



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:42 PM GMT

PDB ID : 3X09
Title : Crystal structure of PIP4KIIBETA F205L complex with AMP
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Deposited on : 2014-10-09
Resolution : 2.70 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 ⓘ symbol.

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AMP	A	501	-	-	-	X
2	AMP	B	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5274 atoms, of which 46 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	315	Total	C	N	O	S	0	0	0
			2592	1648	442	488	14			
1	B	305	Total	C	N	O	S	0	0	0
			2508	1603	431	461	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	205	LEU	PHE	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	205	LEU	PHE	ENGINEERED MUTATION	UNP P78356

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total 33	C 10	H 10	N 5	O 7	P 1	0	0
2	A	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
2	A	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0
2	B	1	Total 35	C 10	H 12	N 5	O 7	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	13	Total	O	0	0
			13	13		

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.

- [illegible]

- Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	108.27Å 183.42Å 107.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.64 – 2.70 70.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.64-2.70) 99.5 (70.37-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.203 , 0.260 0.209 , 0.263	Depositor DCC
R_{free} test set	1478 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.4	EDS
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.020 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 29563 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5274	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.45	0/2643	0.62	0/3554
1	B	0.44	0/2559	0.59	0/3439
All	All	0.45	0/5202	0.60	0/6993

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	2592	0	2563	104	0
1	B	2508	0	2490	149	0
2	A	69	34	36	3	0
2	B	23	12	12	3	0
3	A	23	0	0	3	0
3	B	13	0	0	1	0
All	All	5228	46	5101	248	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 24.

