Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 06:43 PM GMT

PDB ID	:	3X01
Title	:	Crystal structure of PIP4KIIBETA complex with AMP
Authors	:	Takeuchi, K.; Lo, Y.H.; Sumita, K.; Senda, M.; Terakawa, J.; Dimitoris, A.; Locasale, J.W.; Sasaki, M.; Yoshino, H.; Zhang, Y.; Kahoud, E.R.; Takano, T.; Yokota, T.; Emerling, B.; Asara, J.A.; Ishida, T.; Shimada, I.; Daikoku, T.; Cantley, L.C.; Senda, T.; Sasaki, A.T.
Deposited on	:	2014-10-09
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

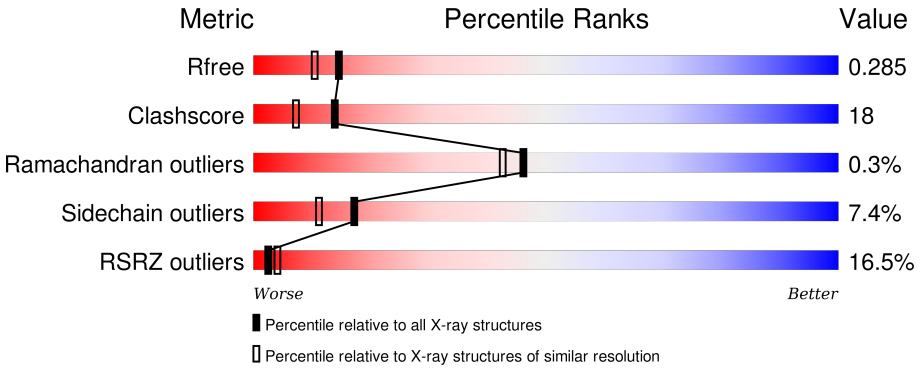
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	9% 55% 22% · 20%
1	B	393	17% 52% 20% · 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5309 atoms, of which 48 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.

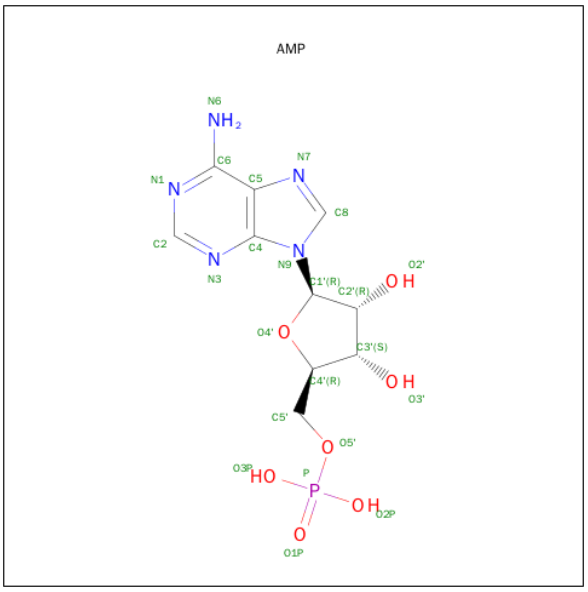
- Molecule 1 is a protein called Phosphatidylinositol 5-phosphate 4-kinase type-2 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2595	1651	442	488	14			
1	B	298	Total	C	N	O	S	0	0	0
			2468	1583	423	449	13			

There are 14 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
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

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



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		
2	B	1	Total	C	H	N	O	P	0	0
			35	10	12	5	7	1		

- Molecule 3 is water.

