Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:54 AM GMT

PDB ID	:	2V92
Title	:	CRYSTAL STRUCTURE OF THE REGULATORY FRAGMENT OF MAMMALIAN AMPK IN COMPLEXES WITH ATP-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	:	2007-08-20
Resolution	:	2.40 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

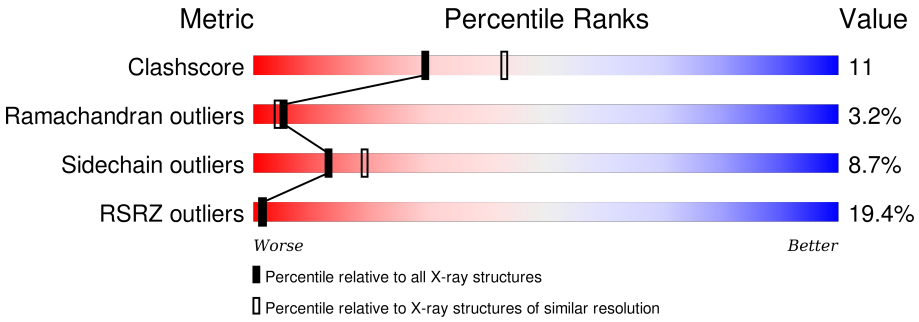
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	157	8% 39% 22% 35%
2	B	87	25% 67% 15% 16%
3	E	330	18% 71% 17% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4324 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.

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

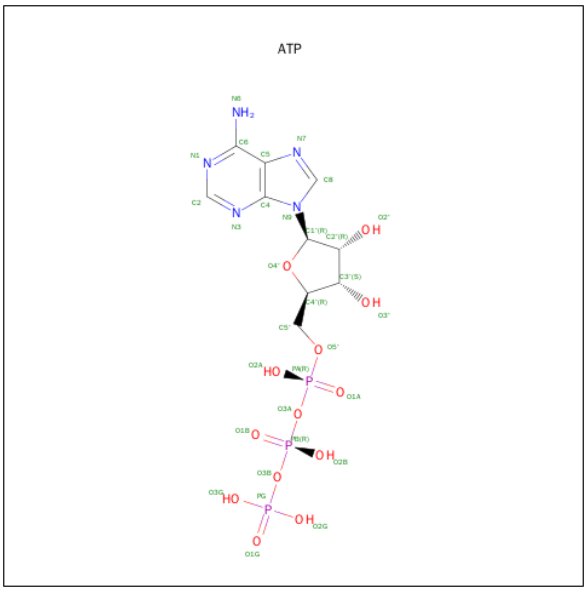
- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			595	388	102	102	3			

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

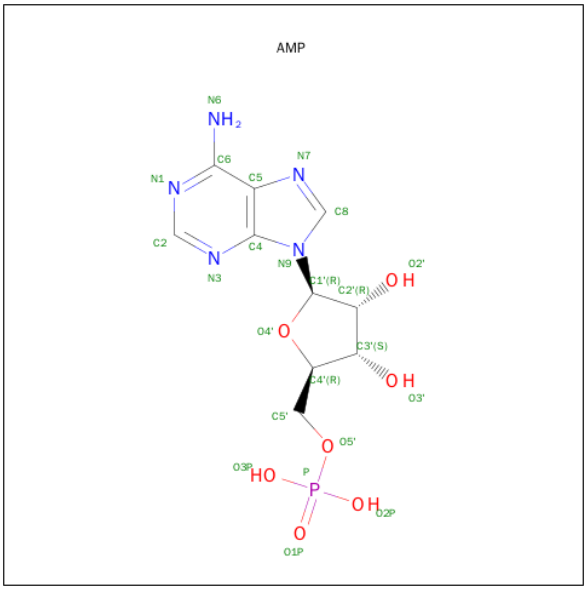
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	304	Total	C	N	O	S	0	0	0
			2441	1584	407	443	7			

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



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

- Molecule 5 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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