All (248) 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:218:LYS:HE2	1:B:403:TYR:OH	1.43	1.18
1:B:225:GLU:HG2	1:B:241:ASN:HB2	1.25	1.14
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.31	1.11
1:A:42:ILE:H	1:A:42:ILE:HD12	1.22	1.01
1:B:222:VAL:HG12	1:B:223:ALA:H	1.28	0.97
1:A:77:ILE:HD11	1:B:77:ILE:CD1	1.95	0.97
1:B:94:LYS:HB2	1:B:190:THR:HB	1.45	0.96
1:B:222:VAL:HG12	1:B:223:ALA:N	1.80	0.96
1:A:138:ARG:HH11	1:A:138:ARG:HG2	1.30	0.93
1:B:110:PHE:CE2	1:B:182:GLN:HG2	2.04	0.92
1:A:155:GLU:N	1:A:155:GLU:OE2	2.05	0.90
1:B:179:LEU:HG	1:B:263:LYS:HG2	1.53	0.89
1:B:218:LYS:HZ3	1:B:278:ASP:HA	1.35	0.89
1:A:415:LEU:O	1:A:416:THR:HG23	1.75	0.87
1:A:77:ILE:CD1	1:B:77:ILE:HD11	2.04	0.87
1:B:222:VAL:CG1	1:B:223:ALA:H	1.88	0.86
1:B:218:LYS:CE	1:B:278:ASP:C	2.44	0.86
1:B:218:LYS:NZ	1:B:278:ASP:HA	1.91	0.84
1:B:139:PHE:O	1:B:139:PHE:CD2	2.29	0.84
1:B:258:LYS:O	1:B:262:GLU:HG2	1.77	0.83
1:B:218:LYS:HE2	1:B:403:TYR:HH	1.38	0.82
1:A:204:VAL:HG23	2:A:501:AMP:C6	2.14	0.82
1:B:139:PHE:O	1:B:139:PHE:HD2	1.61	0.82
1:A:166:LYS:HD2	1:A:274:LEU:HD21	1.61	0.81
1:B:215:TYR:HB3	1:B:217:LEU:HD21	1.61	0.80
1:B:225:GLU:CG	1:B:241:ASN:HB2	2.08	0.80
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.45	0.80
1:B:78:LYS:HD2	1:B:94:LYS:HE2	1.63	0.80
1:A:138:ARG:HH11	1:A:138:ARG:CG	1.94	0.80
1:B:268:VAL:HG12	1:B:404:SER:HB2	1.63	0.80
1:A:42:ILE:CD1	1:A:42:ILE:H	1.95	0.79
1:B:252:VAL:CG1	1:B:256:SER:HB2	2.10	0.79
1:B:118:GLN:O	1:B:122:THR:HB	1.82	0.79
1:B:218:LYS:HG2	1:B:403:TYR:OH	1.82	0.79
1:B:218:LYS:CE	1:B:403:TYR:OH	2.29	0.78
1:A:42:ILE:N	1:A:42:ILE:HD12	1.98	0.78
1:B:219:GLY:O	1:B:406:ARG:HD3	1.83	0.77
1:A:67:MET:HA	1:A:67:MET:HE2	1.67	0.77
1:B:222:VAL:CG1	1:B:223:ALA:N	2.47	0.77
1:B:218:LYS:HE3	1:B:278:ASP:O	1.83	0.77
1:B:236:PRO:HG2	1:B:238:PHE:CE1	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:HB3	1:A:351:MET:CE	2.16	0.76
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.66	0.76
1:B:218:LYS:NZ	1:B:278:ASP:CA	2.50	0.74
1:B:277:MET:O	1:B:278:ASP:HB2	1.87	0.73
1:B:252:VAL:HG13	1:B:256:SER:HB2	1.69	0.73
1:B:34:LYS:NZ	1:B:122:THR:HG21	2.04	0.72
1:B:236:PRO:HG2	1:B:238:PHE:HE1	1.52	0.72
1:B:288:VAL:CG1	1:B:339:PRO:HB2	2.18	0.72
1:A:295:GLU:O	1:A:298:VAL:HG12	1.90	0.71
1:B:218:LYS:HE3	1:B:278:ASP:C	2.10	0.71
