Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:16 PM GMT

PDB ID	:	4EAL
Title	:	Co-crystal of AMPK core with ATP soaked with AMP
Authors	:	Chen, L.; Wang, J.; Zhang, Y.-Y.; Yan, S.F.; Neumann, D.; Schlattner, U.; Wang, Z.-X.; Wu, J.-W.
Deposited on	:	2012-03-22
Resolution	:	2.51 Å(reported)

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

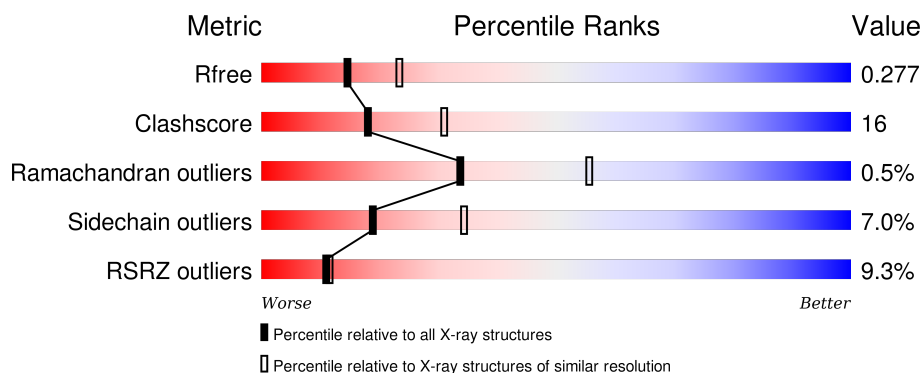|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.51 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	Percentile Ranks	Value
Rfree		0.277
Clashscore		16
Ramachandran outliers		0.5%
Sidechain outliers		7.0%
RSRZ outliers		9.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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 <=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	106	17% / 54% 29% • 13%
2	B	72	6% / 32% 25% • 42%
3	C	330	5% / 58% 22% 5% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3493 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 5'-AMP-activated protein kinase catalytic subunit alpha-1, linker, 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			770	492	136	137	5			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLY	-	EXPRESSION TAG	UNP P54645
A	390	PRO	-	EXPRESSION TAG	UNP P54645
A	391	HIS	-	EXPRESSION TAG	UNP P54645
A	392	MET	-	EXPRESSION TAG	UNP P54645
A	393	GLY	-	EXPRESSION TAG	UNP P54645
A	523	GLY	-	LINKER	UNP P54645
A	524	GLY	-	LINKER	UNP P54645
A	525	GLY	-	LINKER	UNP P54645
A	526	GLY	-	LINKER	UNP P54645
A	527	GLY	-	LINKER	UNP P54645
A	528	GLY	-	LINKER	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	S	0	0	0
