



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:52 PM GMT

PDB ID : 1VHL  
Title : Crystal structure of dephospho-CoA kinase with adenosine-5'-diphosphate  
Authors : Structural GenomiX  
Deposited on : 2003-12-01  
Resolution : 1.65 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

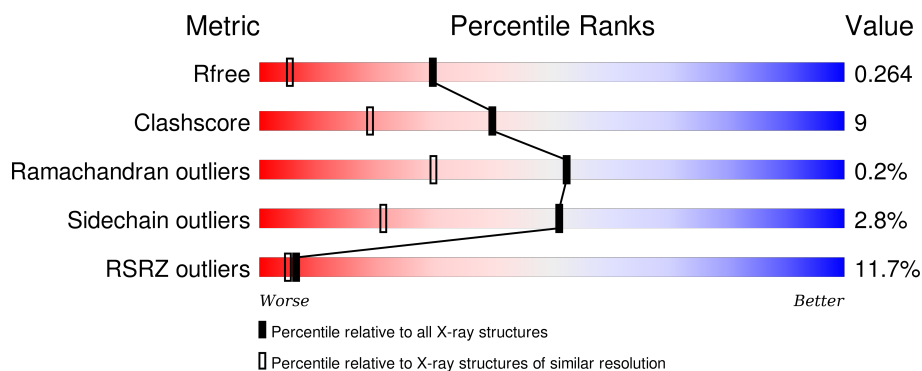
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 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))
$R_{free}$	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	218	<div> <div>11%</div> <div>81%</div> <div>12%</div> <div>5%</div> </div>
1	B	218	<div> <div>3%</div> <div>86%</div> <div>8%</div> <div>5%</div> </div>
1	C	218	<div> <div>18%</div> <div>68%</div> <div>15%</div> <div>16%</div> </div>

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
2	ACT	B	217	-	-	X	-
2	ACT	C	217	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5263 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 Dephospho-CoA kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	1	0
			1580	989	288	301	2			
1	B	208	Total	C	N	O	S	0	3	0
			1595	1000	291	302	2			
1	C	183	Total	C	N	O	S	0	3	0
			1378	869	249	258	2			

There are 39 discrepancies between the modelled and reference sequences:

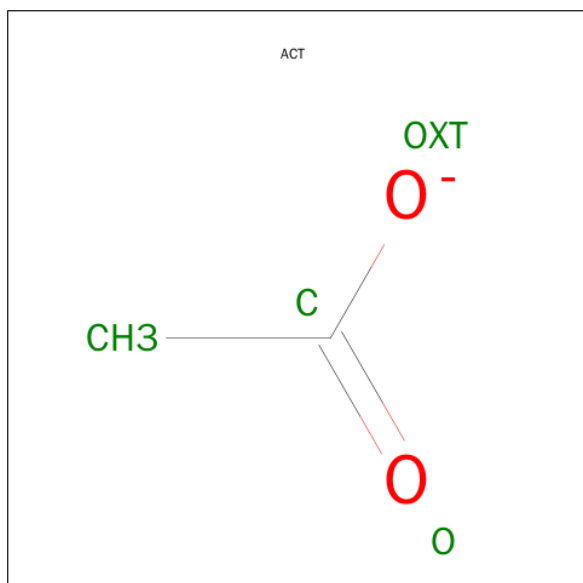
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP P0A6I9
A	0	SER	-	cloning artifact	UNP P0A6I9
A	1	LEU	-	cloning artifact	UNP P0A6I9
A	207	GLU	-	cloning artifact	UNP P0A6I9
A	208	GLY	-	cloning artifact	UNP P0A6I9
A	209	GLY	-	cloning artifact	UNP P0A6I9
A	210	SER	-	cloning artifact	UNP P0A6I9
A	211	HIS	-	cloning artifact	UNP P0A6I9
A	212	HIS	-	cloning artifact	UNP P0A6I9
A	213	HIS	-	cloning artifact	UNP P0A6I9
A	214	HIS	-	cloning artifact	UNP P0A6I9
A	215	HIS	-	cloning artifact	UNP P0A6I9
A	216	HIS	-	cloning artifact	UNP P0A6I9
B	-1	MET	-	cloning artifact	UNP P0A6I9
B	0	SER	-	cloning artifact	UNP P0A6I9
B	1	LEU	-	cloning artifact	UNP P0A6I9
B	207	GLU	-	cloning artifact	UNP P0A6I9
B	208	GLY	-	cloning artifact	UNP P0A6I9
B	209	GLY	-	cloning artifact	UNP P0A6I9
B	210	SER	-	cloning artifact	UNP P0A6I9
B	211	HIS	-	cloning artifact	UNP P0A6I9
B	212	HIS	-	cloning artifact	UNP P0A6I9
B	213	HIS	-	cloning artifact	UNP P0A6I9

