



## wwPDB EM Map/Model Validation Report ⓘ

Jun 29, 2016 – 01:29 PM EDT

PDB ID : 5FWM  
EMDB ID: : 3342  
Title : Atomic cryoEM structure of Hsp90-Cdc37-Cdk4 complex  
Authors : Verba, K.A.; Wang, R.Y.R.; Arakawa, A.; Liu, Y.; Yokoyama, S.; Agard, D.A.  
Deposited on : 2016-02-18  
Resolution : 8.00 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

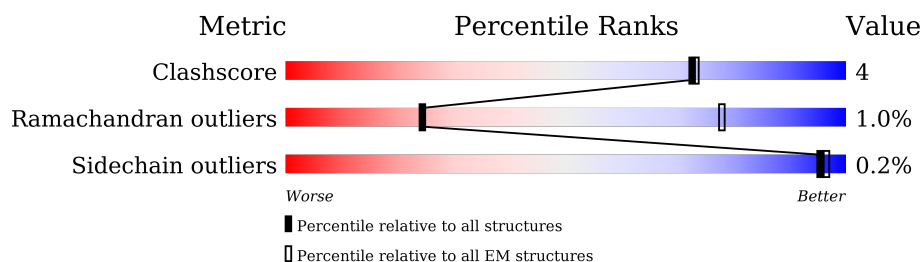
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	727	
1	B	727	
2	E	378	
3	K	310	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 29596 atoms, of which 14789 are hydrogens and 0 are deuteriums.

In the tables below, 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 HEAT SHOCK PROTEIN HSP 90 BETA.

Mol	Chain	Residues	Atoms							AltConf	Trace
1	A	638	Total	C	H	N	O	S	0	0	
			10399	3280	5226	870	1000	23			
1	B	630	Total	C	H	N	O	S	0	0	
			10242	3235	5139	856	989	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P08238
A	-1	GLY	-	EXPRESSION TAG	UNP P08238
A	0	PHE	-	EXPRESSION TAG	UNP P08238
B	-2	GLY	-	EXPRESSION TAG	UNP P08238
B	-1	GLY	-	EXPRESSION TAG	UNP P08238
B	0	PHE	-	EXPRESSION TAG	UNP P08238

- Molecule 2 is a protein called HSP90 CO-CHAPERONE CDC37.

Mol	Chain	Residues	Atoms							AltConf	Trace
2	E	259	Total	C	H	N	O	P	S	0	0
			4307	1358	2125	383	425	1	15		

- Molecule 3 is a protein called CYCLIN-DEPENDENT KINASE 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	291	Total	C	H	N	O	S	0	0
			4584	1463	2299	403	408	11		

There are 7 discrepancies between the modelled and reference sequences:

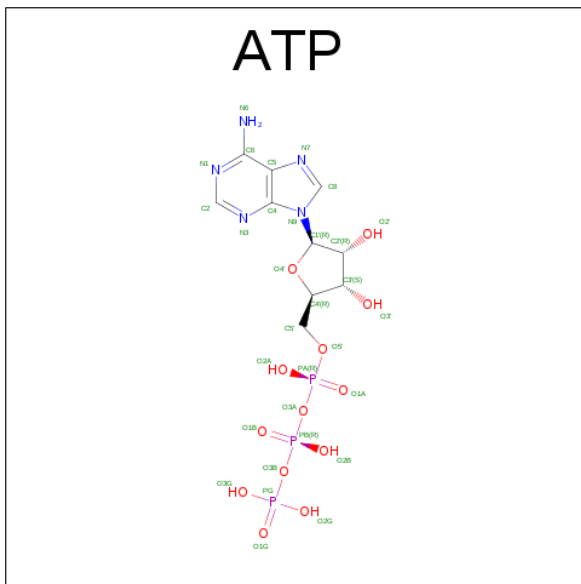
Chain	Residue	Modelled	Actual	Comment	Reference
K	-6	GLY	-	EXPRESSION TAG	UNP P11802
K	-5	ALA	-	EXPRESSION TAG	UNP P11802
K	-4	MET	-	EXPRESSION TAG	UNP P11802

