



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:38 PM GMT

PDB ID : 1GKZ  
Title : BRANCHED-CHAIN ALPHA-KETOACID DEHYDROGENASE KINASE  
(BCK) COMPLEXED WITH ADP  
Authors : Machius, M.; Chuang, J.L.; Wynn, R.M.; Tomchick, D.R.; Chuang, D.T.  
Deposited on : 2001-08-22  
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

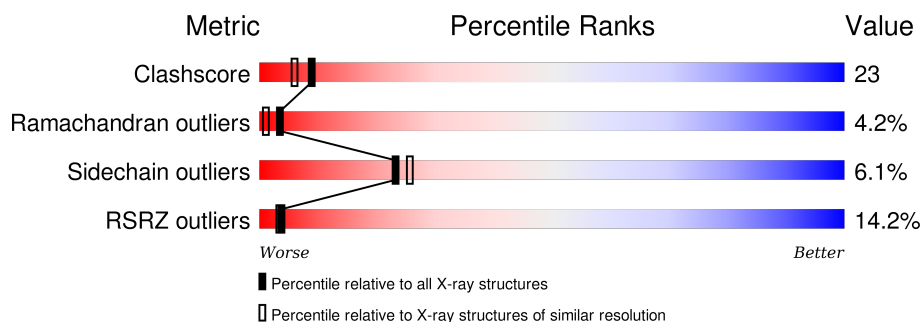
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	388	

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	XE	A	501	-	-	X	-
4	XE	A	502	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 2757 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 [3-METHYL-2-OXOBUTANOATE DEHYDROGENASE [LIPOAMIDE]] KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	42	5	0
			2598	1650	477	458	13			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

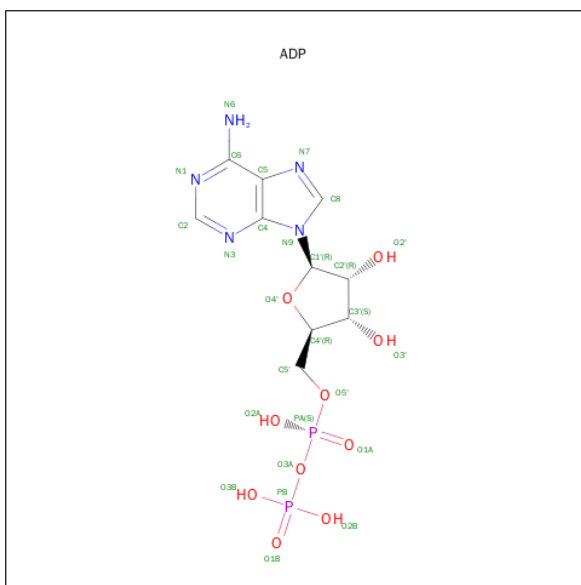
- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	K	0	0
			1	1		

- Molecule 4 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Xe	0	0
			2	2		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	
			27	10	5	10	2	

