



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 08:09 AM EDT

PDB ID : 5I0N  
Title : PI4K IIalpha bound to calcium  
Authors : Baumlova, A.; Boura, E.  
Deposited on : 2016-02-04  
Resolution : 2.28 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

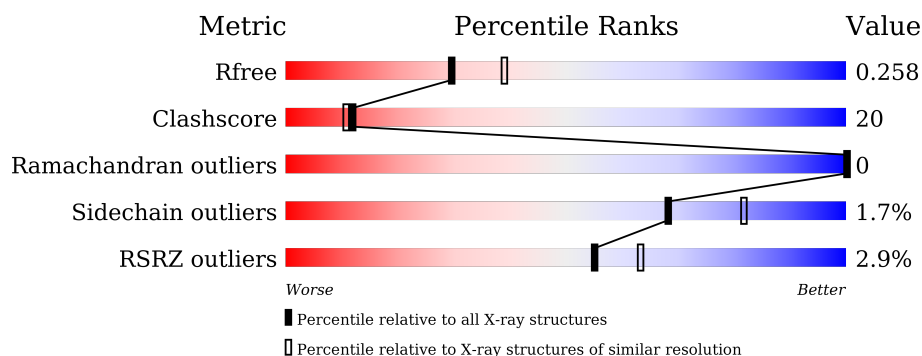
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
$R_{free}$	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	556	<div> <div>3%</div> <div>58%</div> <div>29%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4252 atoms, of which 24 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.

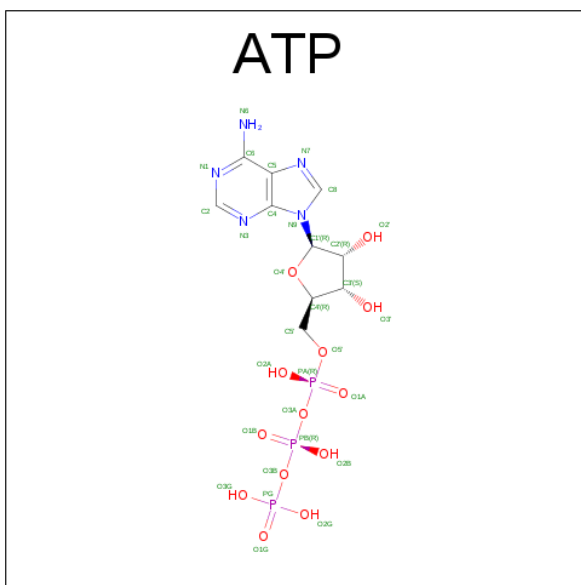
- Molecule 1 is a protein called Phosphatidylinositol 4-kinase type 2-alpha, Lysozyme, Phosphatidylinositol 4-kinase type 2-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	1	0
			3942	2535	683	715	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	GLY	-	expression tag	UNP Q9BTU6
A	73	ALA	-	expression tag	UNP Q9BTU6
A	74	MET	-	expression tag	UNP Q9BTU6
A	75	GLY	-	expression tag	UNP Q9BTU6
A	1001	GLY	-	linker	UNP Q9BTU6
A	1002	THR	-	linker	UNP Q9BTU6
A	1003	GLY	-	linker	UNP Q9BTU6
A	1056	THR	CYS	conflict	UNP D9IEF7
A	1099	ALA	CYS	conflict	UNP D9IEF7

