



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:43 pm GMT

PDB ID : 1B39  
Title : HUMAN CYCLIN-DEPENDENT KINASE 2 PHOSPHORYLATED ON THR 160  
Authors : Brown, N.R.; Noble, M.E.M.; Lawrie, A.M.; Morris, M.C.; Tunnah, P.; Divita, G.; Johnson, L.N.; Endicott, J.A.  
Deposited on : 1998-12-17  
Resolution : 2.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

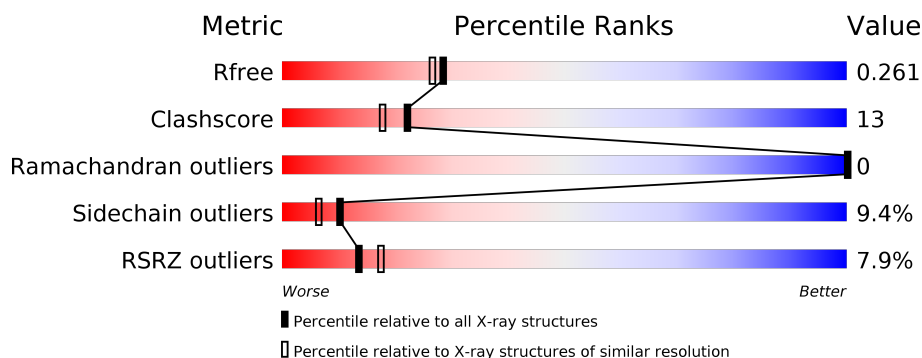
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	299	<div> <div>8%</div> <div>57%</div> <div>31%</div> <div>8%</div> <div>• •</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2515 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.

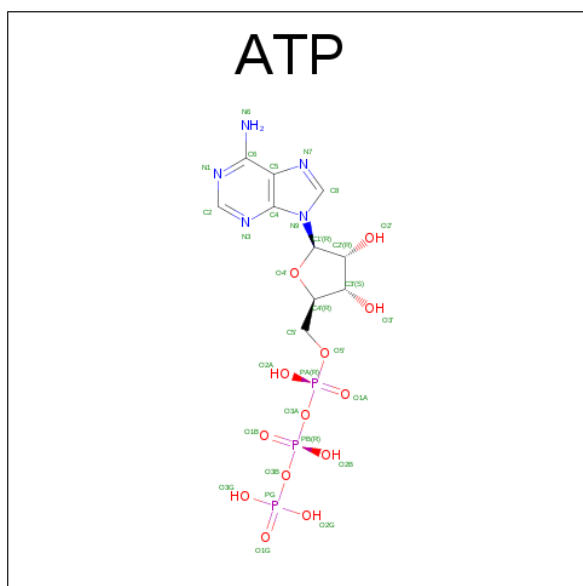
- Molecule 1 is a protein called PROTEIN (CELL DIVISION PROTEIN KINASE 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	0	0
			2338	1525	397	408	8			

- 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 ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

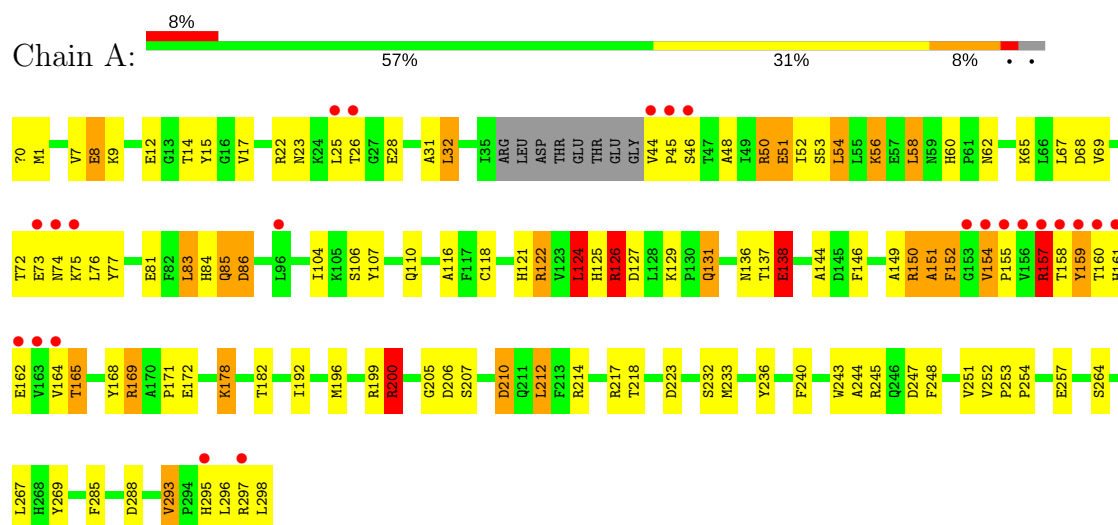
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total 145	O 145	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 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: PROTEIN (CELL DIVISION PROTEIN KINASE 2)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.42Å 71.66Å 72.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 22.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.10) 95.6 (22.02-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.200 , 0.270 0.191 , 0.261	Depositor DCC
$R_{free}$ test set	839 reflections (5.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 81.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2515	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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, 0.333 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: MG, ACE, ATP