1:A:260:PHE:CD2	1:A:415:LEU:HD11	2.26	0.70
1:B:139:PHE:C	1:B:139:PHE:CD2	2.64	0.70
1:A:141:THR:HG22	1:A:142:THR:O	1.91	0.70
1:A:204:VAL:HG13	1:A:366:ALA:HB3	1.74	0.70
1:B:243:PHE:HE2	1:B:414:ILE:CG2	2.04	0.70
1:A:204:VAL:HG23	2:A:501:AMP:N6	2.07	0.70
1:A:67:MET:HA	1:A:67:MET:CE	2.22	0.69
1:B:46:LEU:HD21	1:B:149:ILE:HD13	1.72	0.69
1:B:240:ASP:N	1:B:240:ASP:OD1	2.19	0.68
1:A:140:LEU:HB2	1:A:149:ILE:HB	1.76	0.67
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.25	0.67
1:A:208:ARG:HH22	1:A:342:PHE:HA	1.61	0.66
1:A:399:ASN:HB3	1:A:400:PRO:CD	2.24	0.66
1:A:141:THR:CG2	1:A:142:THR:O	2.44	0.66
1:A:94:LYS:HB2	1:A:190:THR:HB	1.78	0.65
1:B:407:PHE:O	1:B:411:MET:HG2	1.97	0.65
1:A:218:LYS:HD2	1:A:403:TYR:OH	1.97	0.65
1:A:219:GLY:O	1:A:406:ARG:HD2	1.96	0.65
1:B:78:LYS:HD2	1:B:94:LYS:CE	2.26	0.65
1:A:349:TYR:CD1	1:A:366:ALA:HB2	2.32	0.65
1:B:268:VAL:CG1	1:B:404:SER:HB2	2.27	0.65
1:B:246:GLU:HG3	1:B:246:GLU:O	1.97	0.64
1:B:191:VAL:O	1:B:192:ASP:HB2	1.97	0.64
1:B:218:LYS:CE	1:B:278:ASP:O	2.44	0.63
1:B:243:PHE:CE2	1:B:414:ILE:CG2	2.81	0.63
1:B:254:GLU:HG2	1:B:258:LYS:HE3	1.79	0.63
1:B:37:ARG:HG2	1:B:88:ASN:OD1	1.98	0.63
1:B:120:SER:O	1:B:142:THR:HB	1.98	0.63
1:B:224:ARG:C	1:B:225:GLU:HG3	2.19	0.62
1:A:399:ASN:HB3	1:A:400:PRO:HD2	1.82	0.62
1:A:399:ASN:CB	1:A:400:PRO:CD	2.77	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LYS:HG2	1:A:279:TYR:O	2.00	0.61
1:B:240:ASP:HB3	1:B:410:PHE:CZ	2.36	0.61
1:B:205:LEU:HG	1:B:211:VAL:HG21	1.81	0.61
1:A:261:LEU:HD21	1:A:412:SER:HA	1.83	0.61
1:A:256:SER:HB3	1:A:351:MET:HE1	1.82	0.61
1:B:238:PHE:HB3	1:B:242:ASP:HB2	1.82	0.60
1:B:218:LYS:CE	1:B:278:ASP:HA	2.31	0.60
1:A:242:ASP:O	1:A:246:GLU:HG2	2.01	0.60
1:B:213:ARG:NH2	1:B:246:GLU:OE1	2.33	0.60
1:A:66:LEU:O	1:A:67:MET:HE2	2.00	0.60
1:A:206:SER:HB2	1:A:364:PHE:CE2	2.37	0.60
1:A:415:LEU:O	1:A:416:THR:CG2	2.47	0.59
1:B:244:LEU:HD11	1:B:410:PHE:HE1	1.67	0.59
1:B:230:GLU:O	1:B:233:LYS:HG2	2.02	0.59
1:B:206:SER:HB2	1:B:364:PHE:CE2	2.38	0.59
1:A:43:LEU:HD21	1:A:140:LEU:HD11	1.85	0.58
1:A:277:MET:O	1:A:278:ASP:HB2	2.03	0.58
1:B:166:LYS:HD2	1:B:274:LEU:HD21	1.85	0.58
1:A:138:ARG:NH1	1:A:138:ARG:CG	2.60	0.58
1:A:224:ARG:O	1:A:241:ASN:OD1	2.22	0.57
1:B:204:VAL:HG23	2:B:501:AMP:C6	2.39	0.57