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

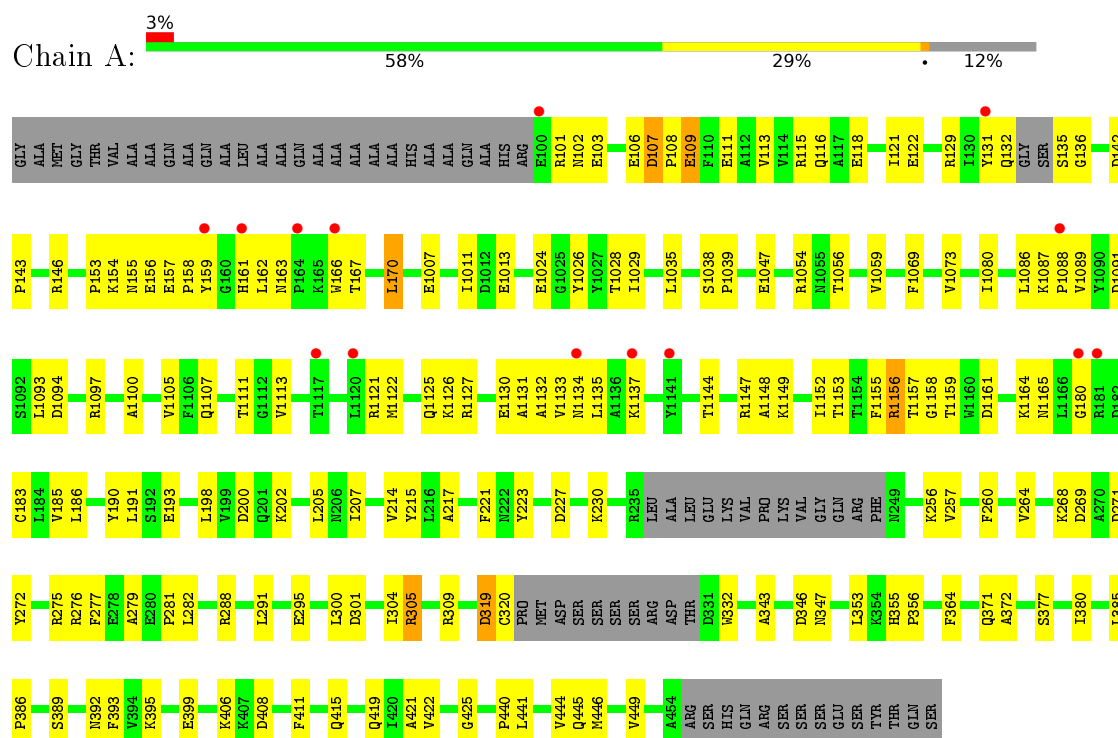
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Ca 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	222	Total O 222 222	0	0



- Molecule 1: Phosphatidylinositol 4-kinase type 2-alpha, Lysozyme, Phosphatidylinositol 4-kinase type 2-alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.88Å 102.03Å 78.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.95 – 2.28 48.95 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.95-2.28) 99.9 (48.95-2.28)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.219 , 0.258 0.219 , 0.258	Depositor DCC
$R_{free}$ test set	1505 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.6	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.9	EDS
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29715 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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, 0.375 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: CA, 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	0.42	3/4035 (0.1%)	0.51	9/5465 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	ILE	C-N	-10.46	1.10	1.34
1	A	305	ARG	C-N	-6.43	1.19	1.34
1	A	108	PRO	N-CD	5.02	1.54	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1158	GLY	O-C-N	-11.60	104.14	122.70
1	A	319	ASP	O-C-N	-9.70	107.18	122.70
1	A	1158	GLY	C-N-CA	8.33	142.53	121.70
1	A	1158	GLY	CA-C-N	8.08	134.97	117.20
1	A	319	ASP	CA-C-N	6.82	132.21	117.20
1	A	304	ILE	C-N-CA	6.79	138.69	121.70
1	A	319	ASP	C-N-CA	6.77	138.62	121.70
1	A	304	ILE	O-C-N	-5.69	113.59	122.70
1	A	107	ASP	C-N-CD	5.50	139.94	128.40

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	3942	0	3919	157	0
2	A	62	24	24	4	0
3	A	2	0	0	0	0
4	A	222	0	0	59	1
All	All	4228	24	3943	159	1

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 20.