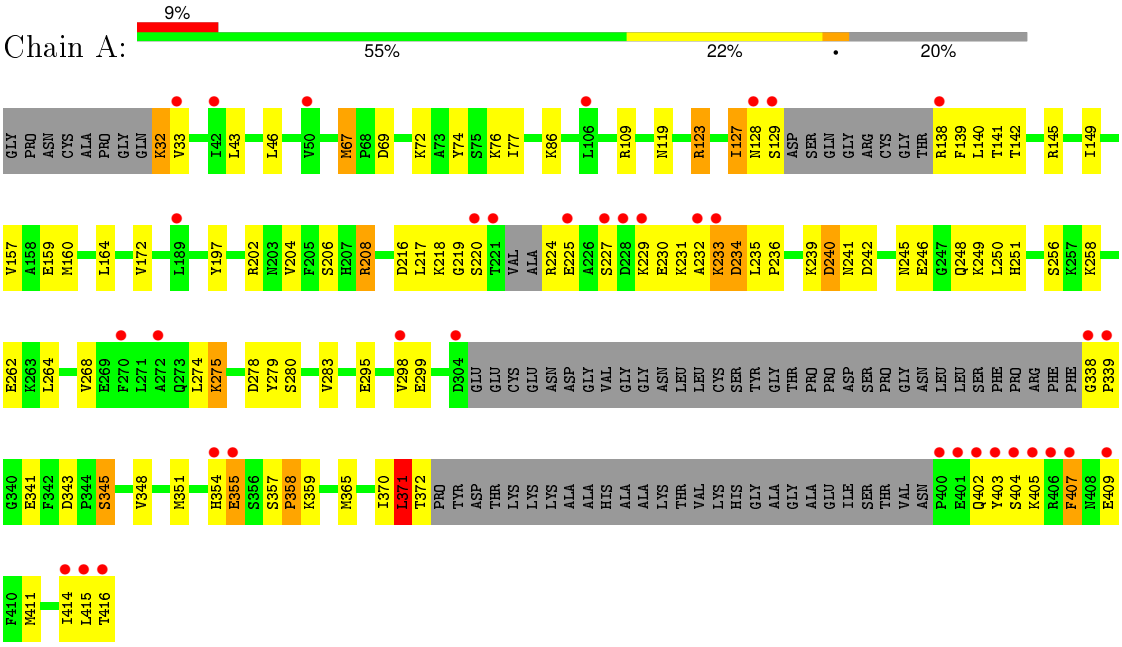
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	51	Total	O	0	0
			51	51		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

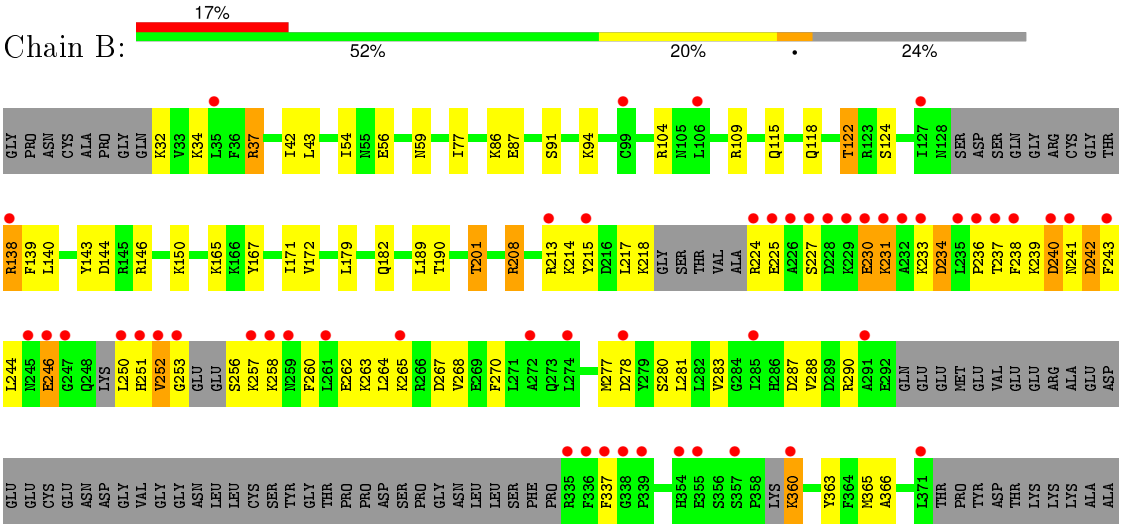
- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta

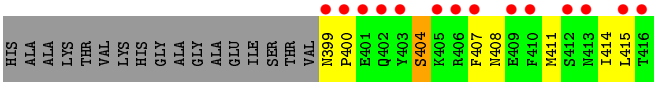
Chain A:



- Molecule 1: Phosphatidylinositol 5-phosphate 4-kinase type-2 beta

Chain B:




