



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:43 PM GMT

PDB ID : 3X07  
Title : Crystal structure of PIP4KIIBETA N203A complex with AMP  
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Deposited on : 2014-10-09  
Resolution : 2.60 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-20026982  
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) : rb-20026982

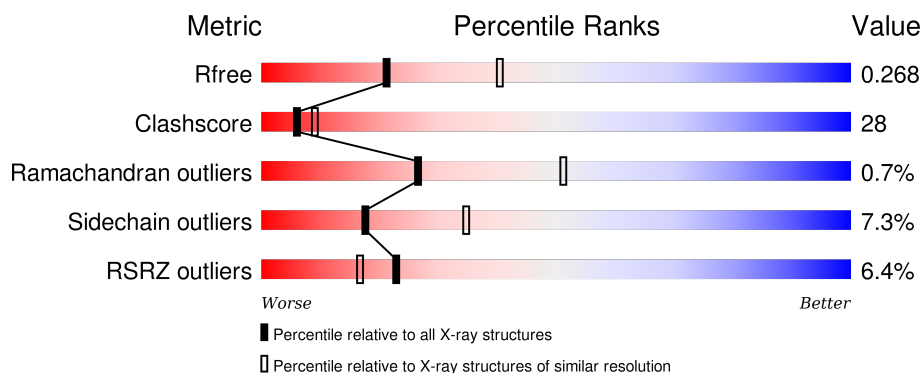
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	393	<div> <div>2%</div> <div>48% 30% 20%</div> </div>
1	B	393	<div> <div>8%</div> <div>45% 24% 5% 26%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5102 atoms, of which 36 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 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2577	1642	438	483	14			
1	B	292	Total	C	N	O	S	0	0	0
			2403	1544	409	437	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLY	-	EXPRESSION TAG	UNP P78356
A	25	PRO	-	EXPRESSION TAG	UNP P78356
A	26	ASN	-	EXPRESSION TAG	UNP P78356
A	27	CYS	-	EXPRESSION TAG	UNP P78356
A	28	ALA	-	EXPRESSION TAG	UNP P78356
A	29	PRO	-	EXPRESSION TAG	UNP P78356
A	30	GLY	-	EXPRESSION TAG	UNP P78356
A	203	ALA	ASN	ENGINEERED MUTATION	UNP P78356
B	24	GLY	-	EXPRESSION TAG	UNP P78356
B	25	PRO	-	EXPRESSION TAG	UNP P78356
B	26	ASN	-	EXPRESSION TAG	UNP P78356
B	27	CYS	-	EXPRESSION TAG	UNP P78356
B	28	ALA	-	EXPRESSION TAG	UNP P78356
B	29	PRO	-	EXPRESSION TAG	UNP P78356
B	30	GLY	-	EXPRESSION TAG	UNP P78356
B	203	ALA	ASN	ENGINEERED MUTATION	UNP P78356

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		
2	A	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	8	Total	O	0	0
			8	8		



I370	TYR	ASP	THR	LYS	LYS	ALA	ALA	HIS	ALA	LYS	THR	VAL	LYS	HIS	GLY	GLY	ALA	ALA	GLU	ILE	SER	THR	VAL	N399	P400	E401	Q402	Y403	S404	K405	R406	F407	N408	E409	F410	M411	S412	N413	I414	LEU	THR		
L371																																											
T372																																											
P373																																											

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.12Å 185.07Å 107.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.56 – 2.60 93.36 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (53.56-2.60) 98.7 (93.36-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.62Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.223 , 0.270 0.227 , 0.268	Depositor DCC
$R_{free}$ test set	1649 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 67.1	EDS
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32995 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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: 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	0.44	0/2629	0.58	0/3533
1	B	0.49	0/2455	0.60	0/3303
All	All	0.46	0/5084	0.59	0/6836

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	2577	0	2540	137	0
1	B	2403	0	2382	158	0
2	A	69	36	36	2	0
3	A	9	0	0	1	0
3	B	8	0	0	1	0
All	All	5066	36	4958	284	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 28.

