



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 12:59 PM BST

PDB ID : 6IE2
Title : Crystal structure of methyladenine demethylase
Authors : Tian, L.F.; Tang, Q.; Chen, Z.Z.; Yan, X.X.
Deposited on : 2018-09-13
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

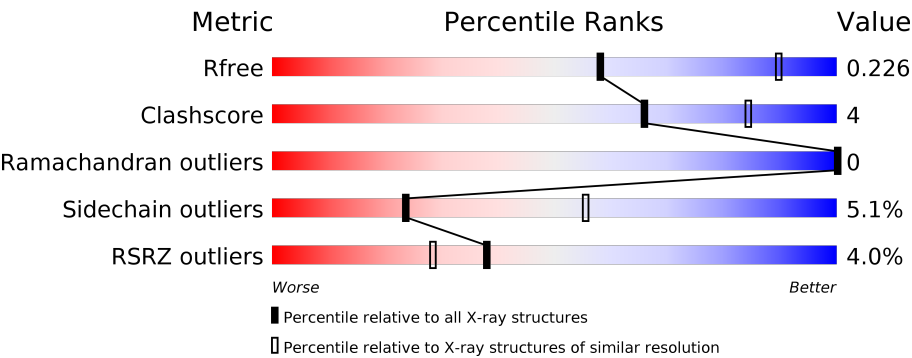
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	389	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%11%..17%</div></div>
1	B	389	<div>3%</div> <div><div></div><div></div><div></div><div></div><div></div></div> <div>73%9%.17%</div>
1	C	389	<div>%</div> <div><div></div><div></div><div></div><div></div><div></div></div> <div>71%11%.17%</div>
1	D	389	<div>4%</div> <div><div></div><div></div><div></div><div></div><div></div></div> <div>74%7%..17%</div>
1	E	389	<div>4%</div> <div><div></div><div></div><div></div><div></div><div></div></div> <div>69%10%.19%</div>
1	F	389	<div>3%</div> <div><div></div><div></div><div></div><div></div><div></div></div> <div>76%6%.17%</div>

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Mol	Chain	Length	Quality of chain
1	G	389	<div><div></div><div>3%</div><div>74%</div><div>8%</div><div>17%</div></div>
1	H	389	<div><div></div><div>9%</div><div>72%</div><div>9%</div><div>17%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20660 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 Nucleic acid dioxygenase ALKBH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2505	1609	427	455	14			
1	B	323	Total	C	N	O	S	0	0	0
			2515	1615	430	456	14			
1	C	323	Total	C	N	O	S	0	0	0
			2521	1619	433	455	14			
1	D	323	Total	C	N	O	S	0	0	0
			2506	1611	426	455	14			
1	E	317	Total	C	N	O	S	0	0	0
			2474	1590	425	445	14			
1	F	324	Total	C	N	O	S	0	0	0
			2533	1627	434	458	14			
1	G	323	Total	C	N	O	S	0	0	0
			2519	1617	435	453	14			
1	H	324	Total	C	N	O	S	0	0	0
			2513	1615	431	453	14			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

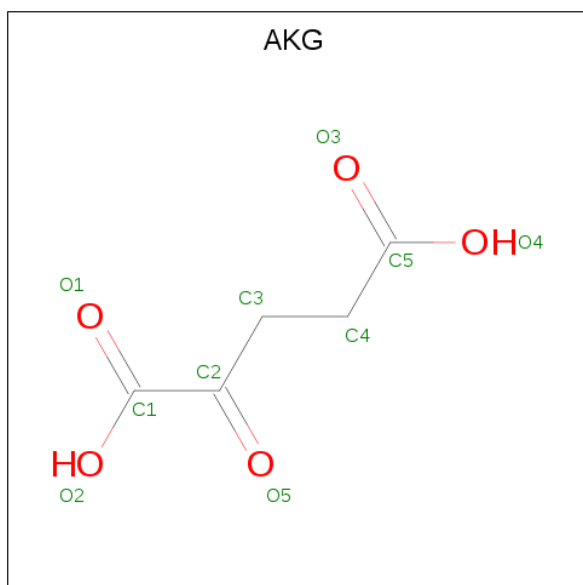
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		
3	G	1	Total	C	O	0	0
			10	5	5		
3	H	1	Total	C	O	0	0
			10	5	5		

