYS:HD2	1.24	1.00
1:D:460:ARG:HD3	1:D:460:ARG:N	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:A:318:SER:HA	1:A:323:GLN:NE2	2.13	0.63
1:D:138:ILE:HG22	1:D:159:PRO:HB2	1.79	0.63
1:D:142:HIS:HB3	6:D:496:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:LEU:O	1:D:468:LEU:HB2	2.00	0.62
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:HA	1:A:100:TRP:CE3	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:A:306:PRO:HG3	1:A:352:TRP:HA	1.85	0.58
1:D:392:ASP:O	1:D:394:PHE:N	2.37	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:290:VAL:HG23	1:A:367:GLY:O	2.08	0.54
1:A:399:PHE:O	1:A:402:ILE:HG22	2.08	0.54
1:D:315:GLU:HB2	1:D:384:MET:CE	2.38	0.54
1:D:356:VAL:HG21	5:D:701:AKG:H41	1.90	0.54
1:A:435:LEU:O	1:A:439:LEU:HD13	2.07	0.53
1:A:197:VAL:HG11	1:A:278:TYR:H	1.74	0.53
1:A:379:LEU:HD13	1:A:438:ALA:HB2	1.90	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:A:290:VAL:HG22	1:A:291:TRP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:OD1	1:D:112:SER:CB	2.57	0.53
1:D:98:ARG:HD2	1:D:106:THR:O	2.09	0.52
1:A:99:ASN:HD22	1:A:101:HIS:H	1.57	0.52
1:D:70:GLU:H	1:D:73[B]:HIS:CD2	2.13	0.52
1:D:290:VAL:HG23	1:D:367:GLY:O	2.10	0.52
1:D:410:LEU:HD13	1:D:432:VAL:CG2	2.39	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:A:313:ARG:HD3	1:A:331:LYS:O	2.09	0.52
1:D:292[A]:TYR:HE2	1:D:299:LYS:HG3	1.73	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:A:194:VAL:HG21	1:A:205:MET:SD	2.50	0.51
1:D:292[A]:TYR:OH	1:D:299:LYS:HE3	2.09	0.51
1:D:459:VAL:HG23	1:D:460:ARG:N	2.25	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:HD3	1:D:460:ARG:H	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:A:215:MET:HA	1:A:215:MET:CE	2.43	0.48
1:D:72:HIS:HD2	1:D:221:LYS:HZ2	1.61	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:103:HIS:O	1:D:199:ARG:HG2	2.14	0.48
1:D:408:LYS:HA	1:D:464:LEU:CD1	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:241:VAL:HG12	1:D:291:TRP:HZ2	1.78	0.47
1:D:256:PRO:HG2	1:D:405:PHE:CE2	2.48	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:194:VAL:HG12	1:D:195:ILE:N	2.30	0.47
1:D:240:GLU:HA	1:D:240:GLU:OE1	2.14	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:A:194:VAL:HG12	1:A:195:ILE:N	2.31	0.46
1:D:99:ASN:HD22	1:D:101:HIS:H	1.63	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:101:HIS:HD2	6:D:513:HOH:O	1.99	0.46
1:A:44:GLN:OE1	1:A:45:PRO:HD2	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:D:460:ARG:HG2	1:D:460:ARG:O	2.16	0.46
1:A:75:VAL:CG1	1:A:199:ARG:HH11	2.20	0.45
1:A:464:LEU:O	1:A:468:LEU:HB2	2.16	0.45
1:D:311:LEU:O	1:D:384:MET:HE1	2.15	0.45
1:A:296:TRP:HB3	6:A:503:HOH:O	2.16	0.45
1:D:460:ARG:HA	1:D:461:PRO:HD2	1.70	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:A:275:GLN:O	1:A:276:ASP:HB2	2.16	0.45
1:A:407:ALA:HB2	1:A:435:LEU:HD21	1.98	0.45
1:D:410:LEU:CD1	1:D:432:VAL:HG22	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG2	1:D:127:ARG:HH11	1.82	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:D:440:LYS:HG2	1:D:465:ILE:HG21	1.98	0.44
1:A:255:TRP:HA	1:A:256:PRO:HD3	1.85	0.44
1:A:54:GLU:O	1:A:80:TYR:HB3	2.18	0.43
1:D:239:VAL:CG1	1:D:240:GLU:N	2.81	0.43
1:D:230:PHE:HB2	1:D:233:THR:OG1	2.19	0.43
1:A:372:ASN:O	1:A:375:ILE:HG13	2.18	0.43
1:D:265:PHE:HA	1:D:267:GLN:HE22	1.83	0.43
1:D:407:ALA:HB3	1:D:464:LEU:HD21	1.99	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:33:PRO:N	1:A:34:PRO:HD3	2.34	0.42
1:A:210:TYR:CZ	1:A:225:VAL:HG23	2.54	0.42
1:A:296:TRP:CZ2	1:A:363:MET:HB2	2.54	0.42
1:D:35:PRO:HB2	1:D:36:PRO:HD2	2.00	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:HE3	1:A:433:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:213:TYR:CE2	1:D:223:LEU:HB2	2.54	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
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: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:467:GLU:CA	1:D:470:LYS:HG2	2.48	0.41
1:D:121:THR:O	1:D:125:GLU:HG3	2.21	0.41
1:D:160:ILE:O	1:D:346:LEU:HD12	2.20	0.41
1:D:177:PHE:CE1	1:D:181:ASP:HB3	2.55	0.41
1:D:246:LYS:HE3	1:D:246:LYS:HB2	1.90	0.41
1:D:255:TRP:HA	1:D:256:PRO:HD3	1.90	0.41
1:A:51:PHE:CG	1:A:71:GLU:HG2	2.55	0.41
1:D:137:ILE:HD13	1:D:336:TYR:CE2	2.56	0.41
1:A:99:ASN:ND2	1:A:102:ARG:H	2.19	0.40
1:A:215:MET:O	1:A:217:PRO:HD3	2.20	0.40
1:D:72:HIS:CE1	1:D:223:LEU:HD11	2.56	0.40
1:D:461:PRO:O	1:D:465:ILE:HG13	2.21	0.40
1:D:174:SER:C	1:D:176:THR:H	2.25	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: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:HG2	1:D:127:ARG:NH1	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 (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	448/488 (92%)	404 (90%)	39 (9%)	5 (1%)	14 42
1	D	448/488 (92%)	401 (90%)	40 (9%)	7 (2%)	9 32
All	All	896/976 (92%)	805 (90%)	79 (9%)	12 (1%)	12 37