All (284) 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:B:225:GLU:HG2	1:B:241:ASN:HB2	1.35	1.08
1:A:42:ILE:H	1:A:42:ILE:HD12	1.11	1.07
1:B:250:LEU:HD22	1:B:414:ILE:HG22	1.41	1.02
1:B:241:ASN:HA	1:B:244:LEU:HD12	1.41	1.01
1:B:243:PHE:HE2	1:B:414:ILE:CG1	1.72	1.01
1:B:243:PHE:HE2	1:B:414:ILE:HG13	1.23	1.00
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.42	0.99
1:B:243:PHE:CE2	1:B:414:ILE:HG13	1.98	0.98
1:A:278:ASP:H	1:A:403:TYR:HE2	1.13	0.97
1:B:252:VAL:CG1	1:B:256:SER:HB2	1.95	0.96
1:B:250:LEU:HD22	1:B:414:ILE:CG2	1.96	0.94
1:B:225:GLU:HG2	1:B:241:ASN:CB	1.96	0.94
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.51	0.93
1:B:277:MET:O	1:B:278:ASP:HB2	1.71	0.88
1:A:141:THR:HG22	1:A:142:THR:O	1.73	0.88
1:A:278:ASP:N	1:A:403:TYR:HE2	1.71	0.88
1:B:264:LEU:HD11	1:B:407:PHE:HE2	1.40	0.87
1:A:42:ILE:CD1	1:A:42:ILE:H	1.84	0.86
1:A:32:LYS:NZ	1:A:32:LYS:HB2	1.91	0.85
1:B:225:GLU:HA	1:B:239:LYS:HB2	1.59	0.84
1:B:243:PHE:CE2	1:B:414:ILE:CG1	2.60	0.83
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.07	0.83
1:A:42:ILE:N	1:A:42:ILE:HD12	1.92	0.83
1:A:77:ILE:HD11	1:B:77:ILE:CD1	2.10	0.81
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.11	0.80
1:B:278:ASP:HB2	1:B:372:THR:HG21	1.61	0.80
1:B:408:ASN:C	1:B:408:ASN:HD22	1.87	0.77
1:B:278:ASP:CB	1:B:372:THR:HG21	2.14	0.77
1:A:67:MET:HE2	1:A:68:PRO:HD3	1.65	0.77
1:A:218:LYS:HD2	1:A:224:ARG:NH1	1.99	0.77
1:B:94:LYS:HB2	1:B:190:THR:HB	1.66	0.76
1:A:399:ASN:HB3	1:A:402:GLN:HB2	1.68	0.76
1:B:243:PHE:CE2	1:B:414:ILE:CD1	2.68	0.75
1:B:407:PHE:O	1:B:411:MET:HG2	1.86	0.75
1:A:109:ARG:CZ	1:A:172:VAL:HG13	2.18	0.74
1:B:243:PHE:CE2	1:B:414:ILE:HD12	2.23	0.73
1:B:252:VAL:HG12	1:B:256:SER:HB2	1.69	0.73
1:B:214:LYS:HE3	1:B:235:LEU:HB3	1.69	0.73
1:A:270:PHE:CZ	1:A:274:LEU:HD11	2.24	0.72
1:A:67:MET:HA	1:A:67:MET:CE	2.19	0.72
1:B:410:PHE:C	1:B:410:PHE:CD1	2.64	0.71
1:B:405:LYS:O	1:B:409:GLU:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:VAL:CG1	1:A:404:SER:HA	2.20	0.70
1:B:249:LYS:HA	1:B:414:ILE:HG23	1.74	0.69
1:B:271:LEU:HD13	1:B:279:TYR:CE2	2.27	0.69
1:B:243:PHE:CZ	1:B:414:ILE:HG21	2.28	0.69
1:B:138:ARG:NH1	1:B:138:ARG:HG3	2.08	0.69
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.75	0.69
1:B:127:ILE:CG2	1:B:128:ASN:N	2.56	0.68
1:B:257:LYS:HD3	1:B:258:LYS:N	2.08	0.68
1:B:243:PHE:CE2	1:B:414:ILE:HG21	2.29	0.68
