



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:08 AM GMT

PDB ID : 2V8Q
Title : CRYSTAL STRUCTURE OF THE REGULATORY FRAGMENT OF MAMMALIAN AMPK IN COMPLEXES WITH AMP
Authors : Xiao, B.; Heath, R.; Saiu, P.; Leiper, F.C.; Leone, P.; Jing, C.; Walker, P.A.; Haire, L.; Eccleston, J.F.; Davis, C.T.; Martin, S.R.; Carling, D.; Gamblin, S.J.
Deposited on : 2007-08-13
Resolution : 2.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

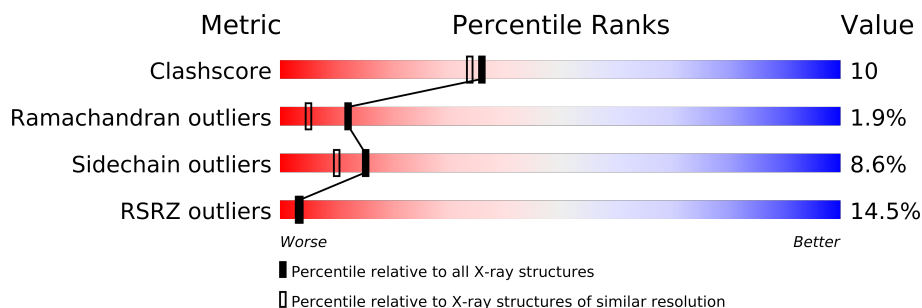
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	157	
2	B	87	
3	E	330	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4381 atoms, of which 0 are hydrogen and 0 are deuterium.

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 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUB-UNIT ALPHA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	0	0
			842	536	149	151	6			

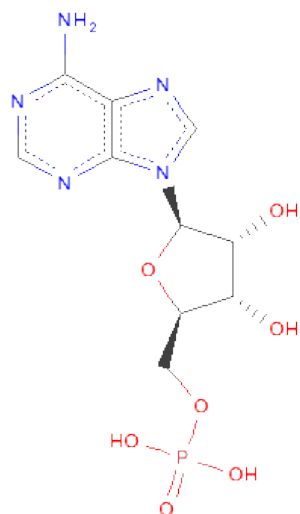
- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			601	392	103	103	3			

- Molecule 3 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	304	Total	C	N	O	S	0	0	0
			2441	1584	407	443	7			

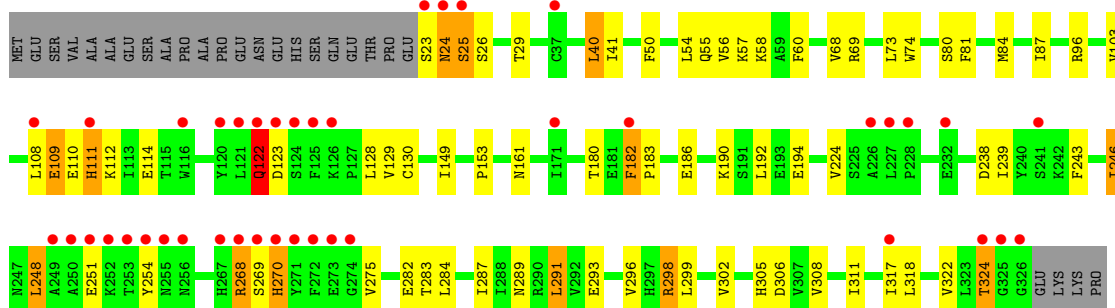
- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total	O	0	0
			87	87		
5	B	50	Total	O	0	0
			50	50		
5	E	291	Total	O	0	0
			291	291		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.52Å 119.39Å 129.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.10) 99.0 (19.98-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.237 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44246 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4381	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	0.48	0/860	0.68	1/1161 (0.1%)
2	B	0.45	0/616	0.66	0/832
3	E	0.47	0/2493	0.66	1/3384 (0.0%)
All	All	0.47	0/3969	0.66	2/5377 (0.0%)

