



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:40 PM GMT

PDB ID : 4PLA  
Title : Crystal structure of phosphatidyl inositol 4-kinase II alpha in complex with ATP  
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Deposited on : 2014-05-16  
Resolution : 2.77 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 (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

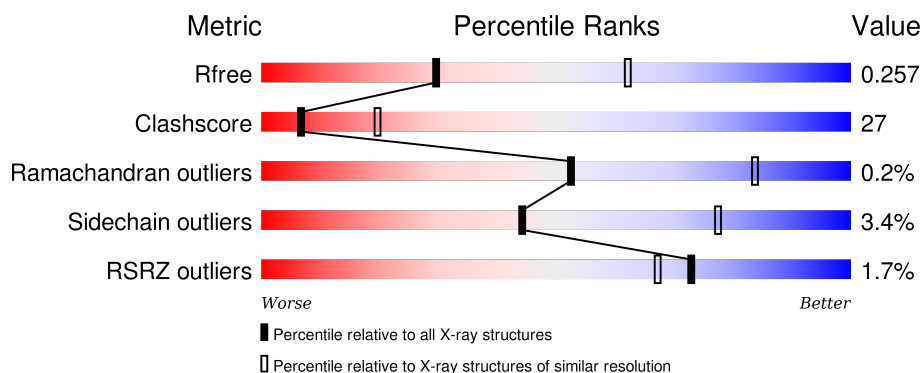
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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></div> <div>47%</div> <div>38%</div> <div>•</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3975 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.

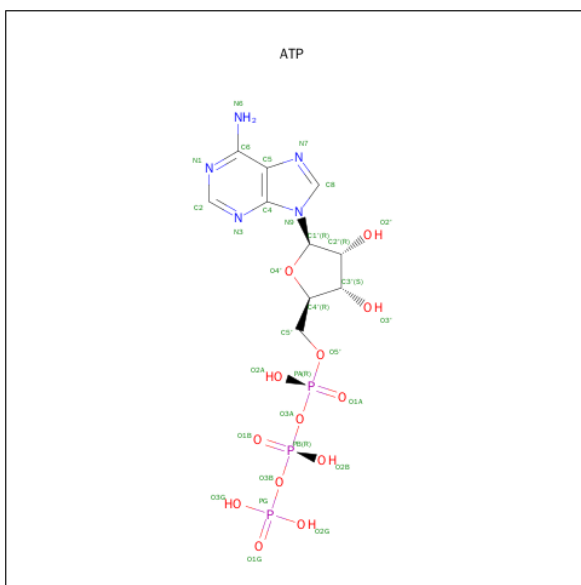
- Molecule 1 is a protein called Chimera protein of Phosphatidylinositol 4-kinase type 2-alpha and Lysozyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3888	2499	670	711	8			

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	engineered mutation	UNP D9IEF7
A	1099	ALA	CYS	engineered mutation	UNP D9IEF7

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




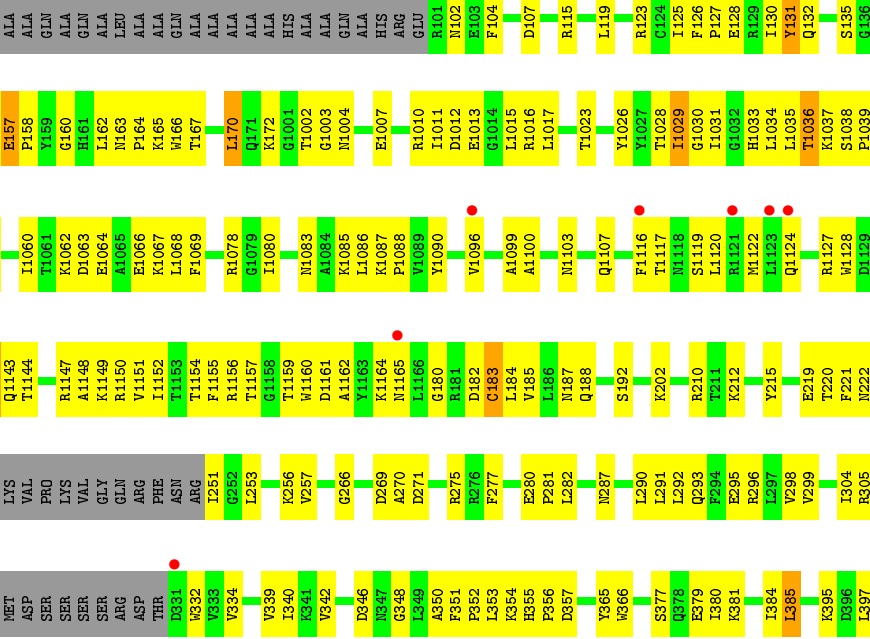
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0
2	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