1:B:218:LYS:CE	1:B:278:ASP:CA	2.83	0.57
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.34	0.56
1:A:51:ASN:HB2	1:A:122:THR:HG21	1.87	0.56
1:B:236:PRO:CG	1:B:238:PHE:CE1	2.88	0.56
1:B:224:ARG:CZ	1:B:239:LYS:HD3	2.37	0.55
1:B:204:VAL:HG23	2:B:501:AMP:N1	2.21	0.55
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.87	0.55
1:B:399:ASN:N	1:B:400:PRO:CD	2.69	0.54
1:A:127:ILE:O	1:A:127:ILE:HG12	2.08	0.54
1:B:218:LYS:HZ3	1:B:278:ASP:CA	2.12	0.54
1:B:34:LYS:HZ3	1:B:122:THR:HG21	1.70	0.54
1:B:34:LYS:HD3	1:B:122:THR:HG23	1.90	0.53
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.38	0.53
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.44	0.53
1:B:355:GLU:N	1:B:355:GLU:OE2	2.42	0.53
1:B:204:VAL:HA	1:B:349:TYR:CD2	2.43	0.53
1:A:241:ASN:O	1:A:245:ASN:HB2	2.08	0.53
1:B:60:VAL:O	1:B:104:ARG:NH2	2.37	0.52
1:A:128:ASN:HB3	1:A:140:LEU:HD23	1.90	0.52
1:B:34:LYS:CE	1:B:122:THR:HG21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:HH2	1:B:77:ILE:HD13	1.74	0.52
1:B:140:LEU:HB2	1:B:149:ILE:HB	1.91	0.52
1:B:189:LEU:N	1:B:189:LEU:HD12	2.24	0.52
1:B:81:ASN:O	1:B:91:SER:HB3	2.10	0.52
1:A:268:VAL:CG1	1:A:404:SER:HA	2.40	0.51
1:B:227:SER:OG	1:B:230:GLU:HB2	2.10	0.51
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.91	0.51
1:B:218:LYS:HE2	1:B:278:ASP:C	2.30	0.51
1:A:234:ASP:O	1:A:236:PRO:HD3	2.11	0.51
1:A:371:LEU:O	1:A:372:THR:CB	2.58	0.51
1:B:166:LYS:HD2	1:B:274:LEU:CD2	2.41	0.50
1:A:343:ASP:OD2	1:A:345:SER:OG	2.26	0.50
1:B:218:LYS:CG	1:B:403:TYR:OH	2.56	0.50
1:B:256:SER:HB3	1:B:351:MET:CE	2.42	0.50
1:B:224:ARG:O	1:B:225:GLU:HG3	2.12	0.50
1:A:204:VAL:HG23	2:A:501:AMP:N1	2.27	0.49
1:B:215:TYR:CB	1:B:217:LEU:HD21	2.36	0.49
1:A:204:VAL:CG1	1:A:366:ALA:HB3	2.40	0.49
1:B:34:LYS:CE	1:B:122:THR:CG2	2.90	0.49
1:B:281:LEU:HD12	1:B:282:LEU:N	2.27	0.49
1:A:274:LEU:O	1:A:275:LYS:HB2	2.12	0.49
1:A:141:THR:CG2	1:A:142:THR:N	2.76	0.49
1:A:256:SER:HB3	1:A:351:MET:HE2	1.94	0.49
1:B:189:LEU:N	1:B:189:LEU:CD1	2.76	0.48
1:A:185:GLY:HA2	3:A:603:HOH:O	2.13	0.48
1:A:109:ARG:NH1	1:A:172:VAL:HG22	2.29	0.48
1:B:218:LYS:NZ	1:B:278:ASP:C	2.66	0.48
1:A:128:ASN:C	1:A:128:ASN:HD22	2.17	0.48
1:A:77:ILE:HG22	1:A:95:PHE:HB3	1.95	0.48
1:B:99:CYS:N	1:B:100:PRO:CD	2.77	0.48
1:A:250:LEU:HD22	1:A:363:TYR:CE2	2.49	0.47