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.59	0.68
1:B:269:GLU:O	1:B:273:GLN:HG3	1.94	0.68
1:A:241:ASN:O	1:A:245:ASN:HB2	1.94	0.68
1:A:169:GLN:O	1:A:172:VAL:HG23	1.94	0.68
1:A:160:MET:HG2	1:A:371:LEU:HD21	1.74	0.67
1:A:127:ILE:O	1:A:128:ASN:HB2	1.94	0.67
1:B:110:PHE:CE1	1:B:182:GLN:HG2	2.29	0.67
1:B:264:LEU:HD11	1:B:407:PHE:CE2	2.27	0.67
1:A:208:ARG:HH22	1:A:342:PHE:HA	1.60	0.67
1:B:225:GLU:HB3	1:B:242:ASP:OD1	1.96	0.66
1:A:214:LYS:HE3	1:A:237:THR:OG1	1.96	0.66
1:B:271:LEU:HD12	1:B:279:TYR:CZ	2.30	0.66
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.26	0.65
1:A:278:ASP:N	1:A:403:TYR:CE2	2.52	0.65
1:B:250:LEU:CD2	1:B:414:ILE:HG22	2.22	0.65
1:B:277:MET:O	1:B:278:ASP:CB	2.45	0.65
1:B:276:ILE:HA	1:B:373:PRO:HG3	1.78	0.65
1:B:243:PHE:HE2	1:B:414:ILE:CD1	2.06	0.64
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.62	0.64
1:A:67:MET:HA	1:A:67:MET:HE2	1.79	0.64
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.79	0.64
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.82	0.63
1:A:349:TYR:CD1	1:A:366:ALA:HB2	2.33	0.63
1:A:66:LEU:HD12	1:A:168:HIS:CE1	2.34	0.62
1:A:218:LYS:HG2	1:A:403:TYR:OH	1.98	0.62
1:A:246:GLU:HG2	1:A:246:GLU:O	1.97	0.62
1:A:278:ASP:CA	1:A:403:TYR:HE2	2.13	0.62
1:B:410:PHE:C	1:B:410:PHE:HD1	2.03	0.62
1:A:56:GLU:OE2	1:B:48:TRP:NE1	2.26	0.62
1:B:127:ILE:HG23	1:B:128:ASN:N	2.14	0.61
1:A:264:LEU:HD21	1:A:411:MET:HB2	1.81	0.61
1:A:32:LYS:HZ2	1:A:32:LYS:HB2	1.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HD22	1:B:283:VAL:HG23	1.82	0.60
1:B:225:GLU:HG2	1:B:241:ASN:HB3	1.83	0.60
1:B:217:LEU:HB3	1:B:411:MET:HE1	1.83	0.60
1:B:166:LYS:HD2	1:B:274:LEU:HD21	1.84	0.59
1:B:238:PHE:HD2	1:B:242:ASP:HB3	1.66	0.59
1:B:271:LEU:CD1	1:B:279:TYR:CZ	2.86	0.59
1:A:260:PHE:CD2	1:A:415:LEU:HD11	2.38	0.59
1:B:217:LEU:H	1:B:217:LEU:HD22	1.69	0.58
1:A:220:SER:CB	1:A:222:VAL:N	2.67	0.58
1:A:250:LEU:HG	1:A:414:ILE:HG22	1.86	0.58
1:A:139:PHE:CE2	2:A:501:AMP:O4'	2.56	0.57
1:A:141:THR:CG2	1:A:145:ARG:HA	2.35	0.57
1:B:281:LEU:HB2	1:B:407:PHE:CZ	2.39	0.57
1:A:208:ARG:NH2	1:A:342:PHE:HA	2.18	0.57
1:B:144:ASP:OD2	1:B:146:ARG:HD2	2.03	0.57
1:B:215:TYR:CD1	1:B:238:PHE:HB2	2.40	0.57
1:A:399:ASN:HA	1:A:402:GLN:HG3	1.87	0.57
1:B:189:LEU:HD12	1:B:189:LEU:N	2.20	0.57
1:B:260:PHE:CE2	1:B:365:MET:CE	2.88	0.56