HIS
ALA
ALA
LYS
THR
VAL
LYS
HIS
GLY
ALA
GLY
ALA
GLU
ILE
SER
THR
VAL
N399
P400
E401
Q402
Y403
S404
K405
R406
F407
N408
E409
F410
M411
S412
N413
T414
L415
T416

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	108.39Å 181.79Å 107.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 – 2.15 70.41 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.40-2.15) 98.0 (70.41-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.14Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, R_{free}	0.246 , 0.279 0.248 , 0.285	Depositor DCC
R_{free} test set	2844 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 62.2	EDS
Estimated twinning fraction	0.005 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.016 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 56894 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5309	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	0.60	1/2647 (0.0%)	0.60	1/3556 (0.0%)
1	B	0.51	0/2519	0.55	0/3382
All	All	0.56	1/5166 (0.0%)	0.58	1/6938 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	SER	C-O	-5.50	1.12	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	371	LEU	N-CA-C	-5.59	95.90	111.00

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	2595	0	2565	95	0
1	B	2468	0	2449	99	0
2	A	69	36	36	5	0
2	B	23	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	55	0	0	2	0
3	B	51	0	0	0	0
All	All	5261	48	5062	188	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 18.

All (188) 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:138:ARG:HH11	1:B:138:ARG:CG	1.60	1.14
1:A:77:ILE:HD11	1:B:77:ILE:HD11	1.16	1.13
1:A:77:ILE:HD11	1:B:77:ILE:CD1	1.79	1.11
1:A:77:ILE:CD1	1:B:77:ILE:HD11	1.81	1.09
1:B:138:ARG:HG2	1:B:138:ARG:HH11	0.97	1.08
1:A:256:SER:HB3	1:A:351:MET:HE2	1.41	1.02
1:A:256:SER:HB3	1:A:351:MET:CE	1.93	0.98
1:B:37:ARG:HH11	1:B:37:ARG:HG2	1.25	0.97
1:A:372:THR:HG22	1:A:372:THR:O	1.63	0.96
1:A:268:VAL:HG12	1:A:404:SER:HB2	1.47	0.95
1:A:217:LEU:HD13	1:A:414:ILE:HD11	1.48	0.94
1:B:250:LEU:HD22	1:B:363:TYR:CD2	2.06	0.89
1:B:138:ARG:HG2	1:B:138:ARG:NH1	1.77	0.88
1:B:268:VAL:HG13	1:B:404:SER:HB2	1.56	0.87
1:A:129:SER:OG	1:A:138:ARG:CG	2.23	0.85
1:B:337:PHE:O	1:B:337:PHE:CD1	2.30	0.85
1:B:260:PHE:CD2	1:B:415:LEU:HD11	2.12	0.84
1:A:229:LYS:O	1:A:232:ALA:HB3	1.80	0.81
1:A:217:LEU:CD1	1:A:414:ILE:HD11	2.10	0.81
1:A:127:ILE:CG2	1:A:128:ASN:N	2.44	0.81
1:B:225:GLU:HG3	1:B:241:ASN:HB2	1.62	0.81
1:A:141:THR:HG22	1:A:142:THR:O	1.81	0.80
1:A:343:ASP:OD2	1:A:345:SER:HB3	1.82	0.80