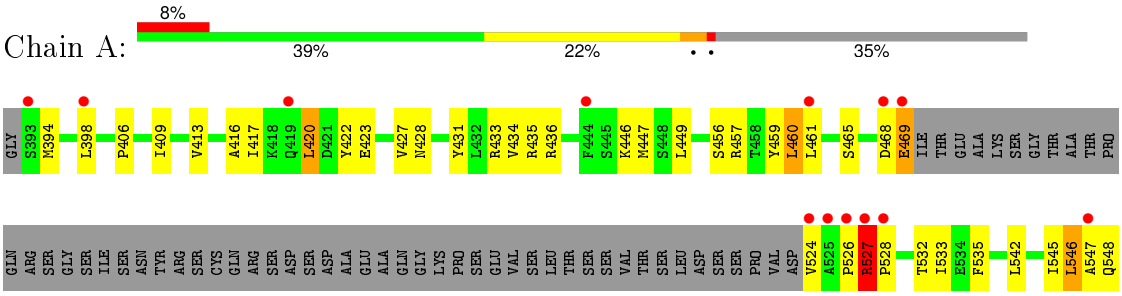
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	72	Total O 72 72	0	0
6	B	47	Total O 47 47	0	0
6	E	242	Total O 242 242	0	0

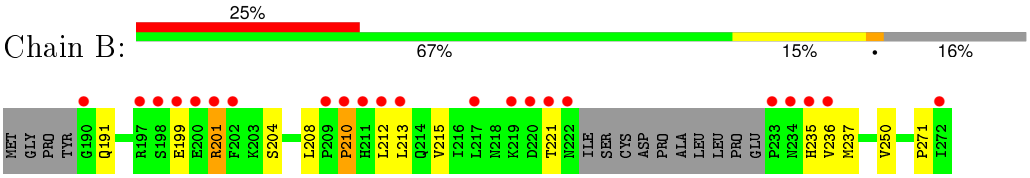
3 Residue-property plots (i)

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.

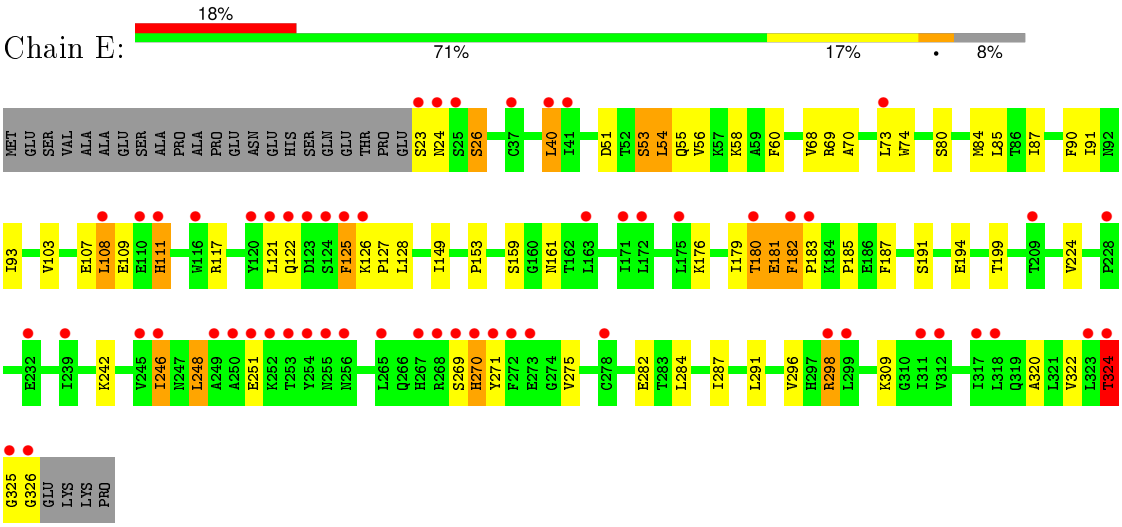
• Molecule 1: 5'-AMP-ACTIVATED PROTEIN KINASE CATALYTIC SUBUNIT ALPHA-1



• Molecule 2: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-2



• Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.96Å 121.03Å 127.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.40) 99.3 (19.92-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.217 , 0.259 0.259 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	54.6	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.4	EDS
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 30129 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4324	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[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, 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	0.47	0/860	0.66	0/1161
2	B	0.47	0/610	0.67	0/825
3	E	0.48	0/2493	0.67	2/3384 (0.1%)
All	All	0.48	0/3963	0.67	2/5370 (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
1	A	0	1
3	E	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	40	LEU	CA-CB-CG	6.08	129.28	115.30
3	E	181	GLU	N-CA-C	-5.38	96.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	527	ARG	Peptide
3	E	182	PHE	Peptide

5.2 Too-close contacts (i)

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	842	0	842	34	0
2	B	595	0	610	5	0
3	E	2441	0	2506	56	0
4	E	62	0	24	7	0
5	E	23	0	12	1	0
6	A	72	0	0	1	0
6	B	47	0	0	0	0
6	E	242	0	0	3	0
All	All	4324	0	3994	90	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 11.