1:A:110:PHE:CZ	1:A:182:GLN:HB3	2.40	0.56
1:B:46:LEU:HD21	1:B:149:ILE:HD13	1.88	0.56
1:B:217:LEU:HB2	1:B:411:MET:CE	2.36	0.56
1:B:277:MET:HE1	1:B:400:PRO:N	2.21	0.55
1:B:240:ASP:O	1:B:244:LEU:HG	2.07	0.55
1:A:241:ASN:O	1:A:245:ASN:CB	2.55	0.55
1:B:252:VAL:HG13	1:B:256:SER:HB2	1.83	0.55
1:A:32:LYS:HZ3	1:A:32:LYS:HB2	1.71	0.55
1:B:281:LEU:HD23	1:B:281:LEU:C	2.27	0.55
1:A:127:ILE:O	1:A:128:ASN:CB	2.53	0.55
1:A:186:MET:HG3	1:A:199:VAL:HG22	1.88	0.55
1:B:243:PHE:HE2	1:B:414:ILE:CG2	2.19	0.55
1:B:408:ASN:ND2	1:B:408:ASN:C	2.59	0.55
1:B:140:LEU:HB2	1:B:149:ILE:HB	1.89	0.55
1:B:240:ASP:HB3	1:B:410:PHE:CE2	2.41	0.55
1:B:276:ILE:HD13	1:B:370:ILE:O	2.07	0.55
1:B:281:LEU:HD22	1:B:283:VAL:CG2	2.37	0.55
1:A:202:ARG:HG3	1:A:203:ALA:N	2.22	0.55
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.20	0.54
1:B:78:LYS:HD2	1:B:94:LYS:HE3	1.88	0.54
1:B:217:LEU:CB	1:B:411:MET:HE1	2.38	0.54
1:B:236:PRO:HB2	1:B:238:PHE:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:PHE:CZ	1:B:414:ILE:CG2	2.91	0.54
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.90	0.54
1:B:260:PHE:CE2	1:B:365:MET:HE3	2.43	0.53
1:B:230:GLU:C	1:B:232:ALA:H	2.11	0.53
1:B:217:LEU:CB	1:B:411:MET:CE	2.86	0.53
1:A:169:GLN:HA	1:A:172:VAL:HG23	1.91	0.53
1:B:217:LEU:HB2	1:B:411:MET:HE3	1.91	0.53
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.24	0.53
1:B:403:TYR:N	1:B:406:ARG:HH21	2.07	0.53
1:A:109:ARG:HG2	1:A:109:ARG:NH1	2.24	0.53
1:A:160:MET:O	1:A:164:LEU:HB2	2.08	0.53
1:A:208:ARG:NH2	1:A:341:GLU:O	2.30	0.53
1:A:139:PHE:CD1	1:A:139:PHE:C	2.81	0.53
1:B:127:ILE:HG22	1:B:128:ASN:HB3	1.90	0.52
1:A:278:ASP:HA	1:A:403:TYR:CE2	2.45	0.52
1:A:168:HIS:O	1:A:172:VAL:HG22	2.09	0.52
1:B:139:PHE:C	1:B:139:PHE:CD1	2.82	0.52
1:B:250:LEU:CD2	1:B:414:ILE:CG2	2.78	0.52
1:A:145:ARG:HH21	1:A:207:HIS:C	2.11	0.52
1:A:54:ILE:HG21	1:A:118:GLN:HB2	1.91	0.52
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.75	0.51
1:A:169:GLN:C	1:A:172:VAL:HG23	2.30	0.51
1:B:271:LEU:HD13	1:B:279:TYR:CD2	2.45	0.51
1:A:278:ASP:CA	1:A:403:TYR:CE2	2.93	0.51
1:A:354:HIS:HD2	1:A:355:GLU:H	1.59	0.51
1:B:78:LYS:CD	1:B:94:LYS:HE2	2.34	0.51
1:A:169:GLN:HA	1:A:172:VAL:CG2	2.40	0.51
1:A:189:LEU:N	1:A:189:LEU:HD12	2.26	0.51
1:B:241:ASN:HA	1:B:244:LEU:CD1	2.27	0.51
1:B:236:PRO:HG2	1:B:238:PHE:HE1	1.77	0.50
1:B:238:PHE:HD2	1:B:242:ASP:CB	2.24	0.50