			340	226	57	55	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	199	MET	-	EXPRESSION TAG	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	285	Total 2279	C 1475	N 383	O 414	S 7	0	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
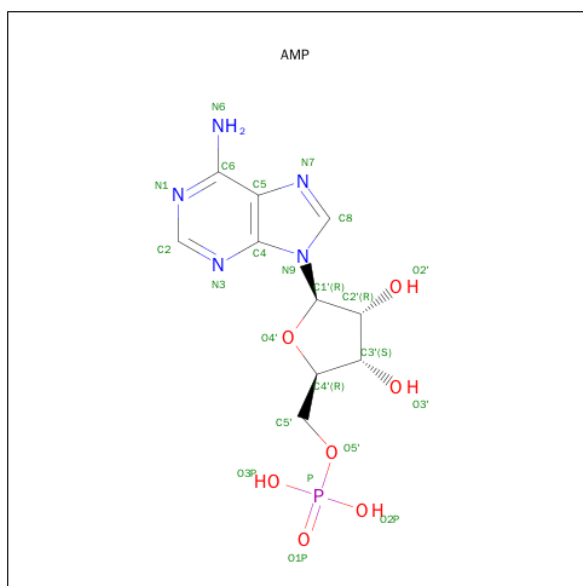
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0
4	C	1	Total 23	C 10	N 5	O 7	P 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	O 7	0	0
5	B	7	Total 7	O 7	0	0
5	C	44	Total 44	O 44	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.
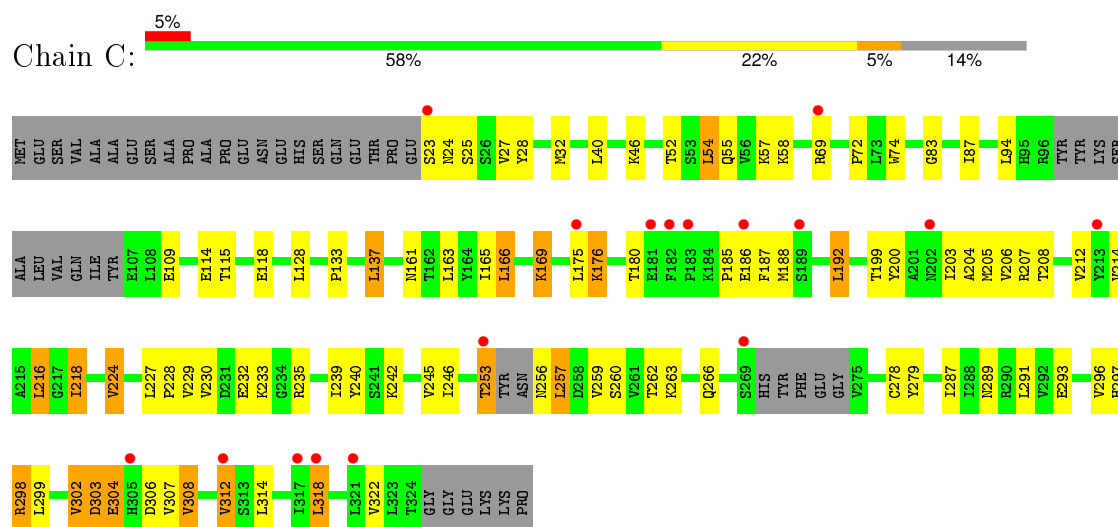
• Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1, linker, 5'-AMP-activated protein kinase catalytic subunit alpha-1
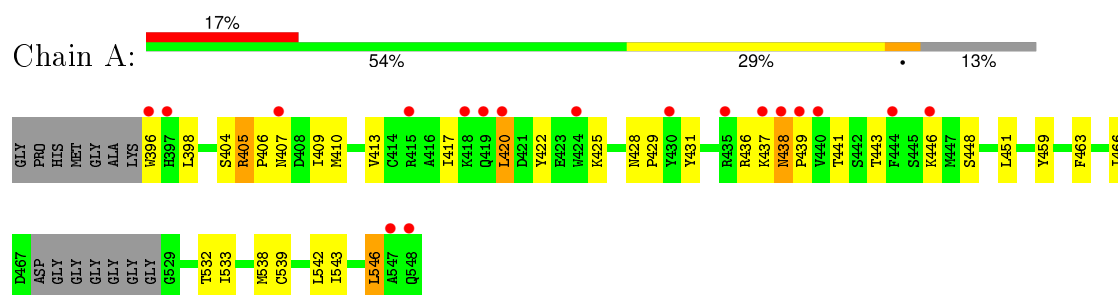
• Molecule 2: 5'-AMP-activated protein kinase subunit beta-1
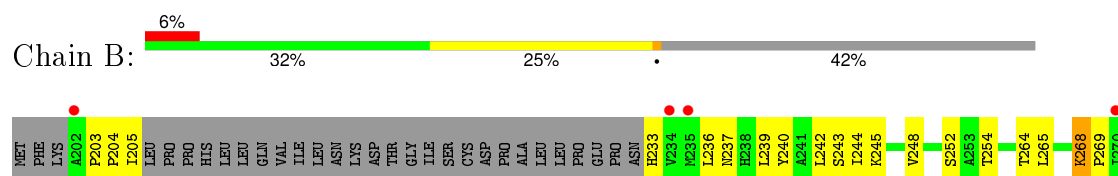
• Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.85Å 40.50Å 77.74Å 90.00° 105.53° 90.00°	Depositor
Resolution (Å)	24.97 – 2.51 24.97 – 2.51	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.97-2.51) 99.5 (24.97-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.73 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.232 , 0.277 0.226 , 0.277	Depositor DCC
R_{free} test set	922 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 18429 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3493	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: 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	0.21	0/786	0.38	0/1058
2	B	0.21	0/348	0.44	0/469
3	C	0.22	0/2321	0.41	0/3146
All	All	0.22	0/3455	0.41	0/4673