1:B:354:HIS:ND1	1:B:356:SER:HB2	2.29	0.47
1:B:254:GLU:CG	1:B:258:LYS:HE3	2.42	0.47
1:B:43:LEU:HD21	1:B:140:LEU:CD1	2.44	0.47
1:A:357:SER:OG	1:A:358:PRO:HD2	2.14	0.47
1:B:218:LYS:HE2	1:B:278:ASP:HA	1.94	0.47
1:A:204:VAL:HG13	1:A:366:ALA:CB	2.43	0.47
1:A:141:THR:HG23	1:A:145:ARG:HA	1.97	0.47
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.44	0.47
1:B:225:GLU:HA	1:B:239:LYS:HB2	1.97	0.47
1:B:289:ASP:O	1:B:292:GLU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:NH2	1:B:239:LYS:HD3	2.31	0.46
1:B:411:MET:O	1:B:414:ILE:HG12	2.15	0.46
1:B:181:PRO:HG2	1:B:370:ILE:HG12	1.96	0.46
1:B:256:SER:O	1:B:260:PHE:HB3	2.16	0.46
1:B:113:ASP:HB3	1:B:116:ASP:OD1	2.16	0.46
1:A:219:GLY:O	1:A:406:ARG:CD	2.62	0.46
1:B:230:GLU:HA	1:B:233:LYS:HD3	1.98	0.46
1:B:79:VAL:O	1:B:92:ARG:HA	2.15	0.46
1:B:243:PHE:CE1	1:B:248:GLN:HB3	2.51	0.45
1:B:233:LYS:CB	1:B:233:LYS:NZ	2.79	0.45
1:A:56:GLU:HG2	3:A:621:HOH:O	2.16	0.45
1:B:57:LEU:O	1:B:104:ARG:NH2	2.50	0.45
1:B:256:SER:HB3	1:B:351:MET:HE2	1.98	0.45
1:B:110:PHE:CZ	1:B:182:GLN:HG2	2.47	0.45
1:A:166:LYS:CD	1:A:274:LEU:HD21	2.40	0.44
1:B:215:TYR:HB3	1:B:217:LEU:CD2	2.41	0.44
1:B:37:ARG:HD3	1:B:88:ASN:OD1	2.17	0.44
1:A:160:MET:O	1:A:164:LEU:HB2	2.16	0.44
1:A:67:MET:HE1	1:A:68:PRO:HD3	1.99	0.44
1:B:96:LYS:HB3	1:B:188:ARG:HB3	1.98	0.44
1:A:43:LEU:O	1:A:47:MET:HG3	2.17	0.44
1:B:104:ARG:HA	1:B:107:ARG:NH1	2.33	0.44
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.84	0.44
1:B:218:LYS:NZ	1:B:278:ASP:O	2.49	0.44
1:A:138:ARG:CB	1:A:138:ARG:NH1	2.81	0.44
1:A:35:LEU:HB3	1:A:88:ASN:ND2	2.33	0.44
1:A:160:MET:CE	1:A:164:LEU:HD13	2.47	0.44
1:B:218:LYS:HG3	1:B:279:TYR:O	2.17	0.44
1:A:218:LYS:HE2	1:A:224:ARG:CZ	2.48	0.43
1:B:159:GLU:O	1:B:162:ASN:HB3	2.18	0.43
1:A:103:PHE:HA	1:A:106:LEU:HB2	2.00	0.43
1:A:251:HIS:O	1:A:353:SER:HA	2.17	0.43
1:B:216:ASP:C	1:B:217:LEU:HD23	2.38	0.43
1:B:251:HIS:HB2	1:B:357:SER:HB2	1.99	0.43
1:A:74:TYR:C	1:A:74:TYR:CD1	2.92	0.43
1:B:219:GLY:N	1:B:240:ASP:OD2	2.52	0.43
1:A:190:THR:HA	1:A:194:VAL:O	2.19	0.43
1:B:371:LEU:O	1:B:372:THR:HG23	2.18	0.43
1:B:225:GLU:HB3	1:B:242:ASP:OD1	2.19	0.43
1:A:186:MET:HG3	1:A:199:VAL:HG22	2.00	0.43
1:A:63:PRO:HB2	1:A:65:MET:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HD12	1:B:79:VAL:HG22	2.01	0.43
1:A:179:LEU:HG	1:A:263:LYS:HB3	2.00	0.43