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 ( $\text{RSRZ} > 2$ ). 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.

- Chain A: 



Amino Acid	Category	Frequency (%)
GLY	Green	47%
ALA	Green	47%
MET	Green	47%
GLY	Green	47%
VAL	Green	47%
ALA	Green	47%
GLN	Green	47%
ALA	Green	47%
GLN	Green	47%
LEU	Green	47%
ALA	Green	47%
ALA	Green	47%
GLN	Green	47%
ALA	Green	47%
ALA	Green	47%
HIS	Green	47%
HIS	Green	47%
ARG	Green	47%
GLU	Green	47%
R101	Yellow	38%
M102	Yellow	38%
F104	Yellow	38%
D107	Yellow	38%
R115	Yellow	38%
L119	Yellow	38%
R123	Yellow	38%
G124	Yellow	38%
F126	Yellow	38%
P127	Yellow	38%
E128	Yellow	38%
H129	Yellow	38%
I130	Yellow	38%
Y131	Yellow	38%
Q132	Yellow	38%
S135	Yellow	38%
G136	Yellow	38%
S137	Yellow	38%
F138	Yellow	38%
F139	Yellow	38%
V140	Yellow	38%
K141	Yellow	38%
D142	Yellow	38%
P143	Yellow	38%

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.74Å 79.54Å 78.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.84 – 2.77 43.74 – 2.77	Depositor EDS
% Data completeness (in resolution range)	93.7 (36.84-2.77) 93.6 (43.74-2.77)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.211 , 0.251 0.213 , 0.257	Depositor DCC
$R_{free}$ test set	809 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.0	EDS
Estimated twinning fraction	0.021 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16191 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3975	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	1/3979 (0.0%)	0.65	1/5396 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	CYS	CB-SG	-5.85	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	385	LEU	C-N-CD	5.78	140.54	128.40

There are no chirality outliers.

There are no planarity outliers.

### 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	3888	0	3866	211	1
2	A	62	24	24	4	0
3	A	1	0	0	0	0
All	All	3951	24	3890	212	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 27.