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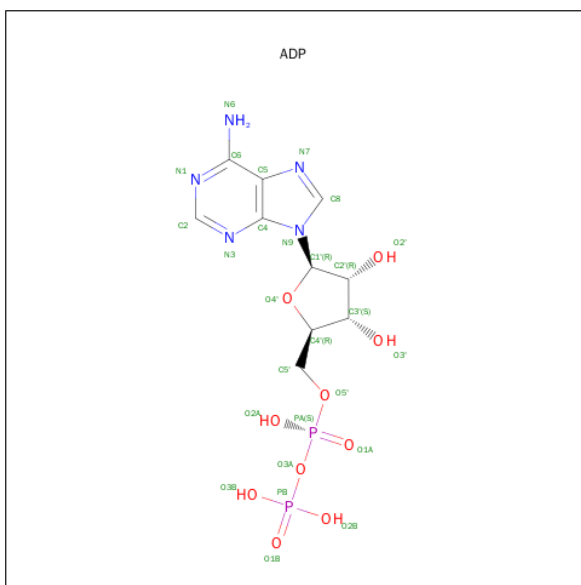
Chain	Residue	Modelled	Actual	Comment	Reference
B	214	HIS	-	cloning artifact	UNP P0A6I9
B	215	HIS	-	cloning artifact	UNP P0A6I9
B	216	HIS	-	cloning artifact	UNP P0A6I9
C	-1	MET	-	cloning artifact	UNP P0A6I9
C	0	SER	-	cloning artifact	UNP P0A6I9
C	1	LEU	-	cloning artifact	UNP P0A6I9
C	207	GLU	-	cloning artifact	UNP P0A6I9
C	208	GLY	-	cloning artifact	UNP P0A6I9
C	209	GLY	-	cloning artifact	UNP P0A6I9
C	210	SER	-	cloning artifact	UNP P0A6I9
C	211	HIS	-	cloning artifact	UNP P0A6I9
C	212	HIS	-	cloning artifact	UNP P0A6I9
C	213	HIS	-	cloning artifact	UNP P0A6I9
C	214	HIS	-	cloning artifact	UNP P0A6I9
C	215	HIS	-	cloning artifact	UNP P0A6I9
C	216	HIS	-	cloning artifact	UNP P0A6I9

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

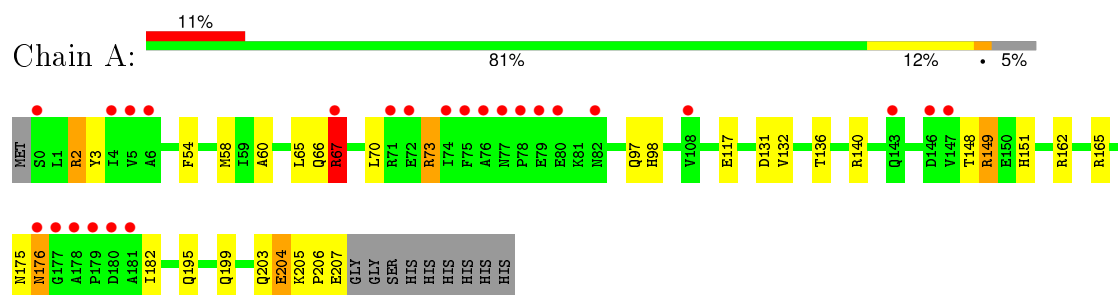
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	263	Total O 263 263	0	0
4	B	253	Total O 253 253	0	0
4	C	159	Total O 159 159	0	0