1:A:243:PHE:CE1	1:A:248:GLN:HG2	2.46	0.50
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.46	0.50
1:B:276:ILE:CG2	1:B:277:MET:N	2.74	0.50
1:B:250:LEU:HD22	1:B:414:ILE:HG21	1.89	0.50
1:A:67:MET:HE2	1:A:68:PRO:CD	2.39	0.50
1:B:213:ARG:CZ	1:B:238:PHE:CZ	2.94	0.50
1:A:35:LEU:HD13	1:A:37:ARG:HH22	1.77	0.49
1:B:79:VAL:O	1:B:92:ARG:HA	2.12	0.49
1:A:224:ARG:O	1:A:241:ASN:HB2	2.12	0.49
1:B:277:MET:HE3	1:B:400:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:HIS:CD2	1:A:355:GLU:N	2.80	0.49
1:B:189:LEU:N	1:B:189:LEU:CD1	2.75	0.49
1:B:227:SER:OG	1:B:230:GLU:HB2	2.12	0.49
1:B:66:LEU:HD12	1:B:168:HIS:CE1	2.47	0.49
1:B:276:ILE:HG22	1:B:277:MET:N	2.27	0.49
1:A:264:LEU:HD11	1:A:407:PHE:CE2	2.44	0.48
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.95	0.48
1:A:250:LEU:HG	1:A:414:ILE:CG2	2.43	0.48
1:B:166:LYS:HD2	1:B:274:LEU:CD2	2.44	0.48
1:B:230:GLU:O	1:B:232:ALA:N	2.46	0.48
1:B:225:GLU:CG	1:B:241:ASN:HB2	2.25	0.48
1:A:264:LEU:CD2	1:A:411:MET:HB2	2.44	0.48
1:A:139:PHE:C	1:A:139:PHE:HD1	2.16	0.48
1:A:261:LEU:HD21	1:A:412:SER:HA	1.96	0.48
1:A:350:ALA:HA	1:A:363:TYR:O	2.14	0.48
1:A:236:PRO:HB2	1:A:238:PHE:CE2	2.49	0.48
1:B:236:PRO:CG	1:B:238:PHE:HE1	2.27	0.47
1:A:225:GLU:HG3	1:A:241:ASN:HB2	1.95	0.47
1:A:213:ARG:NH2	1:A:246:GLU:OE1	2.47	0.47
1:B:208:ARG:HG2	1:B:209:LEU:N	2.28	0.47
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.44	0.47
1:B:213:ARG:NH2	1:B:246:GLU:OE2	2.47	0.47
1:B:277:MET:O	1:B:372:THR:HB	2.13	0.47
1:B:271:LEU:CD1	1:B:279:TYR:CE2	2.96	0.47
1:A:340:GLY:O	1:A:352:LYS:HE2	2.14	0.47
1:B:281:LEU:HB2	1:B:407:PHE:HZ	1.80	0.47
1:A:243:PHE:CZ	1:A:414:ILE:HG23	2.50	0.47
1:B:49:GLY:HA3	1:B:95:PHE:CE2	2.50	0.47
1:A:77:ILE:HG22	1:A:95:PHE:HB3	1.97	0.46
1:A:271:LEU:HD13	1:A:279:TYR:CE2	2.50	0.46
1:B:336:PHE:CD2	1:B:337:PHE:O	2.68	0.46
1:A:109:ARG:NH1	1:A:172:VAL:HG13	2.29	0.46
1:A:153:SER:O	1:A:157:VAL:HG23	2.15	0.46
1:B:82:HIS:CE1	1:B:83:LEU:HG	2.49	0.46
1:A:218:LYS:HE2	1:A:278:ASP:O	2.15	0.46
1:B:410:PHE:O	1:B:410:PHE:CD1	2.68	0.46
1:B:277:MET:CE	1:B:400:PRO:HA	2.46	0.46
1:B:217:LEU:HD22	1:B:217:LEU:N	2.29	0.46
1:B:242:ASP:N	1:B:242:ASP:OD1	2.48	0.46
1:A:168:HIS:O	1:A:172:VAL:CG2	2.64	0.46
1:A:66:LEU:O	1:A:67:MET:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:NZ	2:A:503:AMP:O3P	2.47	0.46
1:B:252:VAL:HG12	1:B:257:LYS:H	1.81	0.46