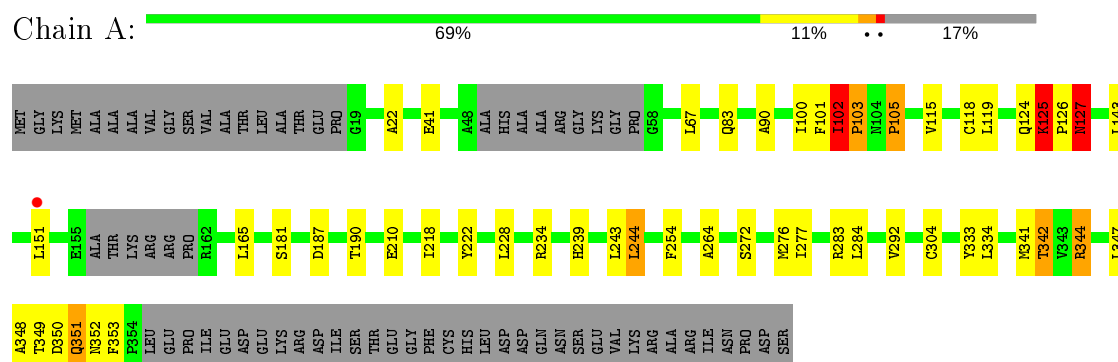
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total 85	O 85	0	0
4	B	68	Total 68	O 68	0	0
4	C	76	Total 76	O 76	0	0
4	D	51	Total 51	O 51	0	0
4	E	60	Total 60	O 60	0	0
4	F	47	Total 47	O 47	0	0
4	G	46	Total 46	O 46	0	0
4	H	53	Total 53	O 53	0	0

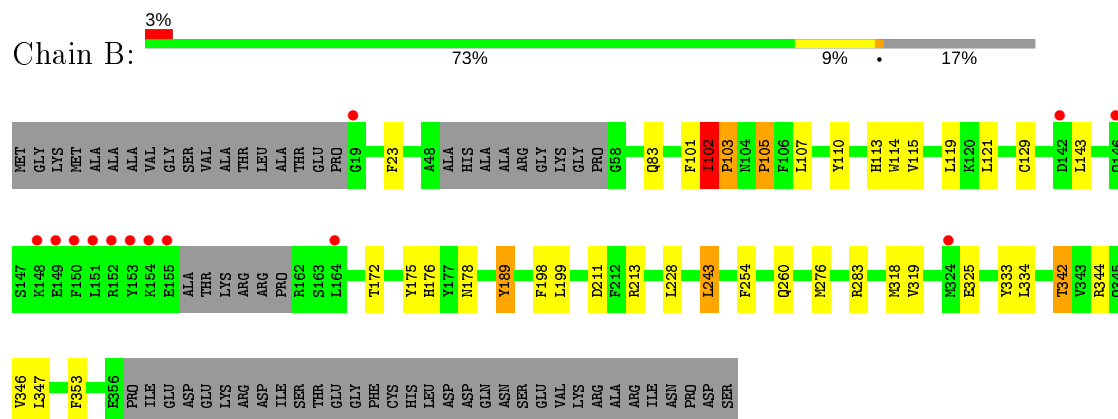
3 Residue-property plots

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.

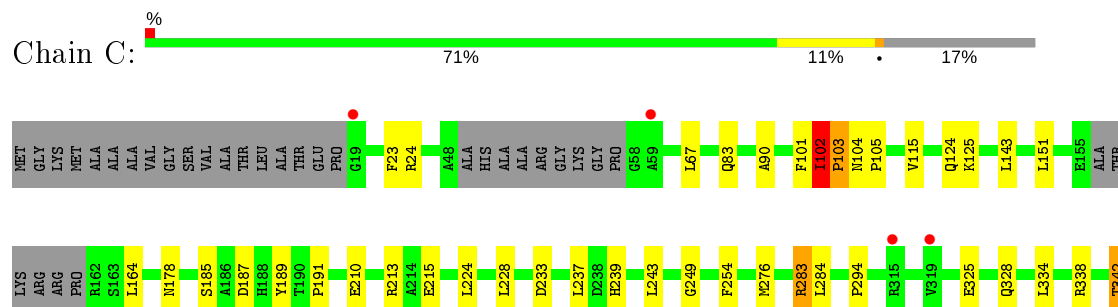
• Molecule 1: Nucleic acid dioxygenase ALKBH1