All (90) 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:413:VAL:HA	1:A:546:LEU:HD12	1.37	1.07
3:E:179:ILE:O	3:E:181:GLU:N	2.04	0.90
3:E:24:ASN:HA	3:E:324:THR:HG21	1.55	0.87
2:B:208:LEU:O	2:B:210:PRO:HD3	1.75	0.86
1:A:532:THR:H	3:E:161:ASN:HD21	1.22	0.86
3:E:269:SER:O	3:E:270:HIS:HB2	1.82	0.80
3:E:84:MET:HE3	3:E:153:PRO:HG3	1.67	0.77
1:A:527:ARG:HB3	1:A:528:PRO:HD3	1.65	0.76
3:E:176:LYS:O	3:E:180:THR:OG1	2.04	0.74
1:A:527:ARG:CB	1:A:528:PRO:HD3	2.19	0.71
3:E:26:SER:HB2	3:E:324:THR:HG23	1.73	0.70
1:A:398:LEU:O	1:A:460:LEU:HD11	1.91	0.69
3:E:282:GLU:HB2	3:E:287:ILE:HD11	1.77	0.67
1:A:447:MET:CE	1:A:542:LEU:HD12	2.25	0.66
1:A:527:ARG:CG	1:A:528:PRO:HD3	2.25	0.65
1:A:416:ALA:HB2	1:A:546:LEU:HB3	1.80	0.64
3:E:24:ASN:HA	3:E:324:THR:CG2	2.28	0.64
2:B:213:LEU:HD12	2:B:237:MET:HE1	1.79	0.64
1:A:542:LEU:O	1:A:546:LEU:HD22	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:296:VAL:HG21	4:E:1327:ATP:C5	2.33	0.62
3:E:242:LYS:HB2	6:E:2036:HOH:O	2.00	0.62
3:E:320:ALA:HB1	3:E:326:GLY:H	1.65	0.62
3:E:125:PHE:HD2	3:E:127:PRO:HD3	1.65	0.61
3:E:55:GLN:HB2	3:E:58:LYS:HD2	1.84	0.60
3:E:296:VAL:CG2	4:E:1327:ATP:C8	2.85	0.59
3:E:87:ILE:HD12	3:E:246:ILE:CG2	2.33	0.59
3:E:93:ILE:HG23	3:E:108:LEU:HD12	1.85	0.58
3:E:107:GLU:HB3	3:E:111:HIS:HE1	1.70	0.56
3:E:23:SER:HB3	3:E:187:PHE:HD2	1.68	0.56
3:E:296:VAL:HG21	4:E:1327:ATP:N7	2.21	0.56
1:A:447:MET:HE1	1:A:542:LEU:HD12	1.85	0.56
1:A:527:ARG:HG3	1:A:528:PRO:HD3	1.87	0.56
1:A:527:ARG:HG3	1:A:528:PRO:CD	2.36	0.55
3:E:69:ARG:NH1	4:E:1328:ATP:O2G	2.40	0.55
3:E:84:MET:CE	3:E:153:PRO:HG3	2.37	0.54
2:B:208:LEU:O	2:B:210:PRO:CD	2.54	0.54
1:A:532:THR:H	3:E:161:ASN:ND2	2.00	0.53
3:E:269:SER:O	3:E:270:HIS:CB	2.56	0.53
3:E:296:VAL:CG2	4:E:1327:ATP:N7	2.72	0.53
1:A:546:LEU:HD23	1:A:547:ALA:HB2	1.91	0.52
3:E:23:SER:HA	3:E:185:PRO:HB3	1.92	0.51
3:E:84:MET:HE3	3:E:128:LEU:HD11	1.92	0.51
1:A:417:ILE:HG23	1:A:422:TYR:HB2	1.92	0.51
3:E:56:VAL:HG13	3:E:60:PHE:CE1	2.46	0.50
3:E:87:ILE:HG21	3:E:242:LYS:O	2.11	0.50
3:E:191:SER:OG	3:E:194:GLU:HG2	2.12	0.50
1:A:420:LEU:HD11	1:A:545:ILE:HG13	1.94	0.50