1:A:357:SER:OG	1:A:358:PRO:HD2	1.82	0.80
1:B:138:ARG:CB	1:B:138:ARG:NH1	2.48	0.77
1:A:234:ASP:O	1:A:236:PRO:HD3	1.86	0.76
1:B:337:PHE:O	1:B:337:PHE:HD1	1.69	0.75
1:A:218:LYS:HG2	1:A:403:TYR:OH	1.87	0.74
1:B:37:ARG:CG	1:B:37:ARG:HH11	2.01	0.74
1:B:138:ARG:NH1	1:B:138:ARG:CG	2.30	0.74
1:A:32:LYS:HG3	1:A:33:VAL:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASP:OD1	1:B:290:ARG:HB2	1.88	0.74
1:A:227:SER:O	1:A:231:LYS:HG3	1.88	0.74
1:B:253:GLY:O	1:B:256:SER:N	2.22	0.73
1:B:138:ARG:CB	1:B:138:ARG:HH11	2.02	0.73
1:B:213:ARG:HH12	1:B:246:GLU:HG3	1.54	0.73
1:B:258:LYS:O	1:B:262:GLU:HG2	1.90	0.72
1:A:268:VAL:CG1	1:A:404:SER:HB2	2.19	0.72
1:B:268:VAL:CG1	1:B:404:SER:HB2	2.21	0.70
1:B:288:VAL:HG21	1:B:360:LYS:HG2	1.73	0.70
1:A:127:ILE:HG22	1:A:128:ASN:N	2.06	0.70
1:A:372:THR:CG2	1:A:372:THR:O	2.34	0.70
1:A:127:ILE:HG22	1:A:128:ASN:HB2	1.73	0.70
1:A:109:ARG:CZ	1:A:172:VAL:HG22	2.22	0.70
1:A:32:LYS:HG3	1:A:33:VAL:H	1.58	0.69
1:B:213:ARG:NH1	1:B:246:GLU:HG3	2.07	0.69
1:A:208:ARG:HB3	1:A:208:ARG:HH11	1.57	0.69
1:B:233:LYS:O	1:B:236:PRO:HD3	1.91	0.68
1:A:129:SER:OG	1:A:138:ARG:HG3	1.93	0.68
1:A:338:GLY:HA3	1:A:341:GLU:OE1	1.93	0.67
1:A:218:LYS:HD2	1:A:224:ARG:CZ	2.25	0.67
1:A:241:ASN:O	1:A:245:ASN:HB2	1.97	0.65
1:B:37:ARG:NH1	1:B:37:ARG:HG2	2.06	0.65
1:B:243:PHE:CE2	1:B:414:ILE:HG22	2.31	0.65
1:B:234:ASP:N	1:B:234:ASP:OD1	2.30	0.64
1:A:208:ARG:NH1	1:A:208:ARG:HB3	2.13	0.64
1:B:250:LEU:CD2	1:B:363:TYR:CD2	2.81	0.63
1:A:141:THR:HG23	1:A:145:ARG:HA	1.78	0.63
1:A:127:ILE:HG22	1:A:128:ASN:CB	2.28	0.63
1:A:67:MET:HA	1:A:67:MET:CE	2.29	0.62
1:A:407:PHE:CD2	1:A:407:PHE:O	2.52	0.62
1:A:407:PHE:CD2	1:A:407:PHE:C	2.72	0.62
1:A:129:SER:OG	1:A:138:ARG:HG2	1.98	0.62
1:A:32:LYS:HB2	1:A:32:LYS:NZ	2.15	0.62
1:B:260:PHE:HD2	1:B:415:LEU:HD11	1.60	0.61
1:A:415:LEU:O	1:A:416:THR:HG23	2.00	0.61
1:A:274:LEU:O	1:A:275:LYS:HB2	1.99	0.61
3:A:632:HOH:O	1:B:56:GLU:HG2	1.99	0.61
1:B:250:LEU:HD22	1:B:363:TYR:CE2	2.35	0.60
1:A:208:ARG:CB	1:A:208:ARG:HH11	2.14	0.60
1:A:217:LEU:CD1	1:A:414:ILE:CD1	2.78	0.60
1:B:118:GLN:O	1:B:122:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LYS:HG3	1:B:258:LYS:N	2.16	0.60
1:B:411:MET:O	1:B:414:ILE:HG12	2.01	0.60
1:A:242:ASP:O	1:A:246:GLU:HG2	2.01	0.60
1:A:219:GLY:N	1:A:240:ASP:OD2	2.34	0.60
1:B:250:LEU:CD2	1:B:363:TYR:CE2	2.85	0.59
1:A:141:THR:CG2	1:A:145:ARG:HA	2.31	0.59
1:B:214:LYS:HE3	1:B:237:THR:OG1	2.02	0.59
1:B:182:GLN:O	1:B:201:THR:HG22	2.03	0.59
1:B:231:LYS:HE3	1:B:238:PHE:HE2	1.67	0.59