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	0.96	1/2397 (0.0%)	2.05	77/3252 (2.4%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	SER	CA-CB	5.91	1.61	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH2	-22.42	109.09	120.30
1	A	199	ARG	NE-CZ-NH2	-17.55	111.53	120.30
1	A	86	ASP	CB-CG-OD1	13.00	130.00	118.30
1	A	138	GLU	OE1-CD-OE2	12.47	138.26	123.30
1	A	122	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	A	223	ASP	CB-CG-OD1	11.65	128.79	118.30
1	A	200	ARG	CA-CB-CG	11.20	138.03	113.40
1	A	245	ARG	NE-CZ-NH1	11.15	125.87	120.30
1	A	200	ARG	NE-CZ-NH2	10.37	125.48	120.30
1	A	58	LEU	CB-CG-CD2	10.36	128.62	111.00
1	A	288	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	A	236	TYR	CB-CG-CD2	-9.42	115.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	TYR	CB-CG-CD1	9.25	126.55	121.00
1	A	233	MET	CA-CB-CG	-9.24	97.60	113.30
1	A	150	ARG	CD-NE-CZ	9.06	136.28	123.60
1	A	245	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	200	ARG	CG-CD-NE	8.68	130.04	111.80
1	A	217	ARG	CD-NE-CZ	8.64	135.69	123.60
1	A	22	ARG	NH1-CZ-NH2	7.96	128.16	119.40
1	A	223	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	257	GLU	CG-CD-OE1	7.26	132.82	118.30
1	A	58	LEU	CB-CG-CD1	-7.06	99.00	111.00
1	A	207	SER	N-CA-CB	6.96	120.94	110.50
1	A	232	SER	CB-CA-C	6.83	123.09	110.10
1	A	243	TRP	CA-CB-CG	6.82	126.66	113.70
1	A	8	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	A	138	GLU	CB-CA-C	-6.59	97.21	110.40
1	A	232	SER	N-CA-CB	-6.44	100.84	110.50
1	A	137	THR	O-C-N	-6.40	112.46	122.70
1	A	196	MET	O-C-N	-6.23	112.73	122.70
1	A	32	LEU	CA-CB-CG	6.22	129.62	115.30
1	A	85	GLN	OE1-CD-NE2	6.17	136.09	121.90
1	A	107	TYR	CB-CG-CD1	6.12	124.67	121.00
1	A	124	LEU	N-CA-CB	6.11	122.63	110.40
1	A	199	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	0	ACE	O-C-N	-5.99	113.11	122.70
1	A	8	GLU	CA-CB-CG	5.80	126.16	113.40
1	A	31	ALA	N-CA-CB	5.79	118.20	110.10
1	A	218	THR	CA-CB-CG2	5.75	120.44	112.40
1	A	50	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	A	199	ARG	N-CA-CB	5.73	120.91	110.60
1	A	152	PHE	CB-CA-C	-5.70	99.00	110.40
1	A	240	PHE	CB-CG-CD1	5.59	124.72	120.80
1	A	106	SER	N-CA-CB	-5.59	102.12	110.50
1	A	245	ARG	CA-CB-CG	5.58	125.67	113.40
1	A	154	VAL	CB-CA-C	-5.56	100.83	111.40
1	A	285	PHE	CA-CB-CG	5.53	127.16	113.90
1	A	81	GLU	N-CA-CB	-5.52	100.66	110.60
1	A	85	GLN	N-CA-CB	-5.51	100.68	110.60
1	A	150	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	172	GLU	OE1-CD-OE2	-5.50	116.69	123.30
1	A	192	ILE	CB-CG1-CD1	5.45	129.15	113.90
1	A	264	SER	N-CA-CB	5.41	118.61	110.50
1	A	104	ILE	CA-C-O	5.37	131.37	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ALA	N-CA-CB	5.34	117.57	110.10
1	A	247	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	85	GLN	CG-CD-OE1	-5.33	110.94	121.60
1	A	165	THR	CA-CB-OG1	-5.33	97.81	109.00
1	A	257	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	A	293	VAL	CA-CB-CG2	5.27	118.80	110.90
1	A	50	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	138	GLU	CB-CG-CD	-5.22	100.11	114.20
1	A	244	ALA	CB-CA-C	-5.21	102.28	110.10
1	A	214	ARG	CD-NE-CZ	-5.20	116.32	123.60
1	A	210	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	A	199	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	A	157	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	169	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	A	212	LEU	CB-CG-CD1	5.14	119.74	111.00
1	A	267	LEU	CB-CG-CD2	5.14	119.73	111.00
1	A	122	ARG	NH1-CZ-NH2	5.13	125.05	119.40
1	A	171	PRO	O-C-N	-5.12	114.52	122.70
1	A	151	ALA	CA-C-N	5.10	128.41	117.20
1	A	126	ARG	CG-CD-NE	-5.07	101.16	111.80
1	A	15	TYR	C-N-CA	-5.02	111.76	122.30
1	A	138	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	A	104	ILE	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	GLU	Mainchain
1	A	269	TYR	Mainchain