3:E:87:ILE:HG12	6:E:2236:HOH:O	2.11	0.50
1:A:428:ASN:HB2	1:A:431:TYR:HB3	1.95	0.49
1:A:449:LEU:HD23	1:A:461:LEU:HD11	1.95	0.48
3:E:69:ARG:NE	4:E:1327:ATP:O2B	2.46	0.48
3:E:181:GLU:HG3	3:E:183:PRO:HD2	1.96	0.48
2:B:236:VAL:O	2:B:236:VAL:HG22	2.13	0.48
1:A:409:ILE:O	1:A:413:VAL:HG13	2.14	0.47
1:A:420:LEU:HD13	1:A:545:ILE:HG21	1.96	0.47
3:E:117:ARG:O	3:E:121:LEU:HB2	2.14	0.47
1:A:423:GLU:CG	1:A:435:ARG:HB3	2.45	0.47
1:A:406:PRO:HG3	1:A:459:TYR:CZ	2.50	0.47
3:E:56:VAL:HG13	3:E:60:PHE:HE1	1.80	0.46
3:E:51:ASP:O	3:E:54:LEU:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HB3	1:A:528:PRO:CD	2.42	0.45
1:A:417:ILE:HG13	1:A:542:LEU:HD21	1.98	0.45
3:E:60:PHE:CE2	3:E:90:PHE:HB2	2.51	0.45
1:A:542:LEU:O	1:A:546:LEU:HD13	2.16	0.45
3:E:51:ASP:OD2	3:E:53:SER:OG	2.28	0.44
2:B:271:PRO:HG2	3:E:53:SER:HB2	1.99	0.44
1:A:527:ARG:CB	1:A:528:PRO:CD	2.91	0.44
1:A:465:SER:HB3	1:A:535:PHE:CD1	2.53	0.44
3:E:248:LEU:O	3:E:251:GLU:HG2	2.18	0.44
3:E:298:ARG:NH1	4:E:1327:ATP:C8	2.86	0.44
3:E:108:LEU:O	3:E:111:HIS:HB2	2.18	0.44
3:E:183:PRO:HD2	6:E:2120:HOH:O	2.17	0.43
1:A:533:ILE:HG21	3:E:74:TRP:CD2	2.53	0.43
3:E:87:ILE:HD12	3:E:246:ILE:HG21	1.99	0.43
1:A:427:VAL:HG21	1:A:433:ARG:HD3	2.00	0.43
3:E:199:THR:HG22	5:E:1329:AMP:O2'	2.19	0.43
3:E:246:ILE:H	3:E:246:ILE:HG13	1.65	0.43
3:E:87:ILE:HD12	3:E:246:ILE:HG23	1.98	0.43
3:E:73:LEU:HD21	3:E:85:LEU:HB2	1.99	0.42
1:A:416:ALA:CB	1:A:546:LEU:HB3	2.47	0.42
3:E:24:ASN:C	3:E:26:SER:H	2.23	0.42
3:E:91:ILE:CD1	3:E:242:LYS:HG2	2.50	0.41
3:E:282:GLU:HB2	3:E:287:ILE:CD1	2.48	0.41
3:E:121:LEU:HD11	3:E:126:LYS:HB2	2.02	0.41
1:A:528:PRO:HA	3:E:80:SER:HB3	2.02	0.41
3:E:24:ASN:CA	3:E:324:THR:HG21	2.38	0.41
1:A:423:GLU:HG3	1:A:435:ARG:HB3	2.02	0.40
3:E:309:LYS:HA	3:E:309:LYS:HD3	1.97	0.40
1:A:446:LYS:HE2	6:A:2053:HOH:O	2.20	0.40
1:A:468:ASP:O	1:A:469:GLU:HG3	2.21	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	98/157 (62%)	94 (96%)	2 (2%)	2 (2%)	9 11
2	B	69/87 (79%)	53 (77%)	10 (14%)	6 (9%)	1 0
3	E	302/330 (92%)	283 (94%)	12 (4%)	7 (2%)	8 8
All	All	469/574 (82%)	430 (92%)	24 (5%)	15 (3%)	5 4