All (159) 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:183:CYS:SG	4:A:1326:HOH:O	1.94	1.24
1:A:288:ARG:NH2	4:A:1302:HOH:O	1.82	1.11
1:A:200:ASP:CG	4:A:1303:HOH:O	1.89	1.10
1:A:346:ASP:HA	4:A:1306:HOH:O	1.53	1.05
1:A:346:ASP:CA	4:A:1306:HOH:O	2.07	1.01
1:A:347:ASN:N	4:A:1306:HOH:O	1.95	1.00
1:A:132:GLN:C	4:A:1307:HOH:O	2.01	0.96
1:A:1047:GLU:OE2	4:A:1304:HOH:O	1.83	0.96
1:A:200:ASP:OD2	4:A:1303:HOH:O	1.83	0.94
1:A:193:GLU:OE2	4:A:1306:HOH:O	1.87	0.93
1:A:1137:LYS:O	4:A:1305:HOH:O	1.86	0.92
1:A:132:GLN:O	4:A:1307:HOH:O	1.88	0.92
1:A:1047:GLU:CD	4:A:1304:HOH:O	2.08	0.91
1:A:1091:ASP:HB2	4:A:1314:HOH:O	1.72	0.88
1:A:1161:ASP:HA	1:A:1164:LYS:HD2	1.53	0.88
1:A:159:TYR:CD1	1:A:186:LEU:HD11	2.10	0.87
1:A:271:ASP:OD1	4:A:1309:HOH:O	1.92	0.87
1:A:193:GLU:CD	4:A:1306:HOH:O	2.14	0.86
1:A:185:VAL:O	4:A:1310:HOH:O	1.93	0.86
1:A:193:GLU:OE1	4:A:1306:HOH:O	1.92	0.85
1:A:129:ARG:HD3	4:A:1330:HOH:O	1.76	0.85
1:A:1091:ASP:N	4:A:1314:HOH:O	2.04	0.83
1:A:103:GLU:OE1	4:A:1312:HOH:O	1.97	0.82
1:A:1047:GLU:HA	4:A:1304:HOH:O	1.80	0.82
1:A:101:ARG:O	4:A:1313:HOH:O	1.99	0.80
1:A:422:VAL:O	4:A:1301:HOH:O	1.99	0.79
1:A:1091:ASP:CB	4:A:1314:HOH:O	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLY:N	4:A:1301:HOH:O	1.81	0.78
1:A:355:HIS:ND1	4:A:1319:HOH:O	2.14	0.78
1:A:421:ALA:O	4:A:1301:HOH:O	2.01	0.78
1:A:102:ASN:N	4:A:1321:HOH:O	2.19	0.76
1:A:425:GLY:CA	4:A:1301:HOH:O	2.28	0.75
1:A:167:THR:HA	1:A:170:LEU:HD22	1.67	0.75
1:A:200:ASP:OD1	4:A:1303:HOH:O	2.00	0.75
1:A:103:GLU:HB3	4:A:1312:HOH:O	1.85	0.74
1:A:422:VAL:C	4:A:1301:HOH:O	2.26	0.73
1:A:1107:GLN:HE22	1:A:1144:THR:HG21	1.52	0.72
1:A:276:ARG:NH2	4:A:1317:HOH:O	2.12	0.72
1:A:154:LYS:NZ	4:A:1331:HOH:O	2.24	0.71
1:A:227:ASP:OD2	4:A:1315:HOH:O	2.08	0.71
1:A:305:ARG:HD2	1:A:364:PHE:CZ	2.26	0.71
1:A:159:TYR:CE1	1:A:186:LEU:HD11	2.30	0.67
1:A:276:ARG:NH1	4:A:1317:HOH:O	2.27	0.67
2:A:1202:ATP:O1G	4:A:1318:HOH:O	2.14	0.66
1:A:155:ASN:HD21	1:A:256:LYS:HE2	1.60	0.66
1:A:135:SER:HB3	4:A:1415:HOH:O	1.95	0.65
1:A:1132:ALA:HB2	1:A:1156:ARG:HG3	1.77	0.65
1:A:191:LEU:HD11	1:A:408:ASP:HB2	1.79	0.64
1:A:371:GLN:NE2	4:A:1334:HOH:O	2.28	0.64
1:A:425:GLY:HA3	4:A:1301:HOH:O	1.96	0.64
1:A:1127:ARG:NH2	4:A:1320:HOH:O	2.31	0.64
1:A:101:ARG:C	4:A:1313:HOH:O	2.33	0.64
1:A:153:PRO:HG2	1:A:156:GLU:HB2	1.79	0.64