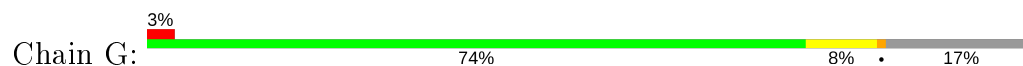


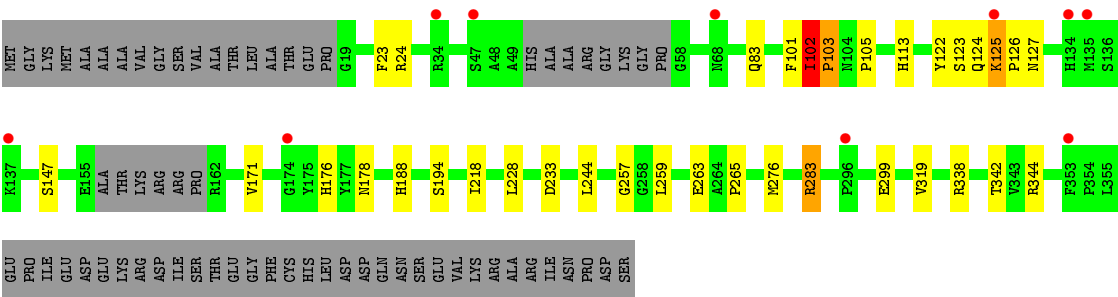
• Molecule 1: Nucleic acid dioxygenase ALKBH1



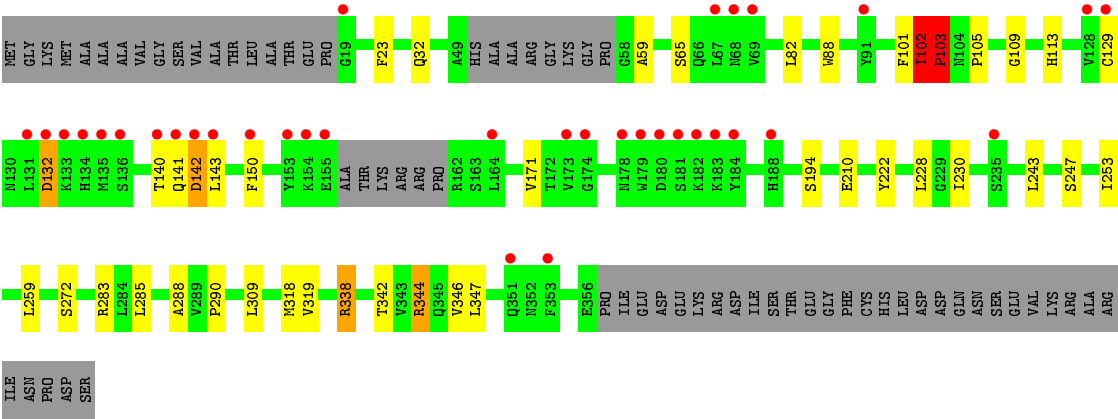
• Molecule 1: Nucleic acid dioxygenase ALKBH1