All (212) 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:438:LYS:HZ2	1:A:446:MET:HE2	0.90	1.05
1:A:438:LYS:NZ	1:A:446:MET:HE2	1.70	1.03
1:A:1141:TYR:OH	1:A:1149:LYS:HE2	1.62	0.98
1:A:123:ARG:HH11	1:A:123:ARG:HG3	1.27	0.97
1:A:398:GLU:OE1	1:A:424:ARG:NH2	2.00	0.93
1:A:438:LYS:HZ2	1:A:446:MET:CE	1.82	0.92
1:A:354:LYS:NZ	1:A:357:ASP:OD1	2.08	0.85
1:A:1165:ASN:O	1:A:180:GLY:HA2	1.75	0.85
1:A:1013:GLU:OE2	1:A:1147:ARG:NH1	2.10	0.84
1:A:119:LEU:HD23	1:A:143:PRO:HG2	1.58	0.84
1:A:1157:THR:OG1	1:A:1159:THR:HG22	1.78	0.83
1:A:130:ILE:HG22	1:A:131:TYR:O	1.79	0.82
1:A:155:ASN:HD21	1:A:256:LYS:HE2	1.42	0.82
1:A:299:VAL:HG11	1:A:384:ILE:HD13	1.61	0.82
1:A:119:LEU:HD23	1:A:143:PRO:CG	2.11	0.80
1:A:162:LEU:O	1:A:222:ASN:ND2	2.14	0.80
1:A:185:VAL:HG11	1:A:188:GLN:OE1	1.83	0.79
1:A:192:SER:HB3	1:A:348:GLY:HA2	1.65	0.78
1:A:1012:ASP:OD1	1:A:1150:ARG:NH1	2.17	0.78
1:A:1063:ASP:O	1:A:1067:LYS:HD3	1.87	0.74
1:A:1023:THR:CG2	1:A:1143:GLN:HG3	2.17	0.74
1:A:202:LYS:HD3	1:A:397:LEU:HD13	1.70	0.73
1:A:1085:LYS:CE	1:A:1117:THR:HG22	2.19	0.72
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.01	0.72
1:A:1119:SER:HB3	1:A:1135:LEU:HD11	1.72	0.69
1:A:1085:LYS:HE2	1:A:1117:THR:HG22	1.75	0.69
1:A:408:ASP:OD2	1:A:410:GLY:N	2.26	0.69
1:A:1041:LEU:O	1:A:1045:LYS:HG3	1.91	0.69
1:A:438:LYS:NZ	1:A:446:MET:CE	2.49	0.69
1:A:1148:ALA:O	1:A:1152:ILE:HG13	1.93	0.69
1:A:1119:SER:CB	1:A:1135:LEU:HD11	2.23	0.69
1:A:228:ARG:O	1:A:231:SER:OG	2.13	0.67
1:A:123:ARG:NH1	1:A:123:ARG:HG3	2.07	0.67
1:A:353:LEU:HD21	1:A:415:GLN:HG2	1.76	0.66
1:A:1127:ARG:HD3	1:A:1130:GLU:HG3	1.76	0.66
1:A:102:ASN:O	1:A:115:ARG:NH1	2.26	0.66
1:A:1133:VAL:O	1:A:1136:ALA:HB3	1.96	0.65
1:A:157:GLU:O	1:A:160:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLU:O	1:A:280:GLU:HG3	1.97	0.64
1:A:1015:LEU:CD2	1:A:1062:LYS:HE2	2.28	0.64
1:A:445:GLN:HA	2:A:1201:ATP:O4'	1.98	0.63
1:A:1140:TRP:O	1:A:1142:ASN:N	2.30	0.63
1:A:130:ILE:HD12	1:A:130:ILE:H	1.64	0.63
1:A:291:LEU:O	1:A:295:GLU:HG3	1.98	0.63
1:A:107:ASP:OD1	1:A:210:ARG:HD3	1.99	0.62
1:A:107:ASP:OD1	1:A:210:ARG:CD	2.47	0.62
1:A:155:ASN:ND2	1:A:256:LYS:HE2	2.15	0.62
1:A:182:ASP:O	1:A:182:ASP:OD1	2.16	0.62
1:A:1127:ARG:HB2	1:A:1130:GLU:HB2	1.82	0.62
1:A:1086:LEU:HD23	1:A:1120:LEU:HD21	1.81	0.62
1:A:406:LYS:HA	1:A:411:PHE:CD2	2.35	0.62
1:A:1120:LEU:O	1:A:1124:GLN:HB2	2.00	0.61
1:A:1119:SER:OG	1:A:1135:LEU:CD1	2.48	0.61