1:A:67:MET:HA	1:A:67:MET:HE2	1.85	0.58
1:A:119:ASN:HB3	1:A:123:ARG:NH1	2.18	0.58
1:B:230:GLU:O	1:B:233:LYS:HG3	2.04	0.58
1:B:243:PHE:HE2	1:B:414:ILE:HG22	1.69	0.58
1:A:407:PHE:O	1:A:411:MET:HG2	2.04	0.57
1:A:230:GLU:O	1:A:233:LYS:HG3	2.05	0.57
1:B:265:LYS:HG3	1:B:408:ASN:HD21	1.70	0.56
1:B:37:ARG:CG	1:B:37:ARG:NH1	2.65	0.56
1:A:216:ASP:O	1:A:224:ARG:NH2	2.38	0.56
1:A:77:ILE:CG1	1:B:77:ILE:HD11	2.36	0.55
1:B:267:ASP:O	1:B:270:PHE:HB3	2.06	0.55
1:B:225:GLU:HG3	1:B:241:ASN:CB	2.35	0.55
1:B:144:ASP:OD2	1:B:146:ARG:HD2	2.07	0.54
1:A:248:GLN:O	1:A:249:LYS:HG2	2.08	0.54
1:A:139:PHE:HZ	2:A:501:AMP:C4	2.25	0.54
1:B:283:VAL:HG22	1:B:365:MET:HG2	1.89	0.54
1:A:46:LEU:HD21	1:A:149:ILE:HD13	1.90	0.53
1:B:213:ARG:HH12	1:B:246:GLU:CG	2.21	0.53
1:B:277:MET:O	1:B:278:ASP:HB2	2.08	0.53
1:B:208:ARG:NH2	1:B:337:PHE:CG	2.77	0.53
1:B:231:LYS:HE3	1:B:238:PHE:CE2	2.44	0.53
1:B:238:PHE:HD2	1:B:242:ASP:OD2	1.91	0.53
1:A:268:VAL:HG12	1:A:404:SER:CB	2.32	0.53
1:B:227:SER:OG	1:B:230:GLU:HB2	2.09	0.53
1:A:268:VAL:CG1	1:A:404:SER:CB	2.87	0.53
1:A:127:ILE:HG23	1:A:128:ASN:N	2.22	0.52
1:B:238:PHE:HB3	1:B:242:ASP:HB2	1.92	0.52
1:B:288:VAL:CG2	1:B:360:LYS:HG2	2.39	0.52
1:B:86:LYS:HE2	1:B:91:SER:OG	2.09	0.52
1:A:229:LYS:O	1:A:232:ALA:CB	2.54	0.52
1:B:43:LEU:HD21	1:B:140:LEU:HD11	1.91	0.51
1:B:109:ARG:CZ	1:B:172:VAL:HG22	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ASP:O	1:B:244:LEU:HG	2.11	0.51
1:A:370:ILE:HG13	1:A:370:ILE:O	2.10	0.51
1:A:249:LYS:C	1:A:250:LEU:HD23	2.32	0.50
1:B:281:LEU:HD12	1:B:366:ALA:O	2.12	0.50
1:A:69:ASP:O	1:A:72:LYS:HG2	2.12	0.50
1:B:268:VAL:CG1	1:B:404:SER:CB	2.90	0.50
1:B:257:LYS:CG	1:B:258:LYS:N	2.74	0.50
1:B:264:LEU:HD21	1:B:411:MET:HB2	1.93	0.49
1:A:43:LEU:HD21	1:A:140:LEU:HD11	1.95	0.49
1:B:231:LYS:CE	1:B:238:PHE:HE2	2.25	0.49
1:B:224:ARG:NH2	1:B:239:LYS:HE2	2.27	0.49
1:A:283:VAL:HG22	1:A:365:MET:HG2	1.93	0.49
1:A:231:LYS:HA	1:A:236:PRO:HB3	1.95	0.49
1:B:287:ASP:OD1	1:B:290:ARG:CB	2.60	0.49
1:A:69:ASP:HA	1:A:72:LYS:HD3	1.95	0.49
1:A:415:LEU:O	1:A:416:THR:CG2	2.60	0.49
1:B:260:PHE:HD2	1:B:415:LEU:CD1	2.25	0.49
1:B:94:LYS:HB2	1:B:190:THR:HB	1.94	0.48
1:A:358:PRO:HG2	1:A:359:LYS:H	1.78	0.48
1:B:138:ARG:NH1	1:B:138:ARG:HB3	2.26	0.48
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.69	0.48
1:B:224:ARG:HH21	1:B:239:LYS:NZ	2.12	0.48
1:B:42:ILE:HD11	1:B:189:LEU:HD22	1.94	0.48
1:B:230:GLU:O	1:B:236:PRO:HB3	2.12	0.48
1:B:208:ARG:NH2	1:B:337:PHE:CD1	2.82	0.48
1:B:139:PHE:CD1	1:B:139:PHE:O	2.67	0.48