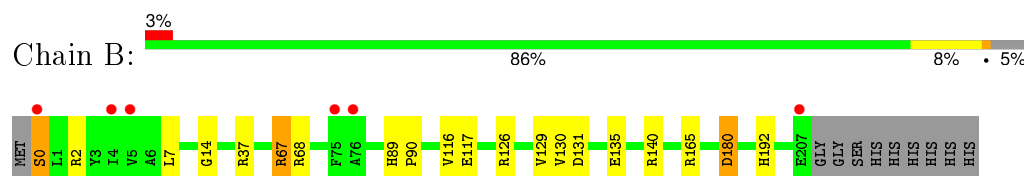
### 3 Residue-property plots [i](#)

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.

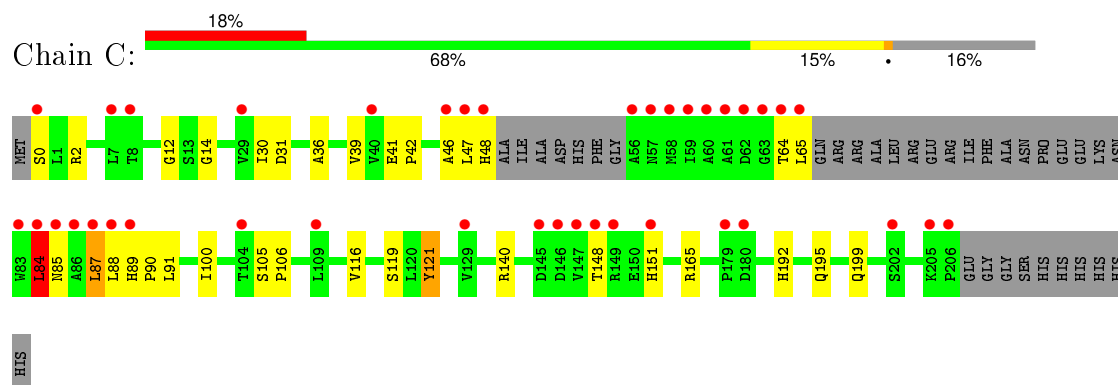
- Molecule 1: Dephospho-CoA kinase



- Molecule 1: Dephospho-CoA kinase



- Molecule 1: Dephospho-CoA kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.62Å 80.52Å 75.31Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	25.15 – 1.65 25.15 – 1.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.15-1.65) 98.5 (25.15-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.65Å)	Xtriage
Refinement program	REFMAC 4	Depositor
R, $R_{free}$	0.224 , 0.284 0.214 , 0.264	Depositor DCC
$R_{free}$ test set	3957 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.9	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78962 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5263	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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: ADP, ACT

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	0.65	0/1610	1.15	7/2198 (0.3%)
1	B	0.72	0/1636	1.18	6/2229 (0.3%)
1	C	0.63	0/1413	1.07	4/1929 (0.2%)
All	All	0.67	0/4659	1.14	17/6356 (0.3%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	TYR	CB-CG-CD1	-9.12	115.53	121.00
1	A	67	ARG	CD-NE-CZ	9.08	136.31	123.60
1	B	180	ASP	CB-CG-OD2	7.96	125.47	118.30
1	B	67	ARG	CD-NE-CZ	6.62	132.86	123.60
1	B	131	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	A	117	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	A	67	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	131	ASP	CB-CG-OD1	6.14	123.82	118.30
1	B	67	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	162	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	117	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	C	121	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	B	140	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	2	ARG	CD-NE-CZ	5.31	131.03	123.60
1	C	165[A]	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	165[B]	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	31	ASP	CB-CG-OD1	5.23	123.01	118.30