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	122	GLN
3	E	180	THR
3	E	270	HIS
1	A	526	PRO
1	A	527	ARG
3	E	26	SER
3	E	70	ALA
3	E	324	THR
3	E	325	GLY
2	B	191	GLN
2	B	199	GLU
2	B	204	SER
2	B	235	HIS
2	B	201	ARG
2	B	210	PRO

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	94/141 (67%)	83 (88%)	11 (12%)	7 8
2	B	67/81 (83%)	62 (92%)	5 (8%)	17 26
3	E	277/299 (93%)	255 (92%)	22 (8%)	15 23
All	All	438/521 (84%)	400 (91%)	38 (9%)	13 19

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

Mol	Chain	Res	Type
1	A	394	MET
1	A	420	LEU
1	A	434	VAL
1	A	436	ARG
1	A	456	SER
1	A	457	ARG
1	A	460	LEU
1	A	469	GLU
1	A	524	VAL
1	A	546	LEU
1	A	548	GLN
2	B	201	ARG
2	B	212	LEU
2	B	215	VAL
2	B	221	THR
2	B	250	VAL
3	E	40	LEU
3	E	53	SER
3	E	54	LEU
3	E	68	VAL
3	E	103	VAL
3	E	108	LEU
3	E	109	GLU
3	E	111	HIS
3	E	125	PHE
3	E	149	ILE
3	E	159	SER
3	E	182	PHE
3	E	224	VAL
3	E	246	ILE
3	E	248	LEU
3	E	271	TYR
3	E	275	VAL
3	E	284	LEU
3	E	291	LEU
3	E	298	ARG
3	E	322	VAL
3	E	324	THR

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

Mol	Chain	Res	Type
2	B	214	GLN
2	B	234	ASN
3	E	24	ASN
3	E	161	ASN

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	$\#\|Z\| > 2$
4	ATP	E	1327	-	24,33,33	1.05	2 (8%)	31,52,52	2.17	8 (25%)
4	ATP	E	1328	-	24,33,33	1.00	2 (8%)	31,52,52	1.97	6 (19%)
5	AMP	E	1329	-	20,25,25	1.00	1 (5%)	22,38,38	2.16	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	ATP	E	1327	-	-	0/18/38/38	0/3/3/3
4	ATP	E	1328	-	-	0/18/38/38	0/3/3/3
5	AMP	E	1329	-	-	0/6/26/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1328	ATP	O4'-C1'	2.21	1.44	1.41
4	E	1327	ATP	O4'-C1'	2.22	1.44	1.41
4	E	1328	ATP	C5-C4	3.00	1.47	1.40
5	E	1329	AMP	C5-C4	3.05	1.47	1.40
4	E	1327	ATP	C5-C4	3.26	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1327	ATP	N3-C2-N1	-8.24	122.58	128.89
5	E	1329	AMP	N3-C2-N1	-8.17	122.64	128.89
4	E	1328	ATP	N3-C2-N1	-7.87	122.87	128.89
4	E	1327	ATP	PA-O3A-PB	-4.23	120.86	132.73
4	E	1327	ATP	C4-C5-N7	-2.81	106.90	109.48
4	E	1328	ATP	PA-O3A-PB	-2.77	124.94	132.73
4	E	1328	ATP	C4-C5-N7	-2.70	106.99	109.48
4	E	1327	ATP	C2'-C1'-N9	-2.64	110.25	114.29
4	E	1328	ATP	O3A-PA-O5'	-2.44	96.46	102.94
4	E	1328	ATP	C2'-C1'-N9	-2.42	110.60	114.29
5	E	1329	AMP	C4-C5-N7	-2.28	107.38	109.48
4	E	1327	ATP	PB-O3B-PG	-2.18	125.36	132.67
4	E	1327	ATP	O3A-PA-O5'	-2.07	97.46	102.94
4	E	1328	ATP	O3G-PG-O2G	2.01	115.05	107.38
5	E	1329	AMP	C2-N1-C6	2.49	123.21	118.77
4	E	1327	ATP	C2-N1-C6	2.53	123.29	118.77
4	E	1327	ATP	O3G-PG-O2G	2.58	117.22	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1327	ATP	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1328	ATP	1	0
5	E	1329	AMP	1	0