● Molecule 1: Nucleic acid dioxygenase ALKBH1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	89.02Å 99.17Å 126.79Å 106.60° 90.42° 93.14°	Depositor
Resolution (Å)	50.01 – 2.80 49.74 – 2.80	Depositor EDS
% Data completeness (in resolution range)	71.2 (50.01-2.80) 71.0 (49.74-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.216 , 0.254 0.223 , 0.226	Depositor DCC
R_{free} test set	3670 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20660	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: MN, 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	0.44	0/2576	0.96	13/3499 (0.4%)
1	B	0.43	0/2586	0.80	5/3513 (0.1%)
1	C	0.43	0/2592	0.78	7/3519 (0.2%)
1	D	0.44	0/2577	1.00	16/3502 (0.5%)
1	E	0.41	0/2543	0.95	17/3452 (0.5%)
1	F	0.40	0/2604	0.76	8/3534 (0.2%)
1	G	0.40	0/2590	0.77	8/3517 (0.2%)
1	H	0.45	0/2584	0.89	11/3512 (0.3%)
All	All	0.42	0/20652	0.87	85/28048 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	3
1	D	0	3
1	E	0	2
1	F	0	1
1	G	0	1
1	H	0	3
All	All	0	17

There are no bond length outliers.

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ILE	CB-CA-C	19.69	150.98	111.60
1	H	102	ILE	CB-CA-C	19.18	149.96	111.60
1	D	153	TYR	CB-CA-C	-18.82	72.76	110.40
1	A	102	ILE	CB-CA-C	18.22	148.03	111.60
1	C	102	ILE	CB-CA-C	16.84	145.28	111.60

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide
1	A	125	LYS	Peptide
1	A	127	ASN	Peptide
1	B	102	ILE	Peptide
1	C	102	ILE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2505	0	2372	29	0
1	B	2515	0	2379	20	0
1	C	2521	0	2395	20	0
1	D	2506	0	2363	18	0
1	E	2474	0	2367	23	0
1	F	2533	0	2410	13	0
1	G	2519	0	2394	14	0
1	H	2513	0	2377	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	4	0	0
3	D	10	0	4	0	0
3	E	10	0	4	0	0
3	F	10	0	4	0	0
3	G	10	0	4	1	0
3	H	10	0	4	0	0
4	A	85	0	0	0	0
4	B	68	0	0	0	0
4	C	76	0	0	0	0
4	D	51	0	0	0	0
4	E	60	0	0	0	0
4	F	47	0	0	0	0
4	G	46	0	0	0	0
4	H	53	0	0	1	0
All	All	20660	0	19089	158	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 4.

The worst 5 of 158 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:E:150:PHE:C	1:E:151:LEU:HD22	1.48	1.34
1:A:101:PHE:CD1	1:A:102:ILE:O	1.81	1.33
1:C:101:PHE:CD1	1:C:102:ILE:O	1.96	1.18
1:E:150:PHE:O	1:E:151:LEU:HD22	0.99	1.17
1:E:150:PHE:O	1:E:151:LEU:CD2	1.94	1.15

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	315/389 (81%)	302 (96%)	13 (4%)	0	100	100
1	B	317/389 (82%)	300 (95%)	17 (5%)	0	100	100
1	C	317/389 (82%)	299 (94%)	18 (6%)	0	100	100
1	D	317/389 (82%)	301 (95%)	16 (5%)	0	100	100
1	E	311/389 (80%)	296 (95%)	15 (5%)	0	100	100
1	F	318/389 (82%)	307 (96%)	11 (4%)	0	100	100
1	G	317/389 (82%)	303 (96%)	14 (4%)	0	100	100
1	H	318/389 (82%)	302 (95%)	16 (5%)	0	100	100
All	All	2530/3112 (81%)	2410 (95%)	120 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	259/331 (78%)	244 (94%)	15 (6%)	20	50
1	B	259/331 (78%)	245 (95%)	14 (5%)	22	53
1	C	260/331 (78%)	246 (95%)	14 (5%)	22	53
1	D	257/331 (78%)	241 (94%)	16 (6%)	18	47
1	E	256/331 (77%)	246 (96%)	10 (4%)	32	66
1	F	261/331 (79%)	248 (95%)	13 (5%)	24	56
1	G	259/331 (78%)	246 (95%)	13 (5%)	24	56
1	H	257/331 (78%)	246 (96%)	11 (4%)	29	62
All	All	2068/2648 (78%)	1962 (95%)	106 (5%)	24	55

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	151	LEU
1	E	32	GLN

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Mol	Chain	Res	Type
1	H	65	SER
1	D	185	SER
1	D	243	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	351	GLN
1	F	32	GLN
1	H	178	ASN
1	E	340	ASN
1	F	113	HIS