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	Cl		
			3	3	0	0

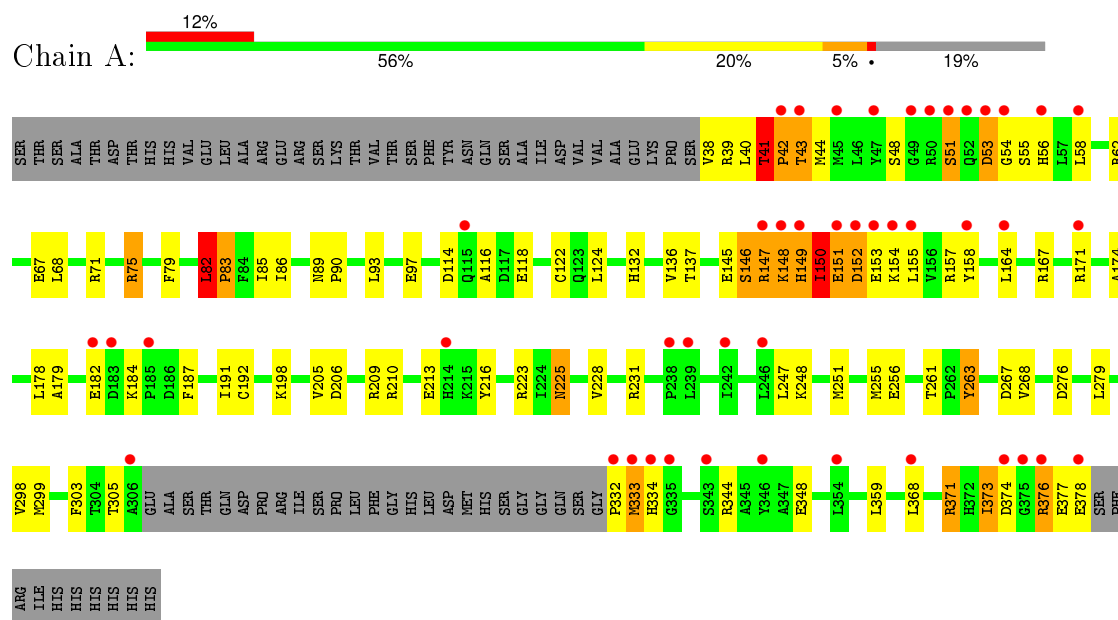
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total	O		
			125	125	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: [3-METHYL-2-OXOBUTANOATE DEHYDROGENASE [LIPOAMIDE]] KINASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	128.92Å 128.92Å 74.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.77 – 2.20 40.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.4 (40.77-2.20) 95.5 (40.77-2.20)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.61 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.268 0.232 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 32075 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2757	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, XE, K, ADP, CL

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	0.77	4/2655 (0.2%)	0.90	10/3583 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	HIS	CB-CG	7.92	1.64	1.50
1	A	153	GLU	C-N	-6.29	1.19	1.34
1	A	150	ILE	N-CA	6.21	1.58	1.46
1	A	149	HIS	CA-C	5.20	1.66	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	LYS	N-CA-C	-8.35	88.46	111.00
1	A	145	GLU	O-C-N	-6.50	112.30	122.70
1	A	149	HIS	C-N-CA	6.12	137.01	121.70
1	A	150	ILE	N-CA-C	6.11	127.49	111.00
1	A	149	HIS	CA-CB-CG	6.09	123.95	113.60
1	A	82	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	149	HIS	CB-CA-C	5.70	121.79	110.40
1	A	148	LYS	N-CA-CB	5.59	120.67	110.60
1	A	268	VAL	N-CA-C	-5.17	97.04	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	GLU	C-N-CA	5.12	134.51	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	TYR	Sidechain

## 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	2598	0	2629	119	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	2	0	0	3	0
5	A	27	0	12	2	0
6	A	3	0	0	0	0
7	A	125	0	0	5	0
All	All	2757	0	2641	120	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 23.