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

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^{th} 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%)	0.95	13 (12%)	5	5	48, 56, 66, 72	0
2	B	73/87 (83%)	1.90	22 (30%)	1	1	41, 57, 87, 94	0
3	E	304/330 (92%)	1.08	58 (19%)	2	1	26, 55, 74, 80	0
All	All	479/574 (83%)	1.18	93 (19%)	1	1	26, 55, 78, 94	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	24	ASN	11.3
3	E	271	TYR	10.2
3	E	125	PHE	8.6
2	B	221	THR	8.4
2	B	222	ASN	8.1
3	E	252	LYS	7.9
3	E	123	ASP	7.8
1	A	527	ARG	7.7
3	E	180	THR	7.4
2	B	220	ASP	7.4
3	E	124	SER	6.8
2	B	233	PRO	6.7
2	B	235	HIS	6.6
3	E	270	HIS	6.5
3	E	267	HIS	6.4
3	E	23	SER	6.2
2	B	201	ARG	5.9
2	B	234	ASN	5.9
3	E	250	ALA	5.6
3	E	182	PHE	5.5
3	E	325	GLY	5.4
3	E	253	THR	5.4
2	B	199	GLU	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	209	PRO	5.3
2	B	210	PRO	5.2
3	E	272	PHE	5.2
3	E	255	ASN	5.0
1	A	524	VAL	4.9
2	B	211	HIS	4.9
2	B	200	GLU	4.9
3	E	120	TYR	4.8
2	B	236	VAL	4.6
1	A	393	SER	4.5
2	B	198	SER	4.4
1	A	528	PRO	4.3
2	B	190	GLY	4.3
3	E	25	SER	4.2
1	A	469	GLU	4.2
1	A	525	ALA	4.1
1	A	468	ASP	3.9
2	B	219	LYS	3.8
3	E	324	THR	3.8
3	E	326	GLY	3.7
3	E	254	TYR	3.7
2	B	272	ILE	3.6
3	E	256	ASN	3.5
3	E	122	GLN	3.4
2	B	197	ARG	3.4
3	E	108	LEU	3.4
3	E	249	ALA	3.4
3	E	171	ILE	3.1
3	E	37	CYS	3.1
3	E	232	GLU	3.1
3	E	265	LEU	3.1
3	E	269	SER	3.0
3	E	323	LEU	2.9
3	E	251	GLU	2.8
2	B	213	LEU	2.8
1	A	526	PRO	2.8
3	E	268	ARG	2.6
3	E	239	ILE	2.6
3	E	312	VAL	2.6
2	B	212	LEU	2.6
1	A	461	LEU	2.5
3	E	175	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	311	ILE	2.5
3	E	111	HIS	2.5
3	E	172	LEU	2.5
3	E	41	ILE	2.4
3	E	317	ILE	2.4
3	E	228	PRO	2.4
3	E	273	GLU	2.4
3	E	245	VAL	2.4
3	E	110	GLU	2.3
3	E	40	LEU	2.3
1	A	444	PHE	2.3
3	E	209	THR	2.2
3	E	116	TRP	2.2
3	E	121	LEU	2.2
2	B	202	PHE	2.2
1	A	398	LEU	2.2
3	E	126	LYS	2.1
3	E	298	ARG	2.1
3	E	163	LEU	2.1
3	E	183	PRO	2.1
1	A	419	GLN	2.1
2	B	217	LEU	2.1
3	E	73	LEU	2.1
3	E	299	LEU	2.1
1	A	547	ALA	2.1
3	E	246	ILE	2.1
3	E	318	LEU	2.1
3	E	278	CYS	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^{th} 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	ATP	E	1328	31/31	0.96	0.11	-1.63	31,39,58,59	0
5	AMP	E	1329	23/23	0.96	0.13	-1.69	39,43,50,51	0
4	ATP	E	1327	31/31	0.95	0.11	-1.74	50,52,57,57	0

6.5 Other polymers (i)

There are no such residues in this entry.