There are no bond length outliers.

There are no bond angle outliers.

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	770	0	772	28	0
2	B	340	0	366	16	0
3	C	2279	0	2359	74	0
4	C	46	0	24	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
5	C	44	0	0	2	0
All	All	3493	0	3521	109	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 16.

All (109) 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)
3:C:253:THR:O	3:C:256:ASN:N	1.86	1.07
3:C:256:ASN:O	3:C:257:LEU:HB2	1.57	1.02
1:A:428:ASN:HB3	1:A:431:TYR:HB3	1.53	0.89
3:C:291:LEU:HD13	3:C:299:LEU:HG	1.57	0.85
3:C:57:LYS:HB3	3:C:109:GLU:HB2	1.58	0.83
1:A:451:LEU:HD11	1:A:459:TYR:HB3	1.68	0.74
3:C:256:ASN:O	3:C:257:LEU:CB	2.34	0.74
2:B:244:ILE:HD12	2:B:244:ILE:H	1.57	0.69
3:C:218:ILE:HD11	3:C:227:LEU:HD22	1.75	0.68
3:C:233:LYS:HD3	3:C:235:ARG:NH2	2.09	0.67
1:A:413:VAL:O	1:A:417:ILE:HG13	1.94	0.67
1:A:532:THR:H	3:C:161:ASN:HD21	1.42	0.65
3:C:218:ILE:HD11	3:C:227:LEU:CD2	2.27	0.65
1:A:428:ASN:CB	1:A:431:TYR:HB3	2.27	0.63
3:C:133:PRO:HG3	3:C:163:LEU:HD12	1.81	0.63
3:C:72:PRO:HG3	3:C:165:ILE:HD11	1.80	0.63
1:A:409:ILE:O	1:A:413:VAL:HG13	2.00	0.61
3:C:40:LEU:HD11	3:C:166:LEU:HD11	1.83	0.60
3:C:23:SER:O	3:C:27:VAL:HG13	2.01	0.59
2:B:243:SER:O	2:B:245:LYS:HG3	2.03	0.58
3:C:25:SER:HA	3:C:185:PRO:HB3	1.86	0.58
3:C:94:LEU:HD13	3:C:216:LEU:HD11	1.86	0.58
3:C:232:GLU:H	3:C:232:GLU:CD	2.09	0.56
3:C:87:ILE:HD11	3:C:246:ILE:HG13	1.87	0.55
3:C:214:VAL:O	3:C:218:ILE:HG23	2.06	0.55
3:C:32:MET:HG3	3:C:322:VAL:HG22	1.89	0.54
1:A:406:PRO:HG3	1:A:459:TYR:CE1	2.43	0.53
1:A:438:ASN:HD22	1:A:439:PRO:HD2	1.73	0.53
3:C:299:LEU:HB2	3:C:312:VAL:HG13	1.91	0.53
3:C:208:THR:HB	3:C:262:THR:HG21	1.91	0.53
3:C:302:VAL:HG13	3:C:303:ASP:O	2.09	0.52
1:A:448:SER:HB3	1:A:466:ILE:HD11	1.91	0.52
3:C:228:PRO:HA	3:C:239:ILE:HD12	1.90	0.52
1:A:410:MET:O	1:A:413:VAL:HG22	2.10	0.52
3:C:224:VAL:O	3:C:242:LYS:HE3	2.10	0.52
3:C:109:GLU:CD	3:C:109:GLU:H	2.13	0.51
1:A:428:ASN:ND2	1:A:429:PRO:HD2	2.26	0.51
1:A:542:LEU:O	1:A:546:LEU:HD22	2.11	0.51
1:A:396:TRP:CH2	2:B:242:LEU:HG	2.46	0.51
3:C:304:GLU:H	3:C:304:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:ALA:HB1	3:C:218:ILE:HD13	1.93	0.50
3:C:192:LEU:HD22	3:C:200:TYR:OH	2.12	0.50
3:C:176:LYS:NZ	3:C:180:THR:HG21	2.26	0.50
1:A:538:MET:O	1:A:542:LEU:HD23	2.12	0.50
3:C:24:ASN:O	3:C:185:PRO:HG3	2.12	0.50
3:C:212:VAL:HG23	3:C:259:VAL:O	2.13	0.49
3:C:296:VAL:HG22	3:C:297:HIS:H	1.77	0.49
3:C:262:THR:O	3:C:266:GLN:HG2	2.13	0.49
3:C:169:LYS:NZ	5:C:535:HOH:O	2.46	0.49
3:C:259:VAL:HG12	3:C:260:SER:O	2.13	0.49
3:C:28:TYR:O	3:C:32:MET:HG2	2.12	0.49
3:C:87:ILE:CD1	3:C:246:ILE:HG13	2.44	0.47
3:C:169:LYS:HB3	3:C:169:LYS:HE2	1.52	0.47