1:A:1015:LEU:HD22	1:A:1062:LYS:HE2	1.80	0.61
1:A:1033:HIS:HD2	1:A:1068:LEU:HB3	1.66	0.61
1:A:1140:TRP:O	1:A:1141:TYR:HB3	2.01	0.61
1:A:251:ILE:O	1:A:251:ILE:HG12	2.01	0.60
1:A:1026:TYR:CZ	1:A:1037:LYS:HD3	2.35	0.60
1:A:377:SER:O	1:A:380:ILE:HG22	2.02	0.60
1:A:305:ARG:O	1:A:305:ARG:HG3	2.01	0.60
1:A:1038:SER:HG	1:A:1040:SER:HG	1.46	0.60
1:A:305:ARG:NH1	1:A:306:ASN:O	2.35	0.59
1:A:231:SER:HA	1:A:251:ILE:O	2.03	0.59
1:A:290:LEU:HD13	1:A:340:ILE:HG21	1.85	0.59
1:A:137:SER:OG	2:A:1202:ATP:O2B	2.17	0.58
1:A:1023:THR:HG21	1:A:1144:THR:HG23	1.85	0.58
1:A:1086:LEU:HD23	1:A:1120:LEU:CD2	2.32	0.58
1:A:1010:ARG:NH2	1:A:1066:GLU:OE1	2.35	0.58
1:A:130:ILE:HD12	1:A:138:TYR:HA	1.85	0.58
1:A:119:LEU:HD23	1:A:143:PRO:HG3	1.87	0.57
1:A:1100:ALA:HB1	1:A:1151:VAL:CG1	2.34	0.57
1:A:135:SER:HB2	1:A:164:PRO:HG2	1.85	0.57
1:A:293:GLN:HB3	1:A:342:VAL:HB	1.85	0.57
1:A:277:PHE:O	1:A:281:PRO:HA	2.03	0.57
1:A:131:TYR:O	1:A:132:GLN:CD	2.43	0.57
1:A:154:LYS:O	1:A:157:GLU:HB2	2.04	0.57
1:A:1023:THR:HG21	1:A:1143:GLN:HG3	1.86	0.56
1:A:142:ASP:HB2	1:A:143:PRO:HD2	1.87	0.56
1:A:1002:THR:O	1:A:1004:ASN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASP:OD2	1:A:275:ARG:NH2	2.38	0.56
1:A:185:VAL:HG11	1:A:188:GLN:CD	2.26	0.56
1:A:1100:ALA:HB3	1:A:1155:PHE:CE1	2.41	0.55
1:A:123:ARG:NH1	1:A:123:ARG:CG	2.65	0.55
1:A:304:ILE:HD12	1:A:350:ALA:CB	2.37	0.55
1:A:107:ASP:OD1	1:A:210:ARG:NE	2.39	0.55
1:A:1054:ARG:NH2	1:A:1064:GLU:OE1	2.40	0.54
1:A:450:ILE:HD12	1:A:452:GLU:HB2	1.88	0.54
1:A:142:ASP:HB2	1:A:143:PRO:CD	2.37	0.54
1:A:1026:TYR:HB3	1:A:1034:LEU:HD11	1.90	0.54
1:A:438:LYS:HD2	1:A:446:MET:CE	2.38	0.54
1:A:1033:HIS:CD2	1:A:1068:LEU:HD13	2.43	0.53
1:A:1141:TYR:HA	1:A:1148:ALA:CB	2.39	0.53
1:A:271:ASP:HB2	1:A:311:ASN:HB3	1.91	0.53
1:A:119:LEU:CD2	1:A:143:PRO:HG2	2.35	0.52
1:A:1119:SER:OG	1:A:1134:ASN:HB2	2.09	0.52
1:A:1029:ILE:HG12	1:A:1030:GLY:H	1.73	0.52
1:A:1041:LEU:CD2	1:A:1045:LYS:HE3	2.39	0.52
1:A:1041:LEU:HG	1:A:1045:LYS:HE3	1.91	0.51
1:A:170:LEU:O	1:A:170:LEU:HD12	2.10	0.51
1:A:1015:LEU:HD21	1:A:1062:LYS:CD	2.41	0.51
1:A:170:LEU:O	1:A:170:LEU:CD1	2.59	0.51
1:A:355:HIS:HE1	1:A:449:VAL:O	1.94	0.51
1:A:1096:VAL:O	1:A:1099:ALA:HB3	2.11	0.51
1:A:1040:SER:OG	1:A:1043:ALA:HB2	2.11	0.50
1:A:438:LYS:HD2	1:A:446:MET:HE3	1.94	0.50
1:A:125:ILE:O	1:A:125:ILE:HG22	2.12	0.50
1:A:221:PHE:HB2	1:A:223:TYR:CE2	2.48	0.49
1:A:305:ARG:NH2	1:A:356:PRO:HG2	2.26	0.49
1:A:104:PHE:CD1	1:A:212:LYS:HD3	2.48	0.49