All (120) 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:147:ARG:HG2	1:A:150:ILE:CB	1.73	1.17
1:A:147:ARG:HG2	1:A:150:ILE:HB	1.10	1.09
1:A:38:VAL:HG11	1:A:48:SER:HB2	1.30	1.07
1:A:147:ARG:CG	1:A:150:ILE:HB	1.94	0.96
1:A:147:ARG:HA	1:A:150:ILE:H	1.30	0.95
1:A:147:ARG:HG2	1:A:150:ILE:CA	2.04	0.87
1:A:38:VAL:HG12	1:A:39:ARG:HG2	1.58	0.85
1:A:150:ILE:HG13	1:A:151:GLU:N	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HA	1:A:150:ILE:HG22	1.61	0.82
1:A:147:ARG:C	1:A:150:ILE:HG22	2.01	0.81
1:A:147:ARG:CA	1:A:150:ILE:HG22	2.12	0.80
1:A:86:ILE:HG12	1:A:146:SER:HB2	1.65	0.78
1:A:299:MET:HE2	1:A:344[A]:ARG:HD3	1.66	0.77
1:A:41:THR:CB	1:A:42:PRO:HD3	2.15	0.77
1:A:42:PRO:CD	1:A:44:MET:HG2	2.16	0.75
1:A:58:LEU:HB3	1:A:62:ARG:NH1	2.01	0.75
1:A:373:ILE:HG22	1:A:374:ASP:N	2.03	0.74
1:A:44:MET:HB3	1:A:71:ARG:HH22	1.53	0.73
1:A:276:ASP:O	1:A:376:ARG:HA	1.87	0.73
1:A:41:THR:OG1	1:A:42:PRO:HD3	1.88	0.72
1:A:38:VAL:HG21	1:A:48:SER:H	1.54	0.72
1:A:147:ARG:HA	1:A:150:ILE:N	2.03	0.72
1:A:58:LEU:HB3	1:A:62:ARG:HH12	1.56	0.71
1:A:39:ARG:HG3	1:A:191:ILE:CD1	2.22	0.70
1:A:179:ALA:O	1:A:182:GLU:HG3	1.91	0.69
1:A:42:PRO:HD2	1:A:44:MET:HG2	1.74	0.68
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.56	0.68
1:A:38:VAL:HG12	1:A:39:ARG:N	2.10	0.66
1:A:223[A]:ARG:HD3	1:A:267:ASP:OD2	1.96	0.66
1:A:248:LYS:HE3	1:A:333:MET:O	1.95	0.65
1:A:62:ARG:HD2	7:A:2003:HOH:O	1.98	0.64
4:A:501:XE:XE	4:A:502:XE:XE	3.72	0.63
1:A:118:GLU:OE2	1:A:122:CYS:SG	2.57	0.63
1:A:83:PRO:HG2	1:A:151:GLU:HG2	1.81	0.62
1:A:151:GLU:CG	1:A:155:LEU:HD13	2.29	0.62
1:A:51:SER:HA	1:A:56:HIS:ND1	2.15	0.62
1:A:167:ARG:HG2	1:A:167:ARG:NH1	2.16	0.61
1:A:83:PRO:CG	1:A:151:GLU:HG2	2.31	0.61
1:A:44:MET:CB	1:A:71:ARG:HH22	2.14	0.61
1:A:209:ARG:O	1:A:213:GLU:HG3	2.00	0.60
1:A:42:PRO:HD3	1:A:44:MET:HG2	1.83	0.59
1:A:151:GLU:O	1:A:152:ASP:C	2.41	0.59
1:A:152:ASP:HB3	1:A:155:LEU:HB2	1.84	0.59
1:A:231:ARG:NH1	7:A:2068:HOH:O	2.34	0.59
1:A:223[B]:ARG:HG3	1:A:223[B]:ARG:HH11	1.68	0.58
1:A:344[A]:ARG:NH2	7:A:2103:HOH:O	2.34	0.58
1:A:371:ARG:CG	1:A:371:ARG:HH11	2.16	0.58
1:A:184:LYS:HE2	1:A:187:PHE:CE1	2.37	0.58
1:A:247:LEU:O	1:A:251:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:HA	7:A:2121:HOH:O	2.04	0.57
1:A:40:LEU:HD12	1:A:40:LEU:N	2.19	0.57
1:A:147:ARG:HG2	1:A:150:ILE:HA	1.86	0.57
1:A:75:ARG:HH11	1:A:75:ARG:HG3	1.70	0.56
1:A:38:VAL:CG1	1:A:48:SER:HB2	2.21	0.56
1:A:332:PRO:O	1:A:333:MET:HB3	2.05	0.56
1:A:147:ARG:CA	1:A:150:ILE:H	2.10	0.55
1:A:39:ARG:HG3	1:A:191:ILE:HD13	1.88	0.55
1:A:298:VAL:HA	1:A:303:PHE:HD2	1.71	0.55
1:A:146:SER:O	1:A:147:ARG:HB2	2.05	0.55
1:A:42:PRO:HD2	1:A:44:MET:H	1.72	0.55
1:A:151:GLU:O	1:A:152:ASP:O	2.24	0.55
1:A:67:GLU:HG3	1:A:71:ARG:HE	1.72	0.55
1:A:79:PHE:HA	1:A:82:LEU:HD22	1.90	0.54