1:A:234:ASP:C	1:A:236:PRO:HD3	2.34	0.48
1:A:264:LEU:HD11	1:A:407:PHE:HE2	1.78	0.47
1:B:242:ASP:N	1:B:242:ASP:OD1	2.47	0.47
1:B:218:LYS:HG3	1:B:224:ARG:NH1	2.29	0.47
1:A:157:VAL:HG21	1:A:197:TYR:CD2	2.50	0.47
1:A:233:LYS:H	1:A:233:LYS:HG3	1.52	0.46
1:A:139:PHE:CE1	2:A:501:AMP:C8	3.04	0.45
1:B:360:LYS:HE3	1:B:360:LYS:HB2	1.70	0.45
1:A:129:SER:OG	1:A:138:ARG:CD	2.65	0.45
1:A:139:PHE:CZ	2:A:501:AMP:C4	3.04	0.45
1:B:54:ILE:HG21	1:B:118:GLN:HB2	1.99	0.45
1:A:298:VAL:HG12	1:A:299:GLU:N	2.31	0.45
1:B:251:HIS:C	1:B:252:VAL:CG1	2.86	0.44
1:B:399:ASN:HB3	1:B:400:PRO:HD3	2.00	0.44
1:B:34:LYS:HE2	1:B:122:THR:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:TYR:CE1	1:B:243:PHE:HD1	2.36	0.44
1:A:256:SER:HB3	1:A:351:MET:HE1	1.89	0.44
1:B:225:GLU:HB3	1:B:242:ASP:OD1	2.18	0.43
1:A:354:HIS:O	1:A:355:GLU:C	2.55	0.43
1:B:138:ARG:CZ	1:B:138:ARG:CB	2.93	0.43
1:B:34:LYS:HE2	1:B:122:THR:HG23	1.99	0.43
1:B:165:LYS:HB2	1:B:165:LYS:HE2	1.90	0.43
1:A:86:LYS:HG2	3:A:609:HOH:O	2.19	0.43
1:A:77:ILE:HD11	1:B:77:ILE:CG1	2.47	0.42
1:B:260:PHE:CD2	1:B:415:LEU:CD1	2.94	0.42
1:A:33:VAL:HG13	1:B:59:ASN:HA	2.02	0.42
1:B:215:TYR:CD1	1:B:243:PHE:HD1	2.36	0.42
1:A:74:TYR:CE1	1:A:76:LYS:HD3	2.54	0.42
1:B:224:ARG:NH1	1:B:240:ASP:OD1	2.52	0.42
1:B:179:LEU:HG	1:B:263:LYS:HG2	2.01	0.42
1:A:140:LEU:HB2	1:A:149:ILE:HB	2.00	0.42
1:B:87:GLU:HA	1:B:87:GLU:OE1	2.19	0.42
1:A:258:LYS:HE3	1:A:262:GLU:OE2	2.19	0.42
1:A:127:ILE:HA	1:A:127:ILE:HD13	1.69	0.42
1:A:295:GLU:O	1:A:298:VAL:HB	2.20	0.42
1:A:139:PHE:HE1	2:A:501:AMP:C8	2.38	0.41
1:A:160:MET:O	1:A:164:LEU:HB2	2.19	0.41
1:A:354:HIS:ND1	1:A:355:GLU:N	2.69	0.41
1:A:159:GLU:OE2	1:A:371:LEU:HA	2.21	0.41
1:B:407:PHE:O	1:B:411:MET:HG2	2.20	0.41
1:A:239:LYS:O	1:A:242:ASP:HB2	2.20	0.41
1:A:204:VAL:HG23	2:A:501:AMP:C6	2.55	0.41
1:A:355:GLU:H	1:A:355:GLU:HG2	1.49	0.40
1:B:217:LEU:HB3	1:B:411:MET:CE	2.52	0.40
1:A:268:VAL:HG13	1:A:279:TYR:OH	2.21	0.40
1:B:124:SER:HB3	1:B:143:TYR:CG	2.56	0.40
1:B:167:TYR:O	1:B:171:ILE:HG12	2.21	0.40
1:A:268:VAL:CG1	1:A:404:SER:HA	2.51	0.40
1:B:250:LEU:HD23	1:B:363:TYR:CE2	2.57	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%)	295 (97%)	8 (3%)	2 (1%)	26 18
1	B	282/393 (72%)	274 (97%)	8 (3%)	0	100 100
All	All	587/786 (75%)	569 (97%)	16 (3%)	2 (0%)	46 42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	PRO
1	A	358	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%)	270 (92%)	23 (8%)	16 9
1	B	278/352 (79%)	259 (93%)	19 (7%)	20 13
All	All	571/704 (81%)	529 (93%)	42 (7%)	17 11