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	1580	0	1562	31	0
1	B	1595	0	1588	16	0
1	C	1378	0	1371	33	0
2	B	4	0	3	4	0
2	C	4	0	3	3	0
3	A	27	0	12	0	0
4	A	263	0	0	9	0
4	B	253	0	0	4	0
4	C	159	0	0	3	0
All	All	5263	0	4539	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (80) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD11	1:C:65:LEU:HB2	1.54	0.88
1:C:148:THR:HG23	1:C:151:HIS:H	1.40	0.85
1:C:84:LEU:HD23	1:C:85:ASN:H	1.46	0.81
1:A:148:THR:HG23	1:A:151:HIS:H	1.47	0.77
1:C:84:LEU:CD2	1:C:85:ASN:H	1.98	0.77
1:A:60:ALA:HB2	1:A:66:GLN:HE21	1.50	0.77
1:B:37:ARG:HH12	1:B:67:ARG:NH1	1.83	0.75
1:A:67:ARG:HH11	1:A:67:ARG:HG3	1.52	0.73
1:C:199:GLN:HG3	4:C:329:HOH:O	1.89	0.71
1:C:14:GLY:H	2:C:217:ACT:H3	1.58	0.69
1:C:192:HIS:HD2	4:C:241:HOH:O	1.76	0.67
1:A:199:GLN:HG3	4:A:303:HOH:O	1.96	0.66
1:B:14:GLY:H	2:B:217:ACT:H1	1.62	0.64
1:A:65:LEU:HB3	1:A:67:ARG:HH12	1.62	0.64
1:C:46:ALA:HB2	1:C:91:LEU:CD1	2.28	0.63
1:C:42:PRO:HD3	1:C:64:THR:HG22	1.80	0.63
1:B:0:SER:HA	4:B:459:HOH:O	1.99	0.62
1:A:54:PHE:HB2	1:A:58:MET:HG3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLN:O	1:C:199:GLN:HG2	1.99	0.61
1:B:135:GLU:HG3	4:B:329:HOH:O	2.01	0.61
1:C:148:THR:HG23	1:C:151:HIS:N	2.15	0.59
1:B:192:HIS:HD2	4:B:295:HOH:O	1.86	0.59
1:B:14:GLY:H	2:B:217:ACT:CH3	2.17	0.57
1:A:207:GLU:HA	4:A:304:HOH:O	2.04	0.56
1:A:195:GLN:O	1:A:199:GLN:HG2	2.06	0.56
1:C:87:LEU:HD23	1:C:88:LEU:HG	1.87	0.56
1:A:205:LYS:HB3	1:A:206:PRO:HD2	1.89	0.55
1:A:206:PRO:O	1:A:207:GLU:C	2.45	0.55
1:C:2:ARG:HG2	1:C:2:ARG:HH21	1.71	0.55
1:B:37:ARG:HH12	1:B:67:ARG:HH11	1.53	0.54
1:A:73:ARG:HH11	1:A:73:ARG:HB2	1.72	0.53
1:C:89:HIS:HB3	1:C:90:PRO:HD3	1.91	0.53
1:B:116:VAL:HG21	1:B:165[B]:ARG:HG2	1.91	0.53
1:A:206:PRO:HG2	4:A:325:HOH:O	2.08	0.53
1:A:98:HIS:HD2	4:A:380:HOH:O	1.93	0.52
1:C:14:GLY:H	2:C:217:ACT:CH3	2.24	0.51
1:A:58:MET:HE3	1:A:58:MET:HA	1.92	0.51
1:A:97:GLN:HG2	4:A:315:HOH:O	2.11	0.50
1:C:47:LEU:CD1	1:C:65:LEU:HB2	2.35	0.50