1:B:260:PHE:CE2	1:B:365:MET:HE1	2.50	0.46
1:A:160:MET:CG	1:A:371:LEU:HD21	2.45	0.46
1:A:77:ILE:HD12	1:B:79:VAL:HG22	1.97	0.45
1:A:243:PHE:HZ	1:A:414:ILE:HG23	1.80	0.45
1:A:169:GLN:CA	1:A:172:VAL:HG23	2.46	0.45
1:A:225:GLU:O	1:A:239:LYS:HG3	2.16	0.45
1:A:350:ALA:HB2	1:A:364:PHE:CD1	2.51	0.45
1:B:206:SER:HA	1:B:347:ASP:OD1	2.17	0.45
1:B:277:MET:HE1	1:B:399:ASN:C	2.37	0.45
1:B:399:ASN:HA	1:B:402:GLN:CB	2.47	0.45
1:A:400:PRO:HG2	1:A:401:GLU:H	1.82	0.45
1:A:224:ARG:O	1:A:225:GLU:HG3	2.15	0.45
1:A:243:PHE:CE1	1:A:248:GLN:CG	3.00	0.45
1:A:49:GLY:HA3	1:A:95:PHE:CE1	2.51	0.44
1:A:94:LYS:HB2	1:A:190:THR:HB	1.99	0.44
1:A:166:LYS:HD2	1:A:274:LEU:HD21	1.98	0.44
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.88	0.44
1:A:82:HIS:HB2	1:B:74:TYR:CZ	2.53	0.44
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.00	0.44
1:A:208:ARG:CB	1:A:208:ARG:NH1	2.80	0.44
1:A:110:PHE:CE1	1:A:182:GLN:HB3	2.53	0.44
1:B:230:GLU:C	1:B:232:ALA:N	2.70	0.44
1:B:150:LYS:HB2	1:B:150:LYS:HE3	1.47	0.44
1:B:104:ARG:HD2	3:B:503:HOH:O	2.17	0.44
1:A:403:TYR:O	1:A:407:PHE:N	2.40	0.43
1:A:43:LEU:O	1:A:47:MET:HG3	2.18	0.43
1:A:59:ASN:HB3	1:B:34:LYS:O	2.18	0.43
1:A:128:ASN:HB2	1:A:140:LEU:HA	2.00	0.43
1:B:48:TRP:HB2	1:B:89:LEU:HD21	2.00	0.43
1:B:414:ILE:O	1:B:414:ILE:HG22	2.19	0.43
1:A:204:VAL:HA	1:A:349:TYR:CD2	2.53	0.43
1:B:179:LEU:HG	1:B:263:LYS:HG2	2.01	0.43
1:B:281:LEU:C	1:B:281:LEU:CD2	2.87	0.43
1:A:258:LYS:NZ	1:A:262:GLU:OE2	2.32	0.43
1:A:246:GLU:CG	1:A:246:GLU:O	2.66	0.43
1:B:57:LEU:O	1:B:104:ARG:NH2	2.51	0.43
1:A:350:ALA:HB2	1:A:364:PHE:CE1	2.53	0.43
1:B:74:TYR:CD1	1:B:74:TYR:C	2.92	0.43
1:A:354:HIS:HD2	1:A:355:GLU:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLY:HA2	3:A:602:HOH:O	2.19	0.43
1:B:399:ASN:N	1:B:400:PRO:CD	2.82	0.42
1:B:188:ARG:C	1:B:189:LEU:HD12	2.39	0.42
1:A:109:ARG:CZ	1:A:172:VAL:CG1	2.93	0.42
1:A:34:LYS:O	1:B:59:ASN:HB3	2.18	0.42
1:B:157:VAL:HG13	1:B:186:MET:HE3	2.01	0.42
1:B:231:LYS:HE2	1:B:238:PHE:CE2	2.54	0.42
1:A:43:LEU:HD21	1:A:140:LEU:CD1	2.49	0.42
1:A:179:LEU:HG	1:A:263:LYS:HB3	2.01	0.42
1:B:250:LEU:H	1:B:250:LEU:HD22	1.85	0.42
1:B:343:ASP:HA	1:B:344:PRO:HD2	1.92	0.42
1:B:213:ARG:NH2	1:B:238:PHE:CE2	2.87	0.42
1:A:270:PHE:CE1	1:A:274:LEU:CD1	3.03	0.42
1:B:238:PHE:CD2	1:B:242:ASP:HB3	2.52	0.42
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.89	0.42