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
2	B	0	3
3	E	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LEU	CA-CB-CG	7.31	132.11	115.30
3	E	40	LEU	CA-CB-CG	6.33	129.87	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	208	LEU	Peptide
2	B	209	PRO	Peptide
2	B	210	PRO	Peptide

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Mol	Chain	Res	Type	Group
3	E	182	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	842	0	842	29	0
2	B	601	0	625	13	0
3	E	2441	0	2506	50	0
4	E	69	0	36	1	0
5	A	87	0	0	1	0
5	B	50	0	0	0	0
5	E	291	0	0	2	0
All	All	4381	0	4009	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:23:SER:HB2	3:E:186:GLU:HB2	1.45	0.96
2:B:208:LEU:O	2:B:210:PRO:HD3	1.69	0.93
2:B:197:ARG:HH11	2:B:197:ARG:HG2	1.38	0.88
3:E:84:MET:HE3	3:E:153:PRO:HG3	1.56	0.86
3:E:108:LEU:O	3:E:111:HIS:HB2	1.81	0.81
1:A:532:THR:H	3:E:161:ASN:HD21	1.25	0.80
3:E:96:ARG:HB3	3:E:108:LEU:HD11	1.65	0.78
3:E:26:SER:HB3	3:E:29:THR:H	1.50	0.76
1:A:413:VAL:HA	1:A:546:LEU:HD12	1.69	0.75
1:A:420:LEU:HD11	1:A:545:ILE:HD12	1.70	0.74
2:B:197:ARG:CG	2:B:197:ARG:HH11	2.01	0.73
1:A:526:PRO:HG2	3:E:128:LEU:HD23	1.70	0.72
1:A:528:PRO:HA	3:E:80:SER:HB3	1.71	0.71
1:A:447:MET:CE	1:A:542:LEU:HD12	2.25	0.66
3:E:69:ARG:HD3	3:E:243:PHE:CD1	2.31	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:541:ASN:O	1:A:545:ILE:HG13	1.99	0.62
1:A:416:ALA:HB2	1:A:546:LEU:HB3	1.83	0.61
3:E:324:THR:HA	5:E:2007:HOH:O	2.01	0.60
3:E:84:MET:CE	3:E:153:PRO:HG3	2.31	0.60
1:A:546:LEU:HD23	1:A:547:ALA:HB2	1.83	0.60
1:A:542:LEU:O	1:A:546:LEU:HD13	2.04	0.58
3:E:87:ILE:HD12	3:E:246:ILE:HG21	1.87	0.56
1:A:417:ILE:HG23	1:A:422:TYR:HB2	1.88	0.55
1:A:416:ALA:CB	1:A:546:LEU:HB3	2.37	0.54
3:E:87:ILE:HD12	3:E:246:ILE:CG2	2.38	0.54
3:E:282:GLU:HB2	3:E:287:ILE:HD11	1.90	0.53
3:E:289:ASN:O	3:E:293:GLU:HG3	2.08	0.53
3:E:248:LEU:O	3:E:251:GLU:HG2	2.09	0.53
2:B:236:VAL:HG13	2:B:236:VAL:O	2.10	0.52
1:A:427:VAL:HG21	1:A:433:ARG:HD3	1.93	0.51
2:B:251:MET:HG3	2:B:272:ILE:HG12	1.93	0.51
2:B:197:ARG:CG	2:B:197:ARG:NH1	2.65	0.51
3:E:283:THR:O	3:E:287:ILE:HD12	2.11	0.51
1:A:428:ASN:HB2	1:A:431:TYR:HB3	1.94	0.49
3:E:24:ASN:C	3:E:25:SER:O	2.50	0.49
3:E:56:VAL:HG13	3:E:60:PHE:CE1	2.47	0.49
3:E:251:GLU:HG3	3:E:254:TYR:H	1.78	0.49