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	67	MET
1	A	123	ARG
1	A	127	ILE

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Mol	Chain	Res	Type
1	A	202	ARG
1	A	206	SER
1	A	208	ARG
1	A	220	SER
1	A	225	GLU
1	A	233	LYS
1	A	234	ASP
1	A	240	ASP
1	A	251	HIS
1	A	275	LYS
1	A	278	ASP
1	A	345	SER
1	A	348	VAL
1	A	355	GLU
1	A	371	LEU
1	A	402	GLN
1	A	405	LYS
1	A	407	PHE
1	A	409	GLU
1	B	32	LYS
1	B	37	ARG
1	B	104	ARG
1	B	115	GLN
1	B	122	THR
1	B	138	ARG
1	B	150	LYS
1	B	201	THR
1	B	208	ARG
1	B	230	GLU
1	B	231	LYS
1	B	234	ASP
1	B	240	ASP
1	B	242	ASP
1	B	246	GLU
1	B	252	VAL
1	B	280	SER
1	B	360	LYS
1	B	404	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	408	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	1.57	5 (22%)	22,38,38	2.03	3 (13%)
2	AMP	A	502	-	22,25,25	0.89	1 (4%)	22,38,38	1.89	3 (13%)
2	AMP	A	503	-	22,25,25	0.99	1 (4%)	22,38,38	2.10	6 (27%)
2	AMP	B	501	-	22,25,25	1.24	3 (13%)	22,38,38	2.13	1 (4%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	AMP	C2'-C1'	-3.39	1.48	1.53
2	A	501	AMP	C4-N3	-3.24	1.30	1.35
2	B	501	AMP	C5-N7	-2.39	1.30	1.39
2	A	501	AMP	C5-N7	-2.38	1.30	1.39
2	A	501	AMP	C2'-C3'	-2.10	1.47	1.53
2	B	501	AMP	C4-N3	-2.09	1.32	1.35
2	B	501	AMP	P-O3P	-2.01	1.47	1.54
2	A	501	AMP	O4'-C4'	-2.01	1.40	1.45
2	A	502	AMP	C5-C4	2.67	1.46	1.40
2	A	503	AMP	C5-C4	3.16	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	AMP	N3-C2-N1	-8.54	122.17	128.87
2	A	503	AMP	N3-C2-N1	-8.00	122.59	128.87
2	A	502	AMP	N3-C2-N1	-7.53	122.95	128.87
2	A	501	AMP	N3-C2-N1	-5.87	124.26	128.87
2	A	501	AMP	C1'-N9-C4	-3.87	122.48	126.81
2	A	501	AMP	O5'-P-O1P	-3.43	98.47	107.08
2	A	503	AMP	C1'-N9-C4	-2.38	124.15	126.81
2	A	503	AMP	O3P-P-O5'	-2.21	100.28	106.72
2	A	503	AMP	N6-C6-N1	2.05	121.96	118.52
2	A	502	AMP	C2-N1-C6	2.10	122.51	118.77
2	A	503	AMP	O2P-P-O1P	2.28	118.06	110.63
2	A	502	AMP	O2P-P-O1P	2.41	118.50	110.63
2	A	503	AMP	C2-N1-C6	2.54	123.30	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	AMP	5	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	315/393 (80%)	1.18	36 (11%) 7 11	30, 61, 111, 138	0
1	B	298/393 (75%)	1.42	65 (21%) 1 2	32, 66, 128, 144	0