1:A:74:TYR:CZ	1:B:82:HIS:HB2	2.54	0.42
1:B:250:LEU:HB3	1:B:363:TYR:CE2	2.55	0.41
1:B:277:MET:HB3	1:B:277:MET:HE3	1.85	0.41
1:B:281:LEU:HD23	1:B:282:LEU:N	2.35	0.41
1:A:67:MET:HA	1:A:67:MET:HE3	1.99	0.41
1:A:225:GLU:C	1:A:239:LYS:HG3	2.41	0.41
1:A:141:THR:HG23	1:A:145:ARG:HA	2.01	0.41
1:A:78:LYS:HB3	1:B:78:LYS:HB3	2.02	0.41
1:B:248:GLN:O	1:B:414:ILE:HD12	2.20	0.41
1:B:399:ASN:HA	1:B:402:GLN:HB3	2.02	0.41
1:B:157:VAL:HG13	1:B:186:MET:CE	2.51	0.41
1:A:49:GLY:HA3	1:A:95:PHE:CZ	2.56	0.41
1:B:268:VAL:HG13	1:B:279:TYR:OH	2.21	0.41
1:B:127:ILE:HG22	1:B:128:ASN:CB	2.51	0.41
1:A:371:LEU:HA	1:A:371:LEU:HD12	1.86	0.41
1:A:208:ARG:HB3	1:A:208:ARG:CZ	2.50	0.41
1:A:78:LYS:HG3	1:A:94:LYS:CG	2.51	0.41
1:A:166:LYS:HD2	1:A:274:LEU:CD2	2.51	0.41
1:B:283:VAL:HG22	1:B:365:MET:HG2	2.02	0.40
1:A:209:LEU:HD11	1:A:342:PHE:HB3	2.03	0.40
1:A:63:PRO:HB2	1:A:65:MET:O	2.22	0.40
1:B:357:SER:HB2	1:B:358:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/393 (77%)	287 (94%)	15 (5%)	2 (1%)	26	51
1	B	278/393 (71%)	260 (94%)	16 (6%)	2 (1%)	26	51
All	All	582/786 (74%)	547 (94%)	31 (5%)	4 (1%)	26	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	231	LYS
1	A	358	PRO
1	A	400	PRO
1	B	354	HIS

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	288/351 (82%)	273 (95%)	15 (5%)	29	54
1	B	271/351 (77%)	245 (90%)	26 (10%)	10	20
All	All	559/702 (80%)	518 (93%)	41 (7%)	17	35

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	42	ILE

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Mol	Chain	Res	Type
1	A	56	GLU
1	A	76	LYS
1	A	139	PHE
1	A	172	VAL
1	A	182	GLN
1	A	240	ASP
1	A	254	GLU
1	A	266	ARG
1	A	280	SER
1	A	295	GLU
1	A	351	MET
1	A	371	LEU
1	A	403	TYR
1	B	104	ARG
1	B	122	THR
1	B	127	ILE
1	B	138	ARG
1	B	139	PHE
1	B	150	LYS
1	B	178	THR
1	B	211	VAL
1	B	217	LEU
1	B	225	GLU
1	B	230	GLU
1	B	240	ASP
1	B	241	ASN
1	B	242	ASP
1	B	244	LEU
1	B	246	GLU
1	B	249	LYS
1	B	250	LEU
1	B	257	LYS
1	B	278	ASP
1	B	285	ILE
1	B	288	VAL
1	B	371	LEU
1	B	399	ASN
1	B	408	ASN
1	B	410	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	HIS
1	B	82	HIS

### 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	$\# Z  > 2$
2	AMP	A	501	-	22,25,25	1.04	1 (4%)	22,38,38	2.20	3 (13%)
2	AMP	A	502	-	22,25,25	1.95	9 (40%)	22,38,38	2.01	5 (22%)
2	AMP	A	503	-	22,25,25	0.94	1 (4%)	22,38,38	1.70	2 (9%)