1:A:53:ASP:O	1:A:55:SER:N	2.41	0.53
1:A:344[B]:ARG:HD2	7:A:2105:HOH:O	2.09	0.53
1:A:344[B]:ARG:O	1:A:348:GLU:HG3	2.09	0.53
1:A:154:LYS:HD3	1:A:158:TYR:OH	2.08	0.53
1:A:58:LEU:O	1:A:62:ARG:HG3	2.09	0.52
1:A:51:SER:HA	1:A:56:HIS:CE1	2.44	0.52
1:A:85:ILE:HD13	1:A:149:HIS:HB3	1.90	0.52
1:A:39:ARG:HH11	1:A:373:ILE:HG21	1.75	0.52
1:A:371:ARG:HG2	1:A:371:ARG:NH1	2.24	0.52
1:A:41:THR:HB	1:A:42:PRO:HD3	1.90	0.52
1:A:136:VAL:HG22	1:A:164:LEU:HD22	1.91	0.51
1:A:147:ARG:HA	1:A:150:ILE:CA	2.40	0.51
1:A:114:ASP:OD1	1:A:116:ALA:HB3	2.11	0.51
1:A:223[B]:ARG:CG	1:A:223[B]:ARG:HH11	2.24	0.50
1:A:68:LEU:HD13	4:A:501:XE:XE	2.90	0.50
1:A:43:THR:HG22	1:A:43:THR:O	2.12	0.50
1:A:171[A]:ARG:HH11	1:A:171[A]:ARG:HG3	1.77	0.50
1:A:147:ARG:HA	1:A:150:ILE:CG2	2.36	0.50
1:A:38:VAL:HG11	1:A:48:SER:CB	2.22	0.50
1:A:150:ILE:CG1	1:A:151:GLU:N	2.66	0.49
1:A:359:LEU:N	1:A:359:LEU:HD12	2.27	0.49
1:A:373:ILE:CG2	1:A:374:ASP:N	2.75	0.49
1:A:225:ASN:HD22	1:A:225:ASN:C	2.16	0.49
1:A:93:LEU:O	1:A:97:GLU:HG3	2.13	0.49
1:A:344[A]:ARG:O	1:A:348:GLU:HG3	2.14	0.48
1:A:40:LEU:O	1:A:41:THR:HG23	2.13	0.48
1:A:261:THR:HG22	1:A:263:TYR:OH	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:CD	1:A:150:ILE:HB	2.43	0.48
1:A:40:LEU:HD12	1:A:40:LEU:H	1.79	0.48
1:A:371:ARG:CG	1:A:371:ARG:NH1	2.75	0.47
1:A:151:GLU:HG3	1:A:155:LEU:HD13	1.97	0.47
1:A:334:HIS:HD2	5:A:601:ADP:O3B	1.98	0.47
1:A:179:ALA:O	1:A:182:GLU:CG	2.61	0.47
1:A:147:ARG:CG	1:A:150:ILE:HA	2.45	0.46
1:A:298:VAL:HA	1:A:303:PHE:CD2	2.50	0.46
1:A:373:ILE:HG22	1:A:374:ASP:H	1.77	0.46
1:A:41:THR:CB	1:A:42:PRO:CD	2.92	0.46
1:A:53:ASP:C	1:A:55:SER:N	2.69	0.45
1:A:136:VAL:HG22	1:A:164:LEU:CD2	2.47	0.45
1:A:206:ASP:HB3	1:A:210:ARG:HH21	1.82	0.44
1:A:147:ARG:CG	1:A:150:ILE:CA	2.89	0.44
1:A:83:PRO:HG3	1:A:151:GLU:HG2	1.99	0.44
1:A:334:HIS:CD2	5:A:601:ADP:O3B	2.70	0.44
1:A:205:VAL:O	1:A:209:ARG:HG3	2.18	0.44
1:A:216:TYR:CD1	1:A:255[A]:MET:HG3	2.53	0.43
1:A:42:PRO:HD2	1:A:43:THR:H	1.83	0.43
1:A:187:PHE:CE2	1:A:192:CYS:HB2	2.54	0.42
1:A:373:ILE:HA	1:A:373:ILE:HD13	1.74	0.42
1:A:154:LYS:HB2	1:A:158:TYR:CZ	2.54	0.42
1:A:132:HIS:CG	4:A:502:XE:XE	3.51	0.42
1:A:155:LEU:C	1:A:155:LEU:HD23	2.40	0.42
1:A:171[A]:ARG:NH1	1:A:171[A]:ARG:HG3	2.35	0.42
1:A:89:ASN:HA	1:A:90:PRO:HD3	1.89	0.42
1:A:174:ALA:O	1:A:178:LEU:HG	2.19	0.41
1:A:223[B]:ARG:CG	1:A:223[B]:ARG:NH1	2.82	0.41
1:A:198:LYS:HD2	1:A:228:VAL:HB	2.03	0.40
1:A:75:ARG:HA	1:A:75:ARG:CZ	2.51	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	317/388 (82%)	291 (92%)	13 (4%)	13 (4%)	3 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	A	51	SER
1	A	147	ARG
1	A	150	ILE
1	A	152	ASP
1	A	333	MET
1	A	373	ILE
1	A	377	GLU
1	A	54	GLY
1	A	146	SER
1	A	41	THR
1	A	376	ARG
1	A	43	THR