3:E:96:ARG:HB3	3:E:108:LEU:CD1	2.40	0.48
3:E:183:PRO:HD2	5:E:2140:HOH:O	2.13	0.48
3:E:69:ARG:NH1	3:E:243:PHE:HB2	2.29	0.48
1:A:427:VAL:CG2	1:A:433:ARG:HD3	2.43	0.47
2:B:262:LYS:NZ	3:E:41:ILE:O	2.43	0.47
1:A:409:ILE:O	1:A:413:VAL:HG13	2.15	0.47
3:E:24:ASN:O	3:E:25:SER:O	2.33	0.46
1:A:441:THR:HG22	1:A:443:THR:HG23	1.97	0.45
1:A:447:MET:HE3	1:A:542:LEU:HD12	1.95	0.45
1:A:423:GLU:CG	1:A:435:ARG:HB3	2.46	0.45
3:E:109:GLU:OE2	3:E:109:GLU:HA	2.16	0.45
2:B:200:GLU:CG	2:B:203:LYS:HB2	2.47	0.45
3:E:291:LEU:HD13	3:E:299:LEU:HG	1.98	0.45
3:E:305:HIS:O	3:E:306:ASP:HB2	2.16	0.45
3:E:246:ILE:H	3:E:246:ILE:HG13	1.69	0.44
1:A:447:MET:HE1	1:A:542:LEU:HD12	1.98	0.44
2:B:208:LEU:HB3	2:B:209:PRO:HD3	1.98	0.44
1:A:542:LEU:O	1:A:546:LEU:HD22	2.16	0.44
1:A:526:PRO:HG3	3:E:130:CYS:SG	2.58	0.44
1:A:533:ILE:HG21	3:E:74:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:401:ARG:NH1	5:A:2014:HOH:O	2.49	0.43
3:E:192:LEU:HG	3:E:287:ILE:HD13	2.01	0.43
3:E:57:LYS:HG3	3:E:109:GLU:HG3	2.00	0.43
1:A:449:LEU:HD23	1:A:461:LEU:HD11	1.99	0.43
3:E:269:SER:O	3:E:270:HIS:HB2	2.19	0.43
2:B:258:ARG:HG3	2:B:263:TYR:CE2	2.54	0.43
3:E:291:LEU:HD23	3:E:317:ILE:CD1	2.48	0.43
3:E:69:ARG:HH11	3:E:243:PHE:HB2	1.84	0.42
1:A:546:LEU:HD23	1:A:547:ALA:CB	2.49	0.42
1:A:423:GLU:HG2	1:A:435:ARG:HB3	2.01	0.42
3:E:269:SER:O	3:E:270:HIS:CB	2.68	0.42
2:B:248:ASP:O	3:E:58:LYS:NZ	2.52	0.42
1:A:532:THR:H	3:E:161:ASN:ND2	2.04	0.42
3:E:84:MET:HE3	3:E:128:LEU:HD11	2.02	0.41
3:E:112:LYS:HG3	3:E:114:GLU:HB2	2.01	0.41
3:E:238:ASP:OD1	3:E:268:ARG:NH2	2.34	0.41
3:E:55:GLN:HB2	3:E:58:LYS:HD2	2.03	0.41
3:E:190:LYS:HB3	3:E:194:GLU:HG3	2.03	0.41
2:B:238:LEU:O	2:B:239:ASN:HB2	2.21	0.41
3:E:73:LEU:O	3:E:81:PHE:HA	2.21	0.41
2:B:269:TYR:HB2	3:E:50:PHE:HD2	1.86	0.41
3:E:122:GLN:HB2	3:E:123:ASP:H	1.75	0.41
1:A:546:LEU:HD23	1:A:547:ALA:N	2.36	0.40
3:E:302:VAL:HG13	3:E:306:ASP:HA	2.02	0.40
3:E:298:ARG:NH1	4:E:1327:AMP:C8	2.90	0.40
3:E:25:SER:O	3:E:26:SER:HB2	2.22	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	98/157 (62%)	96 (98%)	2 (2%)	0	100	100
2	B	69/87 (79%)	58 (84%)	8 (12%)	3 (4%)	4	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	302/330 (92%)	284 (94%)	12 (4%)	6 (2%)	11	5
All	All	469/574 (82%)	438 (93%)	22 (5%)	9 (2%)	12	5