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	AMP	A	501	-	-	0/6/26/26	0/3/3/3
2	AMP	A	502	-	-	0/6/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	503	-	-	0/6/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	AMP	C2'-C1'	-3.21	1.48	1.53
2	A	502	AMP	P-O3P	-3.17	1.43	1.54
2	A	502	AMP	P-O2P	-3.17	1.43	1.54
2	A	502	AMP	O4'-C4'	-2.76	1.38	1.45
2	A	502	AMP	P-O1P	-2.51	1.42	1.50
2	A	502	AMP	P-O5'	-2.48	1.52	1.59
2	A	502	AMP	C2'-C3'	-2.33	1.47	1.53
2	A	502	AMP	C4-N3	-2.29	1.32	1.35
2	A	502	AMP	C5-N7	-2.29	1.31	1.39
2	A	501	AMP	C5-C4	2.02	1.45	1.40
2	A	503	AMP	C5-C4	2.90	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	AMP	N3-C2-N1	-7.86	122.70	128.87
2	A	502	AMP	N3-C2-N1	-7.19	123.22	128.87
2	A	503	AMP	N3-C2-N1	-6.93	123.43	128.87
2	A	502	AMP	C2'-C1'-N9	-2.16	107.69	113.47
2	A	502	AMP	O2P-P-O5'	-2.11	100.58	106.72
2	A	502	AMP	C2-N1-C6	2.07	122.46	118.77
2	A	501	AMP	C2'-C1'-N9	2.25	119.48	113.47
2	A	503	AMP	O2P-P-O1P	2.37	118.35	110.63
2	A	502	AMP	O3P-P-O1P	2.63	119.21	110.63
2	A	501	AMP	C4'-O4'-C1'	3.69	113.56	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	1	0
2	A	503	AMP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	314/393 (79%)	0.58	7 (2%) 65 59	39, 74, 121, 145	0
1	B	292/393 (74%)	0.95	32 (10%) 7 4	25, 76, 144, 160	0
All	All	606/786 (77%)	0.76	39 (6%) 23 17	25, 74, 139, 160	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	251	HIS	6.2
1	B	406	ARG	6.2
1	B	336	PHE	5.8
1	B	250	LEU	5.6
1	B	249	LYS	5.2
1	B	235	LEU	4.8
1	B	211	VAL	4.5
1	B	233	LYS	4.3
1	B	413	ASN	4.1
1	B	290	ARG	3.8
1	B	407	PHE	3.7
1	A	406	ARG	3.5
1	B	355	GLU	3.4
1	B	236	PRO	3.3
1	B	231	LYS	3.3
1	B	363	TYR	3.3
1	B	208	ARG	3.2
1	A	301	ARG	3.0
1	B	238	PHE	3.0
1	B	272	ALA	2.7
1	A	400	PRO	2.7
1	B	212	HIS	2.7
1	A	402	GLN	2.6
1	B	245	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	243	PHE	2.5
1	B	261	LEU	2.4
1	B	400	PRO	2.4
1	B	44	SER	2.4
1	B	264	LEU	2.3
1	A	271	LEU	2.3
1	B	213	ARG	2.3
1	A	338	GLY	2.3
1	B	215	TYR	2.3
1	B	268	VAL	2.2
1	B	287	ASP	2.1
1	B	339	PRO	2.1
1	B	284	GLY	2.1
1	B	279	TYR	2.0
1	A	298	VAL	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(Å <sup>2</sup> )	Q<0.9
2	AMP	A	501	23/23	0.78	0.26	0.63	84,142,184,195	0
2	AMP	A	503	23/23	0.95	0.21	-0.22	58,76,92,94	0
2	AMP	A	502	23/23	0.93	0.21	-0.68	66,84,102,109	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.