1:A:135:SER:N	4:A:1336:HOH:O	2.30	0.63
1:A:1091:ASP:CA	4:A:1314:HOH:O	2.44	0.62
1:A:1087:LYS:HB3	1:A:1088:PRO:HD3	1.82	0.62
1:A:1132:ALA:CB	1:A:1156:ARG:HG3	2.32	0.60
1:A:1130:GLU:OE1	4:A:1320:HOH:O	2.17	0.59
1:A:111:GLU:O	1:A:115:ARG:HG2	2.01	0.59
1:A:1159:THR:HG21	1:A:1161:ASP:OD2	2.04	0.58
1:A:1159:THR:HG23	1:A:1161:ASP:H	1.69	0.58
1:A:1122:MET:CE	1:A:1130:GLU:HB3	2.34	0.57
1:A:159:TYR:OH	1:A:1165:ASN:HB3	2.03	0.57
1:A:200:ASP:OD2	1:A:205:LEU:HB2	2.04	0.57
1:A:1127:ARG:CZ	4:A:1320:HOH:O	2.52	0.56
1:A:142:ASP:HB2	1:A:143:PRO:HD2	1.87	0.56
1:A:305:ARG:HG3	1:A:305:ARG:O	2.06	0.56
1:A:1121:ARG:O	1:A:1125:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:O	1:A:103:GLU:HG2	2.06	0.55
1:A:1080:ILE:CG1	1:A:1105:VAL:HG21	2.37	0.54
1:A:446:MET:O	4:A:1322:HOH:O	2.19	0.53
1:A:215:TYR:CE2	1:A:257:VAL:HB	2.44	0.53
1:A:1089:VAL:O	1:A:1093:LEU:HG	2.09	0.52
1:A:1165:ASN:OD1	1:A:180:GLY:N	2.42	0.52
1:A:157:GLU:HB3	1:A:158:PRO:HD2	1.91	0.52
1:A:277:PHE:CE1	1:A:282:LEU:HD21	2.44	0.52
1:A:1157:THR:OG1	1:A:1159:THR:HG22	2.09	0.52
1:A:305:ARG:CD	1:A:364:PHE:CZ	2.93	0.52
1:A:1125:GLN:O	1:A:1126:LYS:HB2	2.10	0.51
1:A:109:GLU:O	1:A:113:VAL:HG23	2.11	0.51
1:A:121:ILE:HD13	1:A:217:ALA:O	2.11	0.51
1:A:305:ARG:HD2	1:A:364:PHE:HZ	1.70	0.51
1:A:183:CYS:O	1:A:353:LEU:N	2.35	0.50
1:A:142:ASP:HB2	1:A:143:PRO:CD	2.41	0.50
1:A:319:ASP:O	1:A:320:CYS:SG	2.67	0.50
1:A:1122:MET:HE1	1:A:1130:GLU:HB3	1.94	0.50
1:A:214:VAL:HB	1:A:260:PHE:HB2	1.93	0.50
1:A:353:LEU:HD23	1:A:419:GLN:HG3	1.94	0.50
1:A:116:GLN:OE1	4:A:1324:HOH:O	2.20	0.49
1:A:275:ARG:HB2	1:A:275:ARG:CZ	2.42	0.49
1:A:185:VAL:HG12	1:A:353:LEU:HD11	1.94	0.49
1:A:392:ASN:HB2	4:A:1338:HOH:O	2.12	0.49
1:A:1156:ARG:HD3	4:A:1332:HOH:O	2.13	0.48
1:A:1149:LYS:O	1:A:1153:THR:HG23	2.14	0.48
1:A:301:ASP:OD2	1:A:309:ARG:HG2	2.13	0.48
1:A:166:TRP:CE2	1:A:1164:LYS:HG2	2.49	0.48
1:A:1086:LEU:HD21	1:A:1113:VAL:HG12	1.96	0.47
1:A:356:PRO:O	4:A:1325:HOH:O	2.20	0.47
1:A:1127:ARG:HE	1:A:1130:GLU:CD	2.17	0.47
1:A:221:PHE:HB2	1:A:223:TYR:CE2	2.50	0.47
1:A:161[A]:HIS:CE1	1:A:162:LEU:HG	2.50	0.47
1:A:305:ARG:CD	1:A:364:PHE:HZ	2.28	0.47
1:A:1054:ARG:CZ	1:A:1056:THR:HG22	2.45	0.47
2:A:1202:ATP:N3	4:A:1342:HOH:O	2.35	0.47
1:A:445:GLN:HA	2:A:1202:ATP:O4'	2.14	0.47
1:A:136:GLY:O	1:A:153:PRO:HD2	2.14	0.47
1:A:158:PRO:HA	1:A:163:ASN:ND2	2.29	0.47