1:C:41:GLU:HB2	1:C:42:PRO:HD2	1.93	0.50
1:C:119:SER:HA	1:C:121:TYR:CE2	2.49	0.48
1:A:175:ASN:OD1	1:A:182:ILE:HD11	2.14	0.47
1:A:204:GLU:OE2	1:A:204:GLU:HA	2.15	0.47
1:A:65:LEU:HB3	1:A:67:ARG:NH1	2.28	0.47
1:B:37:ARG:NH1	1:B:67:ARG:HH11	2.12	0.47
1:C:89:HIS:HB3	1:C:90:PRO:CD	2.45	0.47
1:C:30:ILE:HD13	1:C:100:ILE:CG1	2.45	0.47
1:A:148:THR:CG2	1:A:151:HIS:HB2	2.44	0.47
1:A:98:HIS:HE1	4:A:422:HOH:O	1.98	0.46
1:B:14:GLY:N	2:B:217:ACT:H1	2.28	0.46
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.23	0.46
1:B:7:LEU:HD11	1:B:130:VAL:CG2	2.46	0.46
1:B:7:LEU:HD11	1:B:130:VAL:HG23	1.99	0.45
1:C:46:ALA:HB2	1:C:91:LEU:HD12	1.98	0.45
1:C:46:ALA:HB2	1:C:91:LEU:HD13	1.99	0.44
1:C:2:ARG:HD3	4:C:358:HOH:O	2.18	0.44
1:A:58:MET:HE1	1:A:70:LEU:N	2.32	0.44
1:C:84:LEU:HD23	1:C:85:ASN:N	2.24	0.44
1:A:67:ARG:NH2	4:A:410:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:HG3	1:A:205:LYS:O	2.18	0.43
1:A:132:VAL:HB	1:A:176:ASN:HB3	2.00	0.43
1:A:136:THR:HG23	1:A:140:ARG:NE	2.34	0.43
1:C:105:SER:HB2	1:C:106:PRO:HD2	2.01	0.43
1:A:54:PHE:CB	1:A:58:MET:HG3	2.49	0.42
1:C:89:HIS:N	1:C:90:PRO:HD2	2.34	0.42
1:A:2:ARG:HG3	4:A:434:HOH:O	2.18	0.42
1:B:68:ARG:HG3	4:B:452:HOH:O	2.19	0.42
1:A:148:THR:OG1	1:A:149:ARG:N	2.54	0.41
1:A:165:ARG:HD3	4:A:266:HOH:O	2.19	0.41
1:C:14:GLY:N	2:C:217:ACT:H3	2.32	0.41
1:C:2:ARG:HG2	1:C:2:ARG:NH2	2.34	0.41
1:B:129:VAL:HG13	1:B:165[B]:ARG:HH11	1.86	0.41
1:C:30:ILE:HD13	1:C:100:ILE:HG12	2.02	0.41
1:C:36:ALA:O	1:C:39:VAL:HG22	2.21	0.41
1:B:14:GLY:HA2	2:B:217:ACT:H1	2.02	0.40
1:A:148:THR:HG22	1:A:151:HIS:HB2	2.04	0.40
1:B:89:HIS:HB3	1:B:90:PRO:HD3	2.03	0.40
1:C:12:GLY:O	1:C:140:ARG:HD2	2.22	0.40
1:C:47:LEU:HA	1:C:47:LEU:HD12	1.93	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	207/218 (95%)	202 (98%)	5 (2%)	0	100	100
1	B	209/218 (96%)	208 (100%)	1 (0%)	0	100	100
1	C	180/218 (83%)	176 (98%)	3 (2%)	1 (1%)	30	9
All	All	596/654 (91%)	586 (98%)	9 (2%)	1 (0%)	52	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	LEU