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	211	HIS
3	E	25	SER
3	E	122	GLN
3	E	270	HIS
3	E	268	ARG
3	E	324	THR
2	B	235	HIS
2	B	208	LEU
3	E	182	PHE

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	94/141 (67%)	85 (90%)	9 (10%)	12	7
2	B	69/81 (85%)	65 (94%)	4 (6%)	28	23
3	E	277/299 (93%)	252 (91%)	25 (9%)	14	9
All	All	440/521 (84%)	402 (91%)	38 (9%)	15	10

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	394	MET
1	A	407	ASN
1	A	420	LEU
1	A	434	VAL
1	A	460	LEU
1	A	469	GLU
1	A	545	ILE

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Mol	Chain	Res	Type
1	A	546	LEU
1	A	548	GLN
2	B	211	HIS
2	B	237	MET
2	B	250	VAL
2	B	272	ILE
3	E	24	ASN
3	E	40	LEU
3	E	54	LEU
3	E	68	VAL
3	E	103	VAL
3	E	109	GLU
3	E	110	GLU
3	E	111	HIS
3	E	122	GLN
3	E	129	VAL
3	E	149	ILE
3	E	180	THR
3	E	224	VAL
3	E	239	ILE
3	E	246	ILE
3	E	248	LEU
3	E	275	VAL
3	E	284	LEU
3	E	291	LEU
3	E	296	VAL
3	E	298	ARG
3	E	308	VAL
3	E	311	ILE
3	E	318	LEU
3	E	322	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	ASN
3	E	122	GLN
3	E	161	ASN
3	E	222	HIS
3	E	247	ASN
3	E	266	GLN
3	E	267	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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$
4	AMP	E	1327	-	25,25,25	1.16	2 (8%)	38,38,38	2.03	8 (21%)
4	AMP	E	1328	-	25,25,25	1.07	2 (8%)	38,38,38	1.97	9 (23%)
4	AMP	E	1329	-	25,25,25	1.21	2 (8%)	38,38,38	1.83	6 (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	AMP	E	1327	-	-	0/10/26/26	0/1/3/3
4	AMP	E	1328	-	-	0/10/26/26	0/1/3/3
4	AMP	E	1329	-	-	0/10/26/26	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1329	AMP	C4-N9	-3.57	1.32	1.37
4	E	1327	AMP	C5-C4	3.43	1.48	1.40
4	E	1329	AMP	C5-C4	3.27	1.47	1.40
4	E	1328	AMP	C5-C4	3.06	1.47	1.40
4	E	1327	AMP	C4-N9	-2.78	1.33	1.37
4	E	1328	AMP	C4-N9	-2.78	1.33	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1327	AMP	N3-C2-N1	-7.59	122.36	128.71
4	E	1328	AMP	N3-C2-N1	-7.33	122.58	128.71
4	E	1329	AMP	N3-C2-N1	-5.91	123.77	128.71
4	E	1329	AMP	N3-C4-N9	5.34	135.07	125.43
4	E	1328	AMP	N3-C4-N9	5.16	134.76	125.43
4	E	1327	AMP	N3-C4-N9	4.95	134.37	125.43
4	E	1329	AMP	C8-N9-C4	3.32	109.44	106.90
4	E	1327	AMP	C4-C5-N7	-3.13	106.84	109.52
4	E	1327	AMP	C8-N9-C4	2.98	109.17	106.90
4	E	1328	AMP	C5-C4-N3	-2.93	119.31	125.70
4	E	1327	AMP	C2-N1-C6	2.83	123.87	118.77
4	E	1328	AMP	C4-C5-N7	-2.76	107.16	109.52