1:A:441:LEU:O	1:A:444:VAL:HG22	2.15	0.47
1:A:1024:GLU:HB3	1:A:1026:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:ILE:HG12	1:A:1105:VAL:HG21	1.96	0.46
1:A:1100:ALA:HB3	1:A:1155:PHE:CE1	2.51	0.46
1:A:1148:ALA:O	1:A:1152:ILE:HG13	2.16	0.46
1:A:1028:THR:HG22	1:A:1029:ILE:N	2.30	0.46
1:A:1122:MET:HE2	1:A:1130:GLU:HB3	1.96	0.46
1:A:279:ALA:O	1:A:281:PRO:HD3	2.15	0.45
1:A:142:ASP:OD1	1:A:146:ARG:N	2.48	0.45
1:A:1007:GLU:O	1:A:1011:ILE:HG13	2.16	0.45
1:A:155:ASN:HA	4:A:1409:HOH:O	2.17	0.45
1:A:1135:LEU:HD23	1:A:1135:LEU:HA	1.78	0.45
1:A:1156:ARG:NH2	4:A:1316:HOH:O	2.12	0.45
1:A:207:ILE:O	1:A:343:ALA:HA	2.17	0.45
1:A:1094:ASP:OD2	1:A:1097:ARG:HD2	2.17	0.45
1:A:291:LEU:O	1:A:295:GLU:HG3	2.17	0.44
1:A:1122:MET:HB2	1:A:1131:ALA:HB2	1.99	0.44
1:A:183:CYS:N	4:A:1326:HOH:O	2.22	0.44
1:A:198:LEU:HD23	1:A:198:LEU:C	2.38	0.44
1:A:230:LYS:HE2	1:A:230:LYS:HB3	1.70	0.44
1:A:425:GLY:HA3	1:A:449:VAL:O	2.18	0.44
1:A:1056:THR:HB	1:A:1059:VAL:O	2.18	0.44
1:A:268:LYS:HD3	1:A:272:TYR:CE1	2.53	0.43
1:A:395:LYS:HE2	1:A:399:GLU:OE2	2.17	0.43
1:A:1038:SER:HA	1:A:1039:PRO:HD3	1.85	0.43
1:A:1035:LEU:O	1:A:1047:GLU:HG2	2.18	0.43
1:A:353:LEU:HD21	1:A:415:GLN:HB3	1.99	0.43
1:A:1069:PHE:O	1:A:1073:VAL:HG23	2.19	0.43
1:A:190:TYR:CZ	1:A:191:LEU:HG	2.54	0.43
1:A:377:SER:O	1:A:380:ILE:HG22	2.18	0.42
1:A:167:THR:O	1:A:170:LEU:HB2	2.19	0.42
1:A:202:LYS:HG2	1:A:393:PHE:CE2	2.54	0.42
1:A:170:LEU:HD12	1:A:170:LEU:HA	1.83	0.42
1:A:275:ARG:HG2	1:A:275:ARG:HH11	1.84	0.42
1:A:1133:VAL:HG12	1:A:1134:ASN:N	2.34	0.42
1:A:1156:ARG:NH1	4:A:1332:HOH:O	2.26	0.42
1:A:372:ALA:O	1:A:440:PRO:HD2	2.20	0.42
1:A:1111:THR:HB	4:A:1365:HOH:O	2.20	0.41
1:A:276:ARG:CZ	4:A:1317:HOH:O	2.50	0.41
1:A:106:GLU:HG2	1:A:107:ASP:N	2.35	0.41
1:A:185:VAL:HG12	1:A:353:LEU:HD21	2.02	0.41
1:A:155:ASN:ND2	1:A:256:LYS:HE2	2.31	0.41
1:A:1013:GLU:OE2	1:A:1147:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.91	0.41
1:A:118:GLU:O	1:A:122:GLU:HG3	2.21	0.41
1:A:205:LEU:CD1	1:A:300:LEU:HB2	2.50	0.41
1:A:309:ARG:NH2	1:A:347:ASN:OD1	2.54	0.41
1:A:385:LEU:HB2	1:A:386:PRO:HD3	2.02	0.40
1:A:221:PHE:HB2	1:A:223:TYR:HE2	1.86	0.40
1:A:264:VAL:HG22	2:A:1201:ATP:N1	2.37	0.40
1:A:157:GLU:HB3	1:A:158:PRO:CD	2.51	0.40
1:A:406:LYS:HA	1:A:411:PHE:CG	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1428:HOH:O	4:A:1455:HOH:O[4_555]	2.00	0.20