3:C:287:ILE:HG23	3:C:299:LEU:HD12	1.96	0.47
3:C:204:ALA:HB1	3:C:218:ILE:CD1	2.45	0.47
3:C:297:HIS:O	3:C:314:LEU:HG	2.15	0.47
3:C:32:MET:CE	3:C:137:LEU:HB3	2.46	0.47
3:C:24:ASN:O	3:C:27:VAL:HG22	2.15	0.46
2:B:203:PRO:HA	2:B:204:PRO:HD3	1.84	0.46
3:C:278:CYS:HB3	3:C:299:LEU:HD13	1.95	0.46
1:A:410:MET:HE2	1:A:410:MET:HB2	1.86	0.46
1:A:396:TRP:CZ3	2:B:242:LEU:HG	2.52	0.45
3:C:240:TYR:HE1	3:C:245:VAL:HG22	1.80	0.45
2:B:244:ILE:HD12	2:B:244:ILE:N	2.29	0.45
3:C:303:ASP:HB2	3:C:307:VAL:H	1.82	0.45
3:C:205:MET:SD	3:C:308:VAL:HG11	2.56	0.45
1:A:438:ASN:HD22	1:A:439:PRO:CD	2.29	0.45
3:C:94:LEU:HD22	3:C:94:LEU:O	2.17	0.45
3:C:206:VAL:HG23	3:C:229:VAL:HA	1.99	0.45
3:C:302:VAL:HG22	3:C:306:ASP:C	2.37	0.44
1:A:533:ILE:HG21	3:C:74:TRP:CD2	2.52	0.44
1:A:441:THR:OG1	1:A:443:THR:HG22	2.17	0.44
3:C:289:ASN:O	3:C:293:GLU:HG2	2.18	0.44
2:B:236:LEU:HD22	2:B:254:THR:O	2.17	0.44
3:C:199:THR:O	3:C:203:ILE:HD11	2.18	0.44
3:C:55:GLN:HB3	3:C:57:LYS:HG2	1.99	0.43
3:C:137:LEU:HD12	3:C:137:LEU:HA	1.89	0.43
1:A:463:PHE:HB2	2:B:239:LEU:HB3	2.00	0.43
2:B:252:SER:HA	2:B:264:THR:O	2.19	0.43
1:A:436:ARG:NH1	1:A:438:ASN:HA	2.34	0.43
3:C:24:ASN:HA	3:C:27:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:O	1:A:439:PRO:HD3	2.19	0.43
3:C:297:HIS:HB2	3:C:298:ARG:CZ	2.48	0.43
2:B:268:LYS:HA	2:B:269:PRO:HD3	1.92	0.43
2:B:265:LEU:HD22	3:C:46:LYS:HE2	2.01	0.43
3:C:115:THR:O	3:C:118:GLU:HB3	2.19	0.43
1:A:533:ILE:HG21	3:C:74:TRP:CE2	2.53	0.43
2:B:269:PRO:HG3	3:C:54:LEU:HA	2.01	0.43
1:A:420:LEU:HB3	1:A:422:TYR:CD2	2.54	0.42
3:C:69:ARG:HD2	5:C:535:HOH:O	2.20	0.42
3:C:260:SER:H	3:C:263:LYS:HE2	1.85	0.42
3:C:260:SER:OG	3:C:263:LYS:HD3	2.20	0.42
3:C:83:GLY:HA2	3:C:128:LEU:HD13	2.01	0.42
1:A:398:LEU:HB2	2:B:240:TYR:CE2	2.55	0.42
3:C:318:LEU:HD13	3:C:318:LEU:HA	1.84	0.41
2:B:244:ILE:CD1	2:B:244:ILE:H	2.29	0.41
2:B:236:LEU:O	2:B:237:ASN:HB2	2.20	0.41
2:B:204:PRO:C	2:B:205:ILE:HD12	2.40	0.41
3:C:52:THR:O	3:C:114:GLU:HG3	2.20	0.41
3:C:185:PRO:HB2	3:C:187:PHE:CD2	2.56	0.41
3:C:207:ARG:HG2	3:C:208:THR:N	2.35	0.41
1:A:539:CYS:O	1:A:543:ILE:HG13	2.20	0.41
3:C:279:TYR:HE2	3:C:303:ASP:O	2.04	0.41
1:A:405:ARG:HH21	1:A:407:ASN:HD22	1.68	0.41
3:C:218:ILE:O	3:C:218:ILE:HD12	2.21	0.40
3:C:230:VAL:HA	3:C:235:ARG:O	2.21	0.40
3:C:185:PRO:HD2	3:C:188:MET:HG3	2.03	0.40
3:C:57:LYS:HG3	3:C:58:LYS:N	2.37	0.40
1:A:425:LYS:HD3	1:A:425:LYS:HA	1.84	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	88/106 (83%)	84 (96%)	3 (3%)	1 (1%)	17	31
2	B	38/72 (53%)	35 (92%)	3 (8%)	0	100	100
3	C	277/330 (84%)	263 (95%)	13 (5%)	1 (0%)	39	61
All	All	403/508 (79%)	382 (95%)	19 (5%)	2 (0%)	34	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	257	LEU
1	A	404	SER