1:A:1086:LEU:CD2	1:A:1120:LEU:HD21	2.42	0.49
1:A:1119:SER:CB	1:A:1135:LEU:CD1	2.89	0.49
1:A:266:GLY:O	1:A:317:LYS:HG3	2.12	0.49
1:A:418:LYS:O	1:A:422:VAL:HG23	2.13	0.49
1:A:1141:TYR:HE1	1:A:1149:LYS:CG	2.26	0.49
1:A:1028:THR:HG22	1:A:1029:ILE:N	2.28	0.48
1:A:126:PHE:CB	1:A:220:THR:HG23	2.42	0.48
1:A:215:TYR:CE2	1:A:257:VAL:HB	2.48	0.48
1:A:1103:ASN:ND2	1:A:1147:ARG:HH21	2.11	0.48
1:A:1054:ARG:HH21	1:A:1064:GLU:CD	2.16	0.48
1:A:166:TRP:CH2	1:A:1164:LYS:CB	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ARG:O	1:A:365:TYR:CD1	2.67	0.48
1:A:1049:ASP:OD1	1:A:1055:ASN:HA	2.14	0.48
1:A:1141:TYR:CE1	1:A:1149:LYS:HG3	2.49	0.47
1:A:1150:ARG:HG3	1:A:1162:ALA:HB1	1.95	0.47
1:A:282:LEU:HB2	1:A:287:ASN:HB2	1.96	0.47
1:A:1159:THR:OG1	1:A:1160:TRP:N	2.47	0.47
1:A:231:SER:O	1:A:232:ARG:HB2	2.13	0.47
1:A:1049:ASP:HB3	1:A:1054:ARG:O	2.13	0.47
1:A:140:VAL:HB	1:A:149:ALA:HB3	1.96	0.47
1:A:1141:TYR:HE1	1:A:1149:LYS:HG3	1.80	0.47
1:A:131:TYR:O	1:A:132:GLN:CG	2.62	0.47
1:A:380:ILE:HD11	1:A:384:ILE:HD12	1.96	0.47
1:A:1135:LEU:N	1:A:1135:LEU:CD1	2.77	0.47
1:A:128:GLU:O	1:A:128:GLU:HG3	2.15	0.46
1:A:310:GLY:H	1:A:313:ASN:HB2	1.80	0.46
2:A:1202:ATP:H8	2:A:1202:ATP:H5'1	1.79	0.46
1:A:1031:ILE:HD12	1:A:1069:PHE:HB2	1.97	0.46
1:A:1107:GLN:OE1	1:A:1140:TRP:NE1	2.45	0.46
1:A:440:PRO:O	1:A:443:LEU:HB3	2.14	0.46
1:A:221:PHE:O	1:A:228:ARG:NH2	2.49	0.46
1:A:1038:SER:HA	1:A:1039:PRO:HD3	1.66	0.46
1:A:1002:THR:C	1:A:1004:ASN:H	2.19	0.46
1:A:298:VAL:HG13	1:A:366:TRP:CH2	2.50	0.46
1:A:1002:THR:C	1:A:1004:ASN:N	2.68	0.46
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.80	0.46
1:A:1122:MET:HB2	1:A:1131:ALA:HB2	1.98	0.46
1:A:406:LYS:HA	1:A:411:PHE:CG	2.51	0.45
1:A:158:PRO:HA	1:A:163:ASN:ND2	2.31	0.45
1:A:1085:LYS:HE2	1:A:1117:THR:CG2	2.45	0.45
1:A:1127:ARG:CD	1:A:1130:GLU:HG3	2.43	0.45
1:A:130:ILE:HD12	1:A:138:TYR:CA	2.46	0.45
1:A:1029:ILE:HD11	1:A:1060:ILE:HG12	1.99	0.45
1:A:130:ILE:HD11	1:A:138:TYR:C	2.37	0.45
1:A:1085:LYS:NZ	1:A:1117:THR:CG2	2.80	0.45
1:A:1036:THR:OG1	1:A:1038:SER:HB3	2.17	0.45
1:A:395:LYS:HE3	1:A:399:GLU:OE2	2.17	0.45
1:A:1085:LYS:NZ	1:A:1117:THR:HG22	2.32	0.44
1:A:102:ASN:O	1:A:115:ARG:NH2	2.48	0.44
1:A:1087:LYS:N	1:A:1088:PRO:CD	2.80	0.44
1:A:351:PHE:N	1:A:352:PRO:CD	2.80	0.44
1:A:1080:ILE:HG21	1:A:1090:TYR:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1004:ASN:HB2	1:A:1160:TRP:CZ2	2.53	0.44
1:A:127:PRO:HA	1:A:139:PHE:O	2.18	0.44