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ASP	-	EXPRESSION TAG	UNP P11802
K	-2	PRO	-	EXPRESSION TAG	UNP P11802
K	-1	GLU	-	EXPRESSION TAG	UNP P11802
K	0	PHE	-	EXPRESSION TAG	UNP P11802

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Mg	0
			1	1	
5	A	1	Total	Mg	0
			1	1	



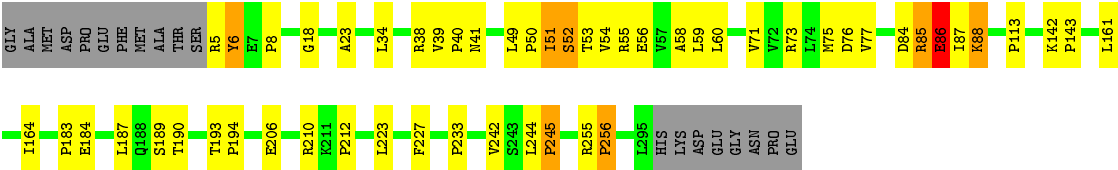
● Molecule 3: CYCLIN-DEPENDENT KINASE 4

Chain K: 

76%

15%

6%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	3800	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4K X 4K)	Depositor

## 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: MG, ATP, SEP

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.95	0/5257	0.57	0/7062
1	B	0.92	0/5187	0.56	0/6972
2	E	0.97	1/2209 (0.0%)	0.50	0/2955
3	K	0.89	1/2342 (0.0%)	0.67	0/3181
All	All	0.93	2/14995 (0.0%)	0.58	0/20170

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
3	K	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	134	GLU	CD-OE2	-5.21	1.20	1.25
3	K	184	GLU	CD-OE2	-5.00	1.20	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	86	GLU	Mainchain,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	5173	5226	5224	38	0
1	B	5103	5139	5137	38	0
2	E	2182	2125	2124	14	0
3	K	2285	2299	2297	46	0
4	A	31	0	12	3	0
4	B	31	0	12	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	14807	14789	14806	125	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.