1:B:204:VAL:HA	1:B:349:TYR:HD2	1.83	0.43
1:B:157:VAL:O	1:B:161:HIS:HD2	2.01	0.43
1:A:218:LYS:HB3	1:A:403:TYR:OH	2.19	0.43
1:B:233:LYS:NZ	1:B:233:LYS:HB3	2.34	0.42
1:B:207:HIS:CE1	1:B:346:VAL:HG11	2.53	0.42
1:B:36:PHE:HD1	1:B:47:MET:HB3	1.84	0.42
1:B:34:LYS:HE2	1:B:122:THR:CG2	2.48	0.42
1:B:64:VAL:HG23	1:B:65:MET:HG2	2.01	0.42
1:A:43:LEU:CD2	1:A:140:LEU:HD11	2.50	0.42
1:A:268:VAL:HG13	1:A:279:TYR:OH	2.20	0.42
2:B:501:AMP:N6	3:B:611:HOH:O	2.52	0.42
1:A:48:TRP:HB2	1:A:89:LEU:HD21	2.01	0.42
1:B:224:ARG:O	1:B:225:GLU:CG	2.67	0.42
1:A:276:ILE:HG22	1:A:277:MET:N	2.35	0.42
1:B:218:LYS:HE2	1:B:278:ASP:CA	2.50	0.42
1:A:206:SER:HB2	1:A:364:PHE:CZ	2.55	0.42
1:A:243:PHE:HZ	1:A:414:ILE:HG23	1.85	0.41
1:A:141:THR:HG23	1:A:142:THR:N	2.34	0.41
1:B:37:ARG:CG	1:B:88:ASN:OD1	2.66	0.41
1:B:233:LYS:HG2	1:B:233:LYS:H	1.53	0.41
1:B:121:VAL:O	1:B:121:VAL:HG12	2.19	0.41
1:A:110:PHE:CE1	1:A:182:GLN:HB3	2.55	0.41
1:B:244:LEU:HD11	1:B:410:PHE:CE1	2.52	0.41
1:B:213:ARG:CZ	1:B:246:GLU:OE1	2.68	0.41
1:A:153:SER:O	1:A:157:VAL:HG23	2.20	0.41
1:B:267:ASP:O	1:B:270:PHE:HB3	2.21	0.41
1:B:288:VAL:HG12	1:B:339:PRO:HB2	1.98	0.41
1:A:283:VAL:HG22	1:A:365:MET:HG2	2.02	0.41
1:A:109:ARG:HG2	3:A:610:HOH:O	2.21	0.41
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.51	0.41
1:A:209:LEU:HD23	1:A:209:LEU:N	2.36	0.41
1:A:60:VAL:HA	1:A:61:PRO:HD2	1.88	0.41
1:A:82:HIS:HB2	1:B:74:TYR:CZ	2.56	0.40
1:B:257:LYS:O	1:B:261:LEU:HG	2.20	0.40
1:A:219:GLY:O	1:A:406:ARG:NE	2.54	0.40
1:B:358:PRO:O	1:B:360:LYS:N	2.54	0.40
1:B:150:LYS:HB2	1:B:150:LYS:HE3	1.88	0.40
1:B:124:SER:HB3	1:B:143:TYR:CD2	2.57	0.40
1:A:50:VAL:HG21	1:A:121:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ILE:HG22	1:B:277:MET:N	2.36	0.40
1:A:205:LEU:HD22	1:A:211:VAL:HG21	2.04	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	305/393 (78%)	285 (93%)	19 (6%)	1 (0%)	46	75
1	B	291/393 (74%)	274 (94%)	16 (6%)	1 (0%)	46	75
All	All	596/786 (76%)	559 (94%)	35 (6%)	2 (0%)	46	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLY
1	A	61	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	293/352 (83%)	276 (94%)	17 (6%)	25	52
1	B	282/352 (80%)	262 (93%)	20 (7%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	575/704 (82%)	538 (94%)	37 (6%)	22	47