1:A:1023:THR:HG22	1:A:1143:GLN:HG3	1.96	0.44
1:A:1133:VAL:HG12	1:A:1134:ASN:N	2.33	0.44
1:A:381:LYS:O	1:A:385:LEU:HB2	2.16	0.44
1:A:404:LEU:HA	1:A:404:LEU:HD12	1.80	0.44
1:A:154:LYS:NZ	1:A:187:ASN:O	2.51	0.44
1:A:1151:VAL:O	1:A:1154:THR:N	2.51	0.43
1:A:1054:ARG:NH2	1:A:1064:GLU:OE2	2.49	0.43
1:A:1007:GLU:O	1:A:1011:ILE:HG13	2.18	0.43
1:A:293:GLN:NE2	1:A:293:GLN:HA	2.33	0.43
1:A:130:ILE:CD1	1:A:138:TYR:CA	2.97	0.43
1:A:156:GLU:OE2	1:A:256:LYS:NZ	2.51	0.43
1:A:292:LEU:O	1:A:296:ARG:HG3	2.17	0.43
1:A:1116:PHE:HB2	1:A:1120:LEU:HD11	2.01	0.43
1:A:257:VAL:HG13	1:A:257:VAL:O	2.19	0.43
1:A:1029:ILE:HD13	1:A:1060:ILE:CD1	2.48	0.42
1:A:1151:VAL:O	1:A:1155:PHE:N	2.48	0.42
1:A:318:TYR:CE1	1:A:339:VAL:CG1	3.02	0.42
1:A:1127:ARG:H	1:A:1127:ARG:HG3	1.56	0.42
1:A:1026:TYR:CE2	1:A:1037:LYS:HD3	2.54	0.42
1:A:126:PHE:CB	1:A:220:THR:CG2	2.97	0.42
1:A:269:ASP:O	1:A:270:ALA:C	2.58	0.42
1:A:1140:TRP:C	1:A:1142:ASN:N	2.73	0.42
1:A:355:HIS:CD2	1:A:448:PRO:HB3	2.54	0.42
1:A:1017:LEU:HA	1:A:1017:LEU:HD23	1.74	0.42
1:A:1159:THR:HG23	1:A:1161:ASP:H	1.84	0.42
1:A:170:LEU:HD22	1:A:1160:TRP:HD1	1.85	0.42
1:A:219:GLU:HA	1:A:253:LEU:CD1	2.50	0.42
1:A:428:LEU:HD23	1:A:428:LEU:C	2.40	0.41
1:A:346:ASP:OD2	2:A:1202:ATP:O1A	2.39	0.41
1:A:183:CYS:SG	1:A:352:PRO:HB3	2.60	0.41
1:A:1138:SER:O	1:A:1140:TRP:O	2.38	0.41
1:A:1141:TYR:HA	1:A:1148:ALA:HB2	2.02	0.41
1:A:1100:ALA:HB1	1:A:1151:VAL:HG13	2.03	0.41
1:A:1128:TRP:HB3	1:A:1156:ARG:HA	2.02	0.41
1:A:1140:TRP:C	1:A:1142:ASN:H	2.19	0.41
1:A:1083:ASN:OD1	1:A:1083:ASN:C	2.59	0.41
1:A:1029:ILE:HD13	1:A:1060:ILE:HD13	2.02	0.41
1:A:232:ARG:HD2	1:A:251:ILE:CG2	2.51	0.41
1:A:1035:LEU:O	1:A:1047:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:HE1	1:A:339:VAL:HG11	1.86	0.41
1:A:223:TYR:CZ	1:A:253:LEU:HB3	2.56	0.41
1:A:280:GLU:CG	1:A:280:GLU:O	2.66	0.41
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.36	0.41
1:A:1029:ILE:CD1	1:A:1060:ILE:HG12	2.51	0.41
1:A:1083:ASN:OD1	1:A:1085:LYS:N	2.54	0.40
1:A:183:CYS:HB3	1:A:184:LEU:HD22	2.04	0.40
1:A:130:ILE:HD13	1:A:137:SER:C	2.41	0.40
1:A:1016:ARG:O	1:A:1030:GLY:HA2	2.21	0.40
1:A:163:ASN:OD1	1:A:165:LYS:N	2.53	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)
1:A:1078:ARG:NH2	1:A:379:GLU:OE2[1_556]	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	477/556 (86%)	462 (97%)	14 (3%)	1 (0%)	52 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1003	GLY