5.3.2 Protein sidechains (i)

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	86/91 (94%)	81 (94%)	5 (6%)	25	45
2	B	38/66 (58%)	35 (92%)	3 (8%)	15	28
3	C	262/299 (88%)	243 (93%)	19 (7%)	17	32
All	All	386/456 (85%)	359 (93%)	27 (7%)	19	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	ARG
1	A	420	LEU
1	A	438	ASN
1	A	446	LYS
1	A	546	LEU
2	B	233	HIS
2	B	248	VAL
2	B	268	LYS
3	C	54	LEU
3	C	137	LEU
3	C	166	LEU

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Mol	Chain	Res	Type
3	C	169	LYS
3	C	175	LEU
3	C	176	LYS
3	C	186	GLU
3	C	192	LEU
3	C	216	LEU
3	C	218	ILE
3	C	224	VAL
3	C	253	THR
3	C	298	ARG
3	C	302	VAL
3	C	303	ASP
3	C	304	GLU
3	C	308	VAL
3	C	312	VAL
3	C	318	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	419	GLN
1	A	428	ASN
1	A	438	ASN
2	B	238	HIS
2	B	255	HIS
3	C	24	ASN
3	C	111	HIS
3	C	161	ASN
3	C	256	ASN
3	C	305	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)

2 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	C	401	-	20,25,25	1.00	1 (5%)	22,38,38	1.93	3 (13%)
4	AMP	C	402	-	20,25,25	1.03	1 (5%)	22,38,38	1.97	3 (13%)

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	C	401	-	-	0/6/26/26	0/3/3/3
4	AMP	C	402	-	-	0/6/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	AMP	C5-C4	3.08	1.47	1.40
4	C	402	AMP	C5-C4	3.16	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	AMP	N3-C2-N1	-6.80	123.69	128.89
4	C	401	AMP	N3-C2-N1	-6.78	123.70	128.89
4	C	402	AMP	C4-C5-N7	-3.35	106.40	109.48
4	C	401	AMP	C4-C5-N7	-2.87	106.84	109.48
4	C	401	AMP	C2'-C1'-N9	-2.15	111.00	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	AMP	O3P-P-O2P	2.15	115.55	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	92/106 (86%)	1.20	18 (19%)	1	1	41, 100, 134, 174	0
2	B	42/72 (58%)	0.71	4 (9%)	10	11	45, 63, 151, 178	0
3	C	285/330 (86%)	0.39	17 (5%)	25	28	36, 62, 106, 161	0
All	All	419/508 (82%)	0.60	39 (9%)	11	11	36, 68, 129, 178	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	23	SER	6.4
1	A	430	TYR	6.0
3	C	253	THR	5.4
1	A	548	GLN	5.2
3	C	321	LEU	4.3
2	B	270	ILE	4.1
3	C	317	ILE	3.9
3	C	269	SER	3.9
2	B	234	VAL	3.7
1	A	444	PHE	3.6
1	A	418	LYS	3.5
3	C	183	PRO	3.5
1	A	397	HIS	3.4
3	C	182	PHE	3.3
3	C	305	HIS	3.3
2	B	202	ALA	3.2
1	A	419	GLN	3.1
1	A	407	ASN	3.0
1	A	424	TRP	2.9
1	A	415	ARG	2.8
1	A	420	LEU	2.7
1	A	437	LYS	2.6
3	C	202	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	440	VAL	2.6
1	A	396	TRP	2.5
1	A	435	ARG	2.5
3	C	318	LEU	2.5
3	C	186	GLU	2.4
3	C	312	VAL	2.4
1	A	446	LYS	2.3
2	B	235	MET	2.3
1	A	439	PRO	2.3
1	A	547	ALA	2.3
3	C	69	ARG	2.2
3	C	213	TYR	2.2
3	C	189	SER	2.2
3	C	175	LEU	2.1
1	A	438	ASN	2.1
3	C	181	GLU	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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	AMP	C	402	23/23	0.94	0.16	-0.31	55,66,73,76	0
4	AMP	C	401	23/23	0.94	0.14	-0.58	44,50,59,66	0

6.5 Other polymers (i)

There are no such residues in this entry.