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/177 (92%)	157 (97%)	5 (3%)	47	16
1	B	165/177 (93%)	161 (98%)	4 (2%)	57	28
1	C	142/177 (80%)	138 (97%)	4 (3%)	51	21
All	All	469/531 (88%)	456 (97%)	13 (3%)	51	21

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	73	ARG
1	A	149	ARG
1	A	176	ASN
1	A	204	GLU
1	B	0	SER
1	B	2	ARG
1	B	126	ARG
1	B	180	ASP
1	C	0	SER
1	C	48	HIS
1	C	84	LEU
1	C	87	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	89	HIS

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Mol	Chain	Res	Type
1	A	97	GLN
1	A	98	HIS
1	A	101	GLN
1	B	154	GLN
1	B	192	HIS
1	C	97	GLN
1	C	192	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 ⓘ

3 ligands are modelled in this entry.

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	ADP	A	217	-	22,29,29	0.97	2 (9%)	27,45,45	2.64	4 (14%)
2	ACT	B	217	-	1,3,3	0.77	0	0,3,3	0.00	-
2	ACT	C	217	-	1,3,3	0.20	0	0,3,3	0.00	-

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	ADP	A	217	-	-	0/12/32/32	0/3/3/3
2	ACT	B	217	-	-	0/0/0/0	0/0/0/0
2	ACT	C	217	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	217	ADP	C5-N7	-2.24	1.31	1.39
3	A	217	ADP	PA-O1A	-2.11	1.43	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	217	ADP	N3-C2-N1	-11.74	119.90	128.89
3	A	217	ADP	C1'-N9-C4	-4.18	120.63	126.94
3	A	217	ADP	C4-C5-N7	-2.75	106.95	109.48
3	A	217	ADP	O5'-PA-O1A	2.22	118.24	109.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	217	ACT	4	0
2	C	217	ACT	3	0

## 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, 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	208/218 (95%)	0.66	25 (12%) <b>6</b> <b>4</b>	12, 21, 45, 59	0
1	B	208/218 (95%)	0.24	6 (2%) 55 56	11, 19, 34, 46	0
1	C	183/218 (83%)	1.04	39 (21%) <b>1</b> <b>1</b>	13, 22, 62, 75	0
All	All	599/654 (91%)	0.63	70 (11%) <b>6</b> <b>5</b>	11, 21, 50, 75	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	PHE	11.3
1	C	83	TRP	10.9
1	A	178	ALA	10.0
1	A	76	ALA	7.5
1	C	58	MET	6.7
1	C	61	ALA	6.4
1	C	47	LEU	6.3
1	A	180	ASP	6.1
1	A	78	PRO	5.9
1	C	48	HIS	5.6
1	A	74	ILE	5.3
1	C	60	ALA	5.2
1	A	79	GLU	5.1
1	C	62	ASP	4.9
1	C	59	ILE	4.5
1	C	84	LEU	4.5
1	C	65	LEU	4.4
1	C	57	ASN	4.4
1	B	76	ALA	4.4
1	A	77	ASN	4.3
1	C	146	ASP	4.2
1	A	80	GLU	4.1
1	C	148	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	177	GLY	3.9
1	C	87	LEU	3.7
1	B	75	PHE	3.7
1	C	86	ALA	3.5
1	A	71	ARG	3.5
1	A	147	VAL	3.5
1	B	207	GLU	3.2
1	A	82	ASN	3.1
1	C	205	LYS	3.0
1	C	63	GLY	3.0
1	C	85	ASN	3.0
1	A	179	PRO	3.0
1	C	147	VAL	2.9
1	B	0	SER	2.9
1	C	64	THR	2.9
1	A	72	GLU	2.8
1	C	179	PRO	2.7
1	C	206	PRO	2.7
1	C	40	VAL	2.7
1	C	46	ALA	2.7
1	A	108	VAL	2.7
1	C	89	HIS	2.7
1	C	88	LEU	2.6
1	B	4	ILE	2.5
1	C	56	ALA	2.5
1	C	180	ASP	2.4
1	C	29	VAL	2.4
1	A	146	ASP	2.4
1	A	176	ASN	2.4
1	B	5	VAL	2.4
1	C	151	HIS	2.4
1	A	5	VAL	2.3
1	A	4	ILE	2.3
1	C	7	LEU	2.3
1	A	67	ARG	2.2
1	C	8	THR	2.2
1	C	104	THR	2.2
1	C	145	ASP	2.2
1	C	109	LEU	2.2
1	C	149[A]	ARG	2.1
1	C	0	SER	2.1
1	A	181	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	GLN	2.1
1	A	0	SER	2.1
1	A	6	ALA	2.1
1	C	202	SER	2.1
1	C	129	VAL	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( $\text{\AA}^2$ )	Q<0.9
2	ACT	B	217	4/4	0.77	0.16	1.19	33,33,35,35	0
3	ADP	A	217	27/27	0.92	0.15	0.13	23,32,33,37	0
2	ACT	C	217	4/4	0.92	0.09	-0.51	33,34,34,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.