### 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	413/473 (87%)	399 (97%)	14 (3%)	44 77

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	TYR
1	A	157	GLU
1	A	167	THR
1	A	170	LEU
1	A	172	LYS
1	A	1029	ILE
1	A	1036	THR
1	A	1042	ASN
1	A	1133	VAL
1	A	1135	LEU
1	A	1137	LYS
1	A	1142	ASN
1	A	332	TRP
1	A	334	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	1033	HIS
1	A	1103	ASN
1	A	187	ASN
1	A	355	HIS

### 5.3.3 RNA [i](#)

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 ⓘ

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	$\# Z  > 2$
2	ATP	A	1201	-	24,33,33	1.01	1 (4%)	31,52,52	2.28	6 (19%)
2	ATP	A	1202	-	24,33,33	1.30	3 (12%)	31,52,52	2.19	6 (19%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1202	ATP	O4'-C4'	-2.54	1.39	1.45
2	A	1202	ATP	C5-N7	-2.17	1.32	1.39
2	A	1202	ATP	C2'-C3'	-2.09	1.47	1.53
2	A	1201	ATP	C5-N7	-2.02	1.32	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ATP	N3-C2-N1	-8.10	122.69	128.89
2	A	1202	ATP	N3-C2-N1	-7.42	123.21	128.89
2	A	1201	ATP	PB-O3B-PG	-5.20	115.23	132.67
2	A	1202	ATP	PB-O3B-PG	-5.03	115.80	132.67
2	A	1201	ATP	PA-O3A-PB	-4.98	118.75	132.73
2	A	1202	ATP	PA-O3A-PB	-4.03	121.41	132.73
2	A	1202	ATP	C4-C5-N7	-3.08	106.64	109.48
2	A	1202	ATP	C2'-C1'-N9	-2.21	110.92	114.29
2	A	1201	ATP	C4-C5-N7	-2.03	107.61	109.48
2	A	1201	ATP	C2-N1-C6	2.05	122.43	118.77
2	A	1202	ATP	O3G-PG-O2G	2.14	115.52	107.38
2	A	1201	ATP	C4'-O4'-C1'	2.15	112.08	109.72

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
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](#)

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, 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	483/556 (86%)	0.31	8 (1%) 73 67	38, 55, 85, 105	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1165	ASN	3.5
1	A	1123	LEU	3.3
1	A	331	ASP	2.5
1	A	1124	GLN	2.5
1	A	1121	ARG	2.4
1	A	1116	PHE	2.2
1	A	135	SER	2.2
1	A	1096	VAL	2.1

### 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	0.88	0.17	-0.79	56,76,112,123	0
2	ATP	A	1202	31/31	0.93	0.18	-1.06	47,66,87,102	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.