All (125) 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:B:609:GLN:HB3	1:B:612:ARG:CG	1.70	1.21
1:B:606:MET:CE	1:B:612:ARG:CZ	2.17	1.20
3:K:49:LEU:O	3:K:49:LEU:HD12	1.56	1.06
1:B:609:GLN:HB3	1:B:612:ARG:HG3	1.39	1.04
1:B:609:GLN:CG	1:B:612:ARG:HG2	1.87	1.04
1:B:609:GLN:CB	1:B:612:ARG:HG2	1.90	1.02
1:B:609:GLN:HB3	1:B:612:ARG:HG2	1.41	0.97
1:B:606:MET:HE3	1:B:612:ARG:CZ	2.01	0.88
1:B:609:GLN:CB	1:B:612:ARG:CG	2.50	0.86
1:B:606:MET:HE1	1:B:612:ARG:CZ	2.06	0.85
4:A:1691:ATP:O2A	4:A:1691:ATP:O2G	2.00	0.80
1:B:606:MET:HE2	1:B:612:ARG:CZ	2.10	0.80
1:B:606:MET:CE	1:B:612:ARG:NH2	2.45	0.79
4:B:1692:ATP:O2G	4:B:1692:ATP:O2B	2.03	0.76
1:B:606:MET:HE3	1:B:612:ARG:NH2	2.00	0.76
2:E:132:LYS:HB3	2:E:133:PRO:HA	1.70	0.72
1:B:606:MET:CE	1:B:612:ARG:NE	2.57	0.68
1:B:609:GLN:HG3	1:B:612:ARG:HG2	1.76	0.65
3:K:39:VAL:HG23	3:K:39:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLN:CG	1:B:612:ARG:CG	2.71	0.63
1:B:606:MET:CE	1:B:612:ARG:NH1	2.61	0.62
1:B:425:ASN:ND2	2:E:131:THR:OG1	2.34	0.61
1:A:279:GLN:O	1:A:279:GLN:HG3	2.02	0.60
1:B:606:MET:HE1	1:B:612:ARG:NE	2.15	0.60
1:B:80:GLN:OE1	1:B:80:GLN:N	2.34	0.60
1:A:221:ARG:HB2	1:A:273:LYS:HB2	1.85	0.58
3:K:75:MET:SD	3:K:76:ASP:HB2	2.44	0.57
2:E:132:LYS:HB3	2:E:133:PRO:CA	2.32	0.57
2:E:131:THR:O	2:E:132:LYS:HB2	2.04	0.56
1:B:609:GLN:HG2	1:B:612:ARG:CD	2.35	0.56
2:E:245:ASP:HB2	3:K:52:SER:HB3	1.87	0.55
1:A:124:SER:OG	1:A:358:ARG:NH1	2.40	0.55
1:A:603:GLU:HB2	3:K:41:ASN:HB3	1.88	0.54
1:A:598:TRP:CZ2	1:A:621:MET:HB2	2.43	0.53
2:E:132:LYS:CB	2:E:133:PRO:HA	2.39	0.52
4:A:1691:ATP:H2'	4:A:1691:ATP:N3	2.24	0.52
1:A:596:TYR:N	1:A:596:TYR:CD1	2.77	0.52
3:K:18:GLY:HA3	3:K:87:ILE:HB	1.92	0.52
3:K:85:ARG:O	3:K:86:GLU:CB	2.58	0.51
1:B:606:MET:HE2	1:B:612:ARG:NH1	2.23	0.51
3:K:51:ILE:O	3:K:52:SER:HB2	2.09	0.51
1:B:606:MET:HE2	1:B:612:ARG:NH2	2.21	0.51
1:A:621:MET:N	3:K:50:PRO:O	2.44	0.50
1:B:606:MET:HE3	1:B:612:ARG:NE	2.25	0.50
3:K:189:SER:OG	3:K:190:THR:N	2.44	0.50
4:A:1691:ATP:O3A	4:A:1691:ATP:O1G	2.30	0.50
1:A:128:GLN:O	1:A:128:GLN:OE1	2.29	0.50
2:E:131:THR:O	2:E:132:LYS:CB	2.59	0.50
3:K:206:GLU:O	3:K:210:ARG:N	2.45	0.50
1:B:609:GLN:HG2	1:B:612:ARG:HD3	1.93	0.50
1:B:609:GLN:HG2	1:B:612:ARG:HG2	1.84	0.49
1:B:220:GLU:HG2	1:B:220:GLU:O	2.13	0.49
3:K:87:ILE:O	3:K:88:LYS:HB2	2.12	0.49
1:A:602:MET:SD	3:K:39:VAL:HB	2.53	0.49
1:A:448:ARG:HD3	3:K:8:PRO:HG3	1.95	0.49
3:K:71:VAL:O	3:K:71:VAL:HG23	2.13	0.48
3:K:142:LYS:HB2	3:K:143:PRO:CD	2.42	0.48
1:A:38:ILE:C	1:A:38:ILE:HD12	2.34	0.48
1:A:486:ILE:O	1:A:486:ILE:HG23	2.14	0.48
1:A:520:TYR:N	1:A:520:TYR:CD1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:255:ARG:O	3:K:256:PRO:C	2.52	0.48
3:K:49:LEU:O	3:K:49:LEU:CD1	2.46	0.48