4	E	1329	AMP	C5-C4-N3	-2.68	119.86	125.70
4	E	1327	AMP	C5-C4-N3	-2.66	119.91	125.70
4	E	1328	AMP	C4'-O4'-C1'	2.61	112.59	109.75
4	E	1329	AMP	C4-C5-N7	-2.40	107.47	109.52
4	E	1328	AMP	C2-N3-C4	2.39	120.82	114.01
4	E	1328	AMP	P-O5'-C5'	2.38	125.06	118.19
4	E	1328	AMP	C2-N1-C6	2.33	122.97	118.77
4	E	1327	AMP	C2-N3-C4	2.26	120.45	114.01
4	E	1327	AMP	O2P-P-O1P	2.07	117.19	110.44
4	E	1329	AMP	C2-N1-C6	2.04	122.45	118.77
4	E	1328	AMP	C3'-C2'-C1'	2.02	104.07	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	102/157 (64%)	0.82	9 (8%)	10 11	34, 43, 49, 63	0
2	B	73/87 (83%)	1.84	20 (27%)	1 1	30, 44, 75, 80	0
3	E	304/330 (92%)	0.91	41 (13%)	4 4	30, 39, 61, 71	0
All	All	479/574 (83%)	1.03	70 (14%)	3 3	30, 40, 67, 80	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	221	THR	11.3
3	E	270	HIS	10.2
3	E	125	PHE	10.1
3	E	23	SER	9.3
3	E	25	SER	8.3
2	B	233	PRO	8.0
3	E	123	ASP	7.9
3	E	271	TYR	7.6
3	E	269	SER	7.1
2	B	235	HIS	7.1
2	B	199	GLU	7.0
2	B	222	ASN	7.0
3	E	182	PHE	6.8
3	E	325	GLY	6.7
2	B	234	ASN	6.7
3	E	24	ASN	6.7
3	E	324	THR	6.3
2	B	210	PRO	6.2
2	B	220	ASP	5.8
3	E	120	TYR	5.8
3	E	326	GLY	5.6
2	B	190	GLY	5.4
2	B	200	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
3	E	108	LEU	5.1
3	E	253	THR	5.1
2	B	236	VAL	4.9
1	A	524	VAL	4.9
3	E	252	LYS	4.9
2	B	211	HIS	4.9
3	E	124	SER	4.7
3	E	272	PHE	4.6
2	B	209	PRO	4.4
3	E	267	HIS	4.3
3	E	255	ASN	4.3
2	B	201	ARG	4.2
2	B	219	LYS	4.2
1	A	469	GLU	4.1
3	E	251	GLU	4.1
3	E	122	GLN	3.9
2	B	198	SER	3.9
1	A	468	ASP	3.6
2	B	272	ILE	3.6
3	E	268	ARG	3.6
1	A	393	SER	3.5
1	A	525	ALA	3.5
3	E	254	TYR	3.4
3	E	273	GLU	3.2
3	E	116	TRP	3.2
2	B	203	LYS	3.0
3	E	126	LYS	3.0
3	E	232	GLU	2.8
2	B	217	LEU	2.8
3	E	317	ILE	2.8
1	A	394	MET	2.7
1	A	461	LEU	2.6
3	E	250	ALA	2.6
3	E	121	LEU	2.6
3	E	274	GLY	2.5
1	A	528	PRO	2.5
3	E	256	ASN	2.4
3	E	171	ILE	2.4
3	E	226	ALA	2.4
3	E	111	HIS	2.4
2	B	247	LYS	2.2
3	E	228	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	249	ALA	2.2
3	E	37	CYS	2.1
3	E	227	LEU	2.1
1	A	527	ARG	2.0
3	E	241	SER	2.0

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 carbohydrates 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. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	AMP	E	1328	23/23	0.11	-1.00	27,29,42,44	0
4	AMP	E	1329	23/23	0.12	-1.11	31,34,35,36	0
4	AMP	E	1327	23/23	0.09	-1.41	33,35,38,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.