All	All	613/786 (77%)	1.30	101 (16%) 2 4	30, 62, 122, 144	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PHE	7.4
1	B	236	PRO	6.6
1	A	221	THR	6.4
1	B	241	ASN	5.8
1	A	339	PRO	5.6
1	B	235	LEU	5.6
1	B	336	PHE	5.3
1	B	339	PRO	5.1
1	B	338	GLY	5.0
1	A	403	TYR	5.0
1	B	228	ASP	4.9
1	A	220	SER	4.9
1	B	229	LYS	4.7
1	B	215	TYR	4.7
1	A	228	ASP	4.6
1	B	405	LYS	4.6
1	B	230	GLU	4.5
1	B	291	ALA	4.5
1	A	405	LYS	4.5
1	B	415	LEU	4.4
1	B	245	ASN	4.3
1	B	213	ARG	4.3
1	B	258	LYS	4.2
1	B	399	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLU	4.0
1	B	243	PHE	4.0
1	B	238	PHE	3.9
1	B	224	ARG	3.8
1	B	138	ARG	3.7
1	A	338	GLY	3.7
1	A	402	GLN	3.7
1	B	253	GLY	3.7
1	B	259	ASN	3.5
1	A	128	ASN	3.5
1	A	416	THR	3.4
1	B	354	HIS	3.4
1	A	233	LYS	3.4
1	A	407	PHE	3.4
1	A	404	SER	3.3
1	B	407	PHE	3.2
1	B	227	SER	3.2
1	A	229	LYS	3.2
1	B	251	HIS	3.1
1	B	261	LEU	3.1
1	B	250	LEU	3.1
1	B	225	GLU	3.1
1	B	335	ARG	3.1
1	B	233	LYS	3.0
1	B	360	LYS	3.0
1	A	225	GLU	3.0
1	B	252	VAL	3.0
1	B	357	SER	3.0
1	B	355	GLU	2.9
1	B	246	GLU	2.8
1	B	265	LYS	2.8
1	B	35	LEU	2.7
1	B	240	ASP	2.7
1	B	278	ASP	2.6
1	A	401	GLU	2.6
1	A	33	VAL	2.6
1	A	138	ARG	2.6
1	B	226	ALA	2.6
1	B	127	ILE	2.5
1	A	409	GLU	2.5
1	A	400	PRO	2.4
1	B	232	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	231	LYS	2.4
1	B	274	LEU	2.4
1	A	189	LEU	2.3
1	B	406	ARG	2.3
1	B	412	SER	2.3
1	A	272	ALA	2.3
1	A	232	ALA	2.3
1	B	285	ILE	2.3
1	B	247	GLY	2.3
1	B	402	GLN	2.3
1	B	257	LYS	2.2
1	B	400	PRO	2.2
1	B	401	GLU	2.2
1	B	272	ALA	2.2
1	A	415	LEU	2.2
1	B	371	LEU	2.2
1	A	354	HIS	2.1
1	B	106	LEU	2.1
1	A	270	PHE	2.1
1	B	237	THR	2.1
1	A	304	ASP	2.1
1	A	106	LEU	2.1
1	A	406	ARG	2.1
1	A	129	SER	2.1
1	A	227	SER	2.1
1	A	50	VAL	2.1
1	A	298	VAL	2.1
1	B	416	THR	2.1
1	B	409	GLU	2.0
1	B	410	PHE	2.0
1	A	42	ILE	2.0
1	A	414	ILE	2.0
1	B	413	ASN	2.0
1	B	403	TYR	2.0
1	B	99	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	AMP	B	501	23/23	0.78	0.24	2.03	72,99,141,144	0
2	AMP	A	503	23/23	0.95	0.17	-0.34	33,45,56,56	0
2	AMP	A	501	23/23	0.85	0.17	-0.43	45,94,156,157	0
2	AMP	A	502	23/23	0.95	0.16	-1.28	42,53,66,73	0

6.5 Other polymers (i)

There are no such residues in this entry.