1:A:473:VAL:HA	1:A:476:MET:SD	2.54	0.48
3:K:142:LYS:HB2	3:K:143:PRO:HD2	1.96	0.47
3:K:210:ARG:O	3:K:210:ARG:HG2	2.14	0.47
3:K:38:ARG:HB3	3:K:86:GLU:N	2.29	0.47
3:K:244:LEU:HB3	3:K:245:PRO:HD2	1.96	0.47
1:B:366:CYS:HA	1:B:369:LEU:HB3	1.97	0.47
3:K:60:LEU:HB3	3:K:73:ARG:HB2	1.97	0.47
1:B:93:MET:SD	4:B:1692:ATP:H1'	2.55	0.46
2:E:245:ASP:HB3	2:E:248:TYR:HB2	1.98	0.46
3:K:84:ASP:HA	3:K:87:ILE:HD12	1.98	0.46
1:A:79:PRO:HA	1:A:193:LEU:HD13	1.96	0.46
1:B:609:GLN:HG2	1:B:612:ARG:CG	2.45	0.46
3:K:187:LEU:HD22	3:K:242:VAL:HG13	1.98	0.46
3:K:73:ARG:HD2	3:K:73:ARG:C	2.36	0.46
1:A:527:GLU:HB2	3:K:5:ARG:HG3	1.97	0.45
1:A:593:THR:HA	3:K:49:LEU:HB2	1.99	0.45
1:B:157:TRP:HE3	1:B:157:TRP:O	2.00	0.45
1:A:456:ARG:HB3	1:A:466:MET:HG2	1.98	0.45
3:K:6:TYR:CD1	3:K:6:TYR:N	2.84	0.45
1:B:93:MET:CE	4:B:1692:ATP:H1'	2.47	0.45
2:E:182:VAL:HB	2:E:231:ARG:HG2	1.99	0.45
1:A:316:LEU:HB2	1:A:337:ARG:HA	1.99	0.44
1:B:83:THR:HG22	1:B:184:HIS:HA	1.99	0.44
3:K:75:MET:SD	3:K:75:MET:C	2.96	0.44
2:E:222:LEU:HB2	2:E:237:PHE:CE2	2.53	0.43
1:A:67:SER:OG	1:A:177:ARG:NH2	2.51	0.43
1:A:624:LYS:HZ2	1:A:624:LYS:HB2	1.83	0.43
1:A:684:ILE:HD13	1:B:658:LEU:HD21	2.00	0.43
1:A:430:TYR:O	1:A:434:SER:N	2.52	0.43
2:E:25:THR:HA	2:E:28:LEU:HB3	2.01	0.43
1:A:10:GLU:N	1:B:171:HIS:HE2	2.16	0.43
2:E:57:CYS:HG	2:E:98:TRP:HE1	1.66	0.43
3:K:161:LEU:HA	3:K:164:ILE:HG12	2.01	0.43
3:K:23:ALA:HB2	3:K:34:LEU:HD11	2.00	0.43
1:A:82:ARG:O	1:A:82:ARG:HG2	2.18	0.43
3:K:183:PRO:O	3:K:187:LEU:HG	2.19	0.43
3:K:223:LEU:HB3	3:K:227:PHE:CE2	2.54	0.43
3:K:55:ARG:O	3:K:58:ALA:HB3	2.19	0.42
1:A:74:ASP:HB2	1:A:87:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:GLU:OE1	1:B:627:GLU:HA	2.18	0.42
2:E:248:TYR:O	2:E:252:PHE:N	2.51	0.42
1:A:128:GLN:CD	1:A:128:GLN:O	2.57	0.42
3:K:6:TYR:HD1	3:K:6:TYR:N	2.17	0.42
1:A:598:TRP:CE3	1:A:622:ALA:HB2	2.54	0.42
3:K:84:ASP:O	3:K:85:ARG:HB2	2.19	0.42
1:A:564:CYS:SG	1:A:628:ILE:HD12	2.60	0.42
1:A:602:MET:HB3	3:K:39:VAL:O	2.20	0.41
3:K:51:ILE:HG22	3:K:52:SER:N	2.35	0.41
1:A:445:SER:HB3	3:K:8:PRO:HB2	2.01	0.41
1:A:621:MET:HA	3:K:53:THR:H	1.86	0.41
1:A:624:LYS:NZ	1:A:624:LYS:HB2	2.35	0.41
1:A:331:ALA:HA	1:A:380:VAL:O	2.21	0.41
1:A:620:MET:SD	3:K:51:ILE:HD12	2.61	0.41
1:B:219:LYS:O	1:B:220:GLU:C	2.59	0.41
2:E:133:PRO:O	2:E:134:GLU:HB2	2.21	0.41
3:K:56:GLU:O	3:K:59:LEU:HB3	2.20	0.41
1:B:148:LYS:C	1:B:148:LYS:HD3	2.42	0.40
1:A:594:SER:HB2	3:K:54:VAL:HB	2.02	0.40
3:K:18:GLY:HA3	3:K:87:ILE:CB	2.52	0.40
3:K:193:THR:N	3:K:194:PRO:HD2	2.36	0.40
1:A:82:ARG:NH1	1:A:187:GLU:OE1	2.55	0.40
1:A:292:ASN:HA	1:A:293:PRO:HD3	1.96	0.40
1:B:551:LYS:NZ	1:B:555:GLU:OE2	2.51	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 PDB entries followed by that with respect to all EM entries.