5.3.3 RNA [i](#)

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	$\# Z > 2$
3	AKG	C	401	2	3,9,9	0.63	0	4,11,11	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AKG	G	401	2	3,9,9	0.33	0	4,11,11	1.23	0
3	AKG	A	401	2	3,9,9	0.70	0	4,11,11	1.29	0
3	AKG	B	401	2	3,9,9	0.27	0	4,11,11	1.41	1 (25%)
3	AKG	D	401	2	3,9,9	0.46	0	4,11,11	0.98	0
3	AKG	E	401	2	3,9,9	0.50	0	4,11,11	1.40	1 (25%)
3	AKG	F	401	2	3,9,9	0.38	0	4,11,11	0.87	0
3	AKG	H	401	2	3,9,9	0.60	0	4,11,11	0.94	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
3	AKG	C	401	2	-	0/3/9/9	-
3	AKG	G	401	2	-	3/3/9/9	-
3	AKG	A	401	2	-	0/3/9/9	-
3	AKG	B	401	2	-	0/3/9/9	-
3	AKG	D	401	2	-	0/3/9/9	-
3	AKG	E	401	2	-	0/3/9/9	-
3	AKG	F	401	2	-	2/3/9/9	-
3	AKG	H	401	2	-	2/3/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	401	AKG	C3-C4-C5	-2.51	108.47	112.67
3	B	401	AKG	C3-C4-C5	-2.43	108.60	112.67

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	401	AKG	C1-C2-C3-C4
3	H	401	AKG	O5-C2-C3-C4
3	F	401	AKG	O5-C2-C3-C4
3	H	401	AKG	C1-C2-C3-C4
3	G	401	AKG	C1-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	401	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, 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	321/389 (82%)	-0.25	1 (0%) 94 93	20, 40, 81, 105	0
1	B	323/389 (83%)	-0.17	13 (4%) 38 28	20, 41, 102, 126	0
1	C	323/389 (83%)	-0.20	4 (1%) 79 73	21, 46, 83, 106	0
1	D	323/389 (83%)	-0.01	16 (4%) 28 19	19, 49, 107, 135	0
1	E	317/389 (81%)	-0.07	14 (4%) 34 24	23, 48, 102, 143	0
1	F	324/389 (83%)	-0.07	10 (3%) 49 39	32, 59, 114, 137	0
1	G	323/389 (83%)	-0.02	10 (3%) 49 39	32, 59, 115, 133	0
1	H	324/389 (83%)	0.26	35 (10%) 5 3	28, 58, 130, 154	0
All	All	2578/3112 (82%)	-0.07	103 (3%) 38 28	19, 51, 107, 154	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	132	ASP	6.6
1	B	153	TYR	6.0
1	B	142	ASP	5.9
1	E	135	MET	5.5
1	H	153	TYR	5.2

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

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
3	AKG	H	401	10/10	0.95	0.20	52,59,63,65	0
3	AKG	G	401	10/10	0.98	0.18	64,67,72,73	0
3	AKG	D	401	10/10	0.98	0.14	34,35,37,37	0
3	AKG	A	401	10/10	0.98	0.16	28,29,31,31	0
3	AKG	E	401	10/10	0.98	0.14	42,53,59,62	0
3	AKG	F	401	10/10	0.98	0.14	62,67,68,69	0
2	MN	E	400	1/1	0.99	0.14	36,36,36,36	0
3	AKG	B	401	10/10	0.99	0.15	25,28,28,30	0
2	MN	C	400	1/1	0.99	0.12	19,19,19,19	0
2	MN	B	400	1/1	0.99	0.15	23,23,23,23	0
3	AKG	C	401	10/10	0.99	0.12	24,27,28,28	0
2	MN	G	400	1/1	0.99	0.13	38,38,38,38	0
2	MN	D	400	1/1	0.99	0.14	19,19,19,19	0
2	MN	F	400	1/1	1.00	0.11	39,39,39,39	0
2	MN	H	400	1/1	1.00	0.14	34,34,34,34	0
2	MN	A	400	1/1	1.00	0.13	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.