### 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	282/340 (83%)	265 (94%)	17 (6%)	24 26

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	53	ASP
1	A	75	ARG
1	A	82	LEU
1	A	83	PRO
1	A	124	LEU

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Mol	Chain	Res	Type
1	A	137	THR
1	A	148	LYS
1	A	150	ILE
1	A	151	GLU
1	A	157	ARG
1	A	225	ASN
1	A	256	GLU
1	A	279	LEU
1	A	305	THR
1	A	368	LEU
1	A	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	334	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	ADP	A	601	3,2	22,29,29	0.93	1 (4%)	27,45,45	1.14	2 (7%)

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	ADP	A	601	3,2	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	ADP	PA-O2A	-2.54	1.44	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	ADP	O2B-PB-O1B	2.16	117.54	110.58
5	A	601	ADP	O3B-PB-O1B	2.75	119.43	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	ADP	2	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	316/388 (81%)	0.60	45 (14%) 4 3	34, 54, 106, 123	9 (2%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	151	GLU	7.6
1	A	375	GLY	7.4
1	A	332	PRO	6.9
1	A	51	SER	6.5
1	A	376	ARG	6.4
1	A	148	LYS	6.0
1	A	149	HIS	5.8
1	A	374	ASP	5.4
1	A	52	GLN	5.4
1	A	378	GLU	5.4
1	A	49	GLY	5.3
1	A	53	ASP	5.2
1	A	50	ARG	4.9
1	A	152	ASP	4.5
1	A	147	ARG	4.3
1	A	334	HIS	4.1
1	A	158	TYR	4.1
1	A	153	GLU	4.0
1	A	214	HIS	3.7
1	A	47	TYR	3.3
1	A	42	PRO	3.2
1	A	335	GLY	3.1
1	A	333	MET	3.1
1	A	171[A]	ARG	3.1
1	A	306	ALA	3.0
1	A	242	ILE	3.0
1	A	58	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	164	LEU	2.8
1	A	54	GLY	2.8
1	A	115	GLN	2.6
1	A	154	LYS	2.6
1	A	185	PRO	2.6
1	A	238	PRO	2.4
1	A	239	LEU	2.4
1	A	346	TYR	2.4
1	A	183	ASP	2.3
1	A	56	HIS	2.3
1	A	354	LEU	2.3
1	A	45	MET	2.3
1	A	182	GLU	2.3
1	A	155	LEU	2.2
1	A	368	LEU	2.2
1	A	43	THR	2.2
1	A	246	LEU	2.1
1	A	343	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	ADP	A	601	27/27	0.97	0.10	-0.91	41,51,57,59	0
3	K	A	402	1/1	0.96	0.10	-1.09	54,54,54,54	0
4	XE	A	502	1/1	0.93	0.06	-2.71	149,149,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	XE	A	501	1/1	0.96	0.05	-5.17	107,107,107,107	0
6	CL	A	701	1/1	0.49	0.35	-	93,93,93,93	0
6	CL	A	703	1/1	0.84	0.14	-	106,106,106,106	0
2	MG	A	401	1/1	0.98	0.07	-	46,46,46,46	0
6	CL	A	702	1/1	0.79	0.07	-	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.