## 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	2338	0	2393	63	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	1	0
4	A	145	0	0	5	0
All	All	2515	0	2405	63	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 13.

All (63) 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:125:HIS:HD2	1:A:127:ASP:H	1.24	0.82
1:A:159:TYR:CE2	1:A:160:THR:HG23	2.15	0.80
1:A:60:HIS:HD2	1:A:62:ASN:H	1.29	0.80
1:A:26:THR:HB	1:A:28:GLU:H	1.53	0.71
1:A:58:LEU:HD21	1:A:118:CYS:SG	2.31	0.71
1:A:48:ALA:O	1:A:52:ILE:HG12	1.93	0.69
1:A:26:THR:HG21	1:A:28:GLU:HB2	1.74	0.68
1:A:60:HIS:CD2	1:A:62:ASN:H	2.11	0.68
1:A:149:ALA:HB1	1:A:154:VAL:HG22	1.78	0.66
1:A:12:GLU:CD	1:A:160:THR:HG21	2.16	0.65
1:A:83:LEU:HD23	4:A:492:HOH:O	1.96	0.64
1:A:51:GLU:HG2	1:A:151:ALA:HB2	1.83	0.60
1:A:54:LEU:N	1:A:54:LEU:HD23	2.19	0.58
1:A:84:HIS:HB3	1:A:298:LEU:HD22	1.87	0.56
1:A:295:HIS:O	1:A:295:HIS:CG	2.58	0.56
1:A:56:LYS:HD2	1:A:69:VAL:HG23	1.89	0.55
1:A:53:SER:O	1:A:56:LYS:HB2	2.08	0.52
1:A:1:MET:HG2	1:A:77:TYR:CZ	2.44	0.52
1:A:158:THR:HG22	1:A:164:VAL:CG2	2.40	0.52
1:A:136:ASN:HB3	4:A:492:HOH:O	2.10	0.52
1:A:126:ARG:NH2	1:A:169:ARG:CZ	2.73	0.52
1:A:14:THR:HA	1:A:158:THR:HB	1.92	0.51
1:A:126:ARG:NH2	1:A:169:ARG:NH2	2.60	0.50
1:A:23:ASN:OD1	1:A:25:LEU:N	2.41	0.50
1:A:200:ARG:HD2	4:A:515:HOH:O	2.13	0.48
1:A:84:HIS:CB	1:A:298:LEU:HD22	2.44	0.48
1:A:124:LEU:HD22	1:A:182:THR:HG22	1.96	0.48
1:A:126:ARG:HH21	1:A:169:ARG:NH2	2.12	0.47
1:A:62:ASN:ND2	1:A:110:GLN:HB3	2.28	0.47
1:A:251:VAL:HG12	1:A:252:VAL:HG13	1.97	0.47
1:A:85:GLN:HG3	1:A:86:ASP:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:THR:HB	1:A:73:GLU:OE1	2.16	0.46
1:A:158:THR:HG22	1:A:164:VAL:HG22	1.98	0.44
1:A:58:LEU:CD2	1:A:118:CYS:SG	3.04	0.44
1:A:205:GLY:HA2	1:A:210:ASP:OD2	2.18	0.44
1:A:125:HIS:HE1	1:A:144:ALA:O	1.99	0.44
1:A:178:LYS:HD3	4:A:432:HOH:O	2.18	0.44
1:A:129:LYS:NZ	3:A:381:ATP:O1G	2.47	0.44
1:A:248:PHE:CD1	1:A:248:PHE:N	2.87	0.43
1:A:45:PRO:HB2	1:A:48:ALA:HB3	2.00	0.43
1:A:131:GLN:CD	1:A:131:GLN:H	2.21	0.43
1:A:161:HIS:O	1:A:162:GLU:C	2.57	0.43
1:A:26:THR:CB	1:A:28:GLU:H	2.28	0.43
1:A:121:HIS:O	1:A:122:ARG:HB2	2.18	0.42
1:A:157:ARG:HD2	1:A:161:HIS:O	2.20	0.42
1:A:26:THR:CG2	1:A:28:GLU:HB2	2.45	0.42
1:A:159:TYR:CD2	1:A:160:THR:HG23	2.55	0.42
1:A:65:LYS:HD3	1:A:67:LEU:HD21	2.01	0.42
1:A:200:ARG:HH11	1:A:200:ARG:HD2	1.71	0.42
1:A:165:THR:HG21	1:A:168:TYR:CE2	2.55	0.42
1:A:14:THR:N	1:A:158:THR:HB	2.35	0.42
1:A:12:GLU:HG3	1:A:160:THR:OG1	2.21	0.41
1:A:44:VAL:HG21	1:A:76:LEU:HB2	2.02	0.41
1:A:253:PRO:HB2	1:A:254:PRO:HD3	2.01	0.41
1:A:9:LYS:HE3	1:A:17:VAL:HG23	2.03	0.41
1:A:206:ASP:HB2	4:A:422:HOH:O	2.21	0.41
1:A:164:VAL:HG12	1:A:165:THR:N	2.36	0.41
1:A:126:ARG:HD2	1:A:126:ARG:HH11	1.71	0.40
1:A:158:THR:N	1:A:162:GLU:O	2.54	0.40
1:A:158:THR:OG1	1:A:162:GLU:HB3	2.21	0.40
1:A:52:ILE:HD11	1:A:152:PHE:CZ	2.56	0.40
1:A:14:THR:CG2	1:A:155:PRO:HD2	2.52	0.40
1:A:7:VAL:O	1:A:8:GLU:HB3	2.21	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	287/299 (96%)	272 (95%)	15 (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	256/263 (97%)	232 (91%)	24 (9%)	10	6