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 (i)

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%)	43 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	396/424 (93%)	382 (96%)	14 (4%)	36 70
All	All	784/848 (92%)	759 (97%)	25 (3%)	39 73

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
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

Sometimes 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

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Mol	Chain	Res	Type
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 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 monosaccharides 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	$\#\|Z\| > 2$
5	AKG	D	701	3	9,9,9	1.04	0	11,11,11	1.65	3 (27%)
4	OXY	A	492	-	1,1,1	1.27	0	-		
5	AKG	A	702	3	9,9,9	1.19	1 (11%)	11,11,11	1.56	4 (36%)
4	OXY	D	492	-	1,1,1	1.27	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
5	AKG	A	702	3	-	0/9/9/9	-
5	AKG	D	701	3	-	0/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	702	AKG	C3-C2	2.18	1.53	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	701	AKG	O2-C1-O1	-2.84	117.11	123.61
5	D	701	AKG	O2-C1-C2	2.59	121.06	113.97
5	A	702	AKG	O2-C1-O1	-2.38	118.15	123.61
5	A	702	AKG	O4-C5-O3	-2.20	117.81	123.30
5	D	701	AKG	O4-C5-O3	-2.17	117.89	123.30
5	A	702	AKG	C3-C2-C1	2.16	119.97	115.97
5	A	702	AKG	O2-C1-C2	2.07	119.62	113.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	701	AKG	1	0
5	A	702	AKG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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%)	-0.34	6 (1%)	77	77	13, 32, 55, 84	0
1	D	448/488 (91%)	-0.35	7 (1%)	72	71	13, 31, 55, 84	0
All	All	895/976 (91%)	-0.34	13 (1%)	73	73	13, 32, 55, 84	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	PRO	3.8
1	D	457	ASP	3.3
1	A	260	VAL	2.9
1	D	429	VAL	2.8
1	D	424	PRO	2.4
1	A	421	GLY	2.4
1	A	258	ASP	2.4
1	A	417	LEU	2.4
1	D	419	GLU	2.4
1	D	422	PHE	2.3
1	D	259	SER	2.3
1	A	262	PRO	2.2
1	D	458	ASN	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 monosaccharides 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^{th} 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
4	OXY	D	492	2/2	0.71	0.66	72,72,72,73	0
5	AKG	D	701	10/10	0.79	0.43	102,103,103,103	0
5	AKG	A	702	10/10	0.86	0.41	97,97,99,99	0
4	OXY	A	492	2/2	0.93	0.50	61,61,61,61	0
3	FE2	A	491	1/1	0.94	0.13	65,65,65,65	0
3	FE2	D	491	1/1	0.98	0.14	69,69,69,69	0
2	ZN	A	490	1/1	0.99	0.06	26,26,26,26	0
2	ZN	A	489	1/1	1.00	0.07	21,21,21,21	0
2	ZN	D	489	1/1	1.00	0.06	30,30,30,30	0
2	ZN	D	490	1/1	1.00	0.05	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.