## 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	478/556 (86%)	460 (96%)	18 (4%)	0	<b>100</b> <b>100</b>

There are no Ramachandran outliers to report.

### 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	417/473 (88%)	410 (98%)	7 (2%)	68 82

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	GLU
1	A	131	TYR
1	A	170	LEU
1	A	1156	ARG
1	A	269	ASP
1	A	332	TRP
1	A	389	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 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
2	ATP	A	1201	3	26,33,33	1.86	8 (30%)	26,52,52	1.73	3 (11%)
2	ATP	A	1202	-	26,33,33	0.95	1 (3%)	26,52,52	1.84	1 (3%)

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	ATP	A	1201	3	-	0/18/38/38	0/3/3/3
2	ATP	A	1202	-	-	0/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ATP	C2'-C1'	-3.51	1.48	1.53
2	A	1201	ATP	PG-O3G	-3.37	1.43	1.54
2	A	1201	ATP	PG-O1G	-2.83	1.41	1.50
2	A	1201	ATP	C5-N7	-2.57	1.30	1.39
2	A	1201	ATP	PA-O2A	-2.54	1.44	1.55
2	A	1201	ATP	PB-O2B	-2.50	1.44	1.55
2	A	1201	ATP	PB-O1B	-2.25	1.43	1.51
2	A	1201	ATP	PG-O2G	-2.13	1.47	1.54
2	A	1202	ATP	C5-C4	2.99	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1202	ATP	N3-C2-N1	-7.56	122.93	128.87
2	A	1201	ATP	N3-C2-N1	-6.45	123.80	128.87
2	A	1201	ATP	C4'-O4'-C1'	2.12	111.89	109.64
2	A	1201	ATP	N6-C6-N1	2.37	122.49	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ATP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1202	ATP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	172:LYS	C	1001:GLY	N	4.16
1	A	1166:LEU	C	180:GLY	N	3.51
1	A	305:ARG	C	306:ASN	N	1.19
1	A	304:ILE	C	305:ARG	N	1.10

## 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, 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	489/556 (87%)	0.21	14 (2%) 55 63	27, 45, 77, 90	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	TRP	4.1
1	A	1137	LYS	3.8
1	A	159	TYR	3.8
1	A	181	ARG	3.6
1	A	180	GLY	3.5
1	A	1134	ASN	3.0
1	A	1088	PRO	2.8
1	A	131	TYR	2.7
1	A	1141	TYR	2.6
1	A	100	GLU	2.2
1	A	164	PRO	2.2
1	A	1117	THR	2.2
1	A	161[A]	HIS	2.0
1	A	1120	LEU	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<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
2	ATP	A	1201	31/31	0.96	0.12	-1.17	30,40,46,50	0
2	ATP	A	1202	31/31	0.95	0.13	-1.36	33,51,70,78	0
3	CA	A	1203	1/1	0.81	0.13	-	38,38,38,38	0
3	CA	A	1204	1/1	0.95	0.13	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.