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	634/727 (87%)	600 (95%)	30 (5%)	4 (1%)	30 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	626/727 (86%)	610 (97%)	15 (2%)	1 (0%)	52	86
2	E	256/378 (68%)	241 (94%)	14 (6%)	1 (0%)	39	80
3	K	285/310 (92%)	240 (84%)	33 (12%)	12 (4%)	3	34
All	All	1801/2142 (84%)	1691 (94%)	92 (5%)	18 (1%)	24	65

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	132	LYS
3	K	52	SER
3	K	85	ARG
3	K	86	GLU
3	K	256	PRO
3	K	77	VAL
3	K	88	LYS
1	A	174	PRO
1	A	281	GLU
3	K	40	PRO
3	K	51	ILE
3	K	113	PRO
1	A	128	GLN
3	K	212	PRO
3	K	233	PRO
1	A	173	GLU
3	K	245	PRO
1	B	127	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	577/653 (88%)	575 (100%)	2 (0%)	94	96
1	B	569/653 (87%)	569 (100%)	0	100	100
2	E	238/340 (70%)	238 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	247/262 (94%)	246 (100%)	1 (0%)	93	96
All	All	1631/1908 (86%)	1628 (100%)	3 (0%)	95	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	ARG
1	A	596	TYR
3	K	6	TYR

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

Mol	Chain	Res	Type
1	B	425	ASN
3	K	98	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
2	SEP	E	13	2	7,9,10	1.57	1 (14%)	8,12,14	1.43	2 (25%)

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
2	SEP	E	13	2	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	SEP	P-O1P	3.22	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	SEP	O-C-CA	-2.00	120.35	125.72
2	E	13	SEP	OG-CB-CA	3.28	111.12	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
4	ATP	A	1691	5	26,33,33	1.15	2 (7%)	26,52,52	1.73	3 (11%)
4	ATP	B	1692	5	26,33,33	1.03	1 (3%)	26,52,52	1.73	4 (15%)

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
4	ATP	A	1691	5	-	0/18/38/38	0/3/3/3
4	ATP	B	1692	5	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1691	ATP	O4'-C1'	2.29	1.44	1.41
4	A	1691	ATP	C5-C4	3.17	1.47	1.40
4	B	1692	ATP	C5-C4	3.20	1.47	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1691	ATP	N3-C2-N1	-6.92	123.43	128.87
4	B	1692	ATP	N3-C2-N1	-6.79	123.54	128.87
4	B	1692	ATP	O2'-C2'-C1'	-2.04	105.24	111.61
4	A	1691	ATP	O2G-PG-O1G	2.03	117.24	110.63
4	A	1691	ATP	O3G-PG-O2G	2.03	114.89	107.44
4	B	1692	ATP	O3G-PG-O2G	2.12	115.24	107.44
4	B	1692	ATP	O2G-PG-O1G	2.31	118.17	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1691	ATP	3	0
4	B	1692	ATP	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.