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LEU
1	A	46	SER
1	A	50	ARG
1	A	51	GLU
1	A	54	LEU
1	A	56	LYS
1	A	68	ASP
1	A	74	ASN
1	A	75	LYS
1	A	83	LEU
1	A	124	LEU
1	A	126	ARG
1	A	131	GLN
1	A	138	GLU
1	A	146	PHE
1	A	150	ARG
1	A	157	ARG
1	A	159	TYR
1	A	178	LYS

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Mol	Chain	Res	Type
1	A	200	ARG
1	A	212	LEU
1	A	293	VAL
1	A	296	LEU
1	A	297	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	59	ASN
1	A	60	HIS
1	A	125	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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
3	ATP	A	381	2	27,33,33	1.30	2 (7%)	25,52,52	1.52	5 (20%)

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	ATP	A	381	2	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	381	ATP	C8-N7	-3.70	1.27	1.34
3	A	381	ATP	C5-N7	-2.23	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	381	ATP	O3'-C3'-C4'	-2.47	103.87	111.09
3	A	381	ATP	C4'-O4'-C1'	2.22	112.13	109.77
3	A	381	ATP	C4-C5-N7	2.58	111.90	109.41
3	A	381	ATP	C1'-N9-C4	3.18	132.14	126.64
3	A	381	ATP	C5-C6-N6	3.57	127.75	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	381	ATP	1	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	290/299 (96%)	0.37	23 (7%) <b>13</b> <b>17</b>	15, 28, 63, 110	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	PRO	12.4
1	A	158	THR	12.4
1	A	160	THR	12.0
1	A	159	TYR	10.3
1	A	154	VAL	9.3
1	A	156	VAL	8.3
1	A	164	VAL	7.5
1	A	74	ASN	7.3
1	A	25	LEU	6.8
1	A	161	HIS	6.8
1	A	162	GLU	4.5
1	A	96	LEU	4.4
1	A	157	ARG	4.4
1	A	163	VAL	4.2
1	A	73	GLU	4.1
1	A	44	VAL	3.9
1	A	295	HIS	3.9
1	A	75	LYS	3.4
1	A	46	SER	3.2
1	A	45	PRO	3.1
1	A	26	THR	2.6
1	A	297	ARG	2.4
1	A	153	GLY	2.3



## 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
3	ATP	A	381	31/31	0.90	0.19	0.40	32,45,50,51	0
2	MG	A	382	1/1	0.64	0.15	-	36,36,36,36	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.