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	42	ILE
1	A	67	MET
1	A	76	LYS
1	A	77	ILE
1	A	127	ILE
1	A	128	ASN
1	A	138	ARG
1	A	141	THR
1	A	149	ILE
1	A	214	LYS
1	A	224	ARG
1	A	234	ASP
1	A	240	ASP
1	A	298	VAL
1	A	356	SER
1	A	406	ARG
1	B	37	ARG
1	B	42	ILE
1	B	104	ARG
1	B	122	THR
1	B	123	ARG
1	B	128	ASN
1	B	138	ARG
1	B	139	PHE
1	B	178	THR
1	B	205	LEU
1	B	208	ARG
1	B	210	THR
1	B	224	ARG
1	B	230	GLU
1	B	233	LYS
1	B	240	ASP
1	B	280	SER
1	B	353	SER
1	B	355	GLU
1	B	401	GLU

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

Mol	Chain	Res	Type
1	A	408	ASN
1	B	115	GLN
1	B	128	ASN
1	B	161	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	1.01	1 (4%)	22,38,38	1.82	5 (22%)
2	AMP	A	502	-	22,25,25	1.04	1 (4%)	22,38,38	1.40	2 (9%)
2	AMP	A	503	-	22,25,25	0.98	1 (4%)	22,38,38	1.50	3 (13%)
2	AMP	B	501	-	22,25,25	0.92	1 (4%)	22,38,38	1.84	5 (22%)

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
2	AMP	A	503	-	-	0/6/26/26	0/3/3/3
2	AMP	B	501	-	-	0/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	AMP	C5-C4	2.89	1.47	1.40
2	B	501	AMP	C5-C4	3.03	1.47	1.40
2	A	502	AMP	C5-C4	3.37	1.48	1.40
2	A	501	AMP	C5-C4	3.54	1.48	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	N3-C2-N1	-6.66	123.64	128.87
2	A	501	AMP	N3-C2-N1	-6.14	124.04	128.87
2	A	503	AMP	N3-C2-N1	-5.44	124.60	128.87
2	A	502	AMP	N3-C2-N1	-4.79	125.11	128.87
2	B	501	AMP	O3P-P-O5'	-2.51	99.40	106.72
2	A	501	AMP	O3P-P-O5'	-2.40	99.73	106.72
2	B	501	AMP	C1'-N9-C4	-2.04	124.53	126.81
2	A	502	AMP	O2P-P-O1P	2.17	117.70	110.63
2	A	501	AMP	N6-C6-N1	2.17	122.16	118.52
2	A	501	AMP	C2-N1-C6	2.19	122.67	118.77
2	A	501	AMP	O2P-P-O1P	2.30	118.14	110.63
2	B	501	AMP	O2P-P-O1P	2.31	118.17	110.63
2	A	503	AMP	N6-C6-N1	2.32	122.41	118.52
2	B	501	AMP	N6-C6-N1	2.36	122.48	118.52
2	A	503	AMP	O2P-P-O1P	2.45	118.62	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	AMP	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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	315/393 (80%)	0.51	4 (1%) 79 79	37, 69, 122, 144	0
1	B	305/393 (77%)	0.78	25 (8%) 14 11	39, 74, 137, 161	0
All	All	620/786 (78%)	0.64	29 (4%) 35 34	37, 71, 134, 161	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	TYR	4.5
1	B	238	PHE	4.3
1	B	415	LEU	4.2
1	B	336	PHE	3.9
1	B	254	GLU	3.7
1	B	211	VAL	3.6
1	B	363	TYR	3.6
1	B	251	HIS	3.5
1	B	219	GLY	3.3
1	B	233	LYS	3.2
1	B	236	PRO	3.2
1	B	218	LYS	3.1
1	B	223	ALA	3.1
1	B	249	LYS	3.1
1	B	258	LYS	2.9
1	B	407	PHE	2.7
1	A	302	ALA	2.6
1	A	340	GLY	2.4
1	B	255	GLU	2.4
1	A	274	LEU	2.3
1	B	416	THR	2.3
1	B	35	LEU	2.3
1	B	179	LEU	2.2
1	B	413	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	230	GLU	2.2
1	B	406	ARG	2.2
1	A	249	LYS	2.1
1	B	231	LYS	2.1
1	B	235	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	AMP	B	501	23/23	0.83	0.43	3.54	118,147,189,194	0
2	AMP	A	501	23/23	0.89	0.35	2.28	64,140,183,194	0
2	AMP	A	502	23/23	0.95	0.19	-0.71	53,69,83,91	0
2	AMP	A	503	23/23	0.95	0.18	-0.93	52,71,87,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.