



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:49 AM GMT

PDB ID : 3Q4Z  
Title : Structure of unphosphorylated PAK1 kinase domain  
Authors : Wang, J.; Wu, J.-W.; Wang, Z.-X.  
Deposited on : 2010-12-26  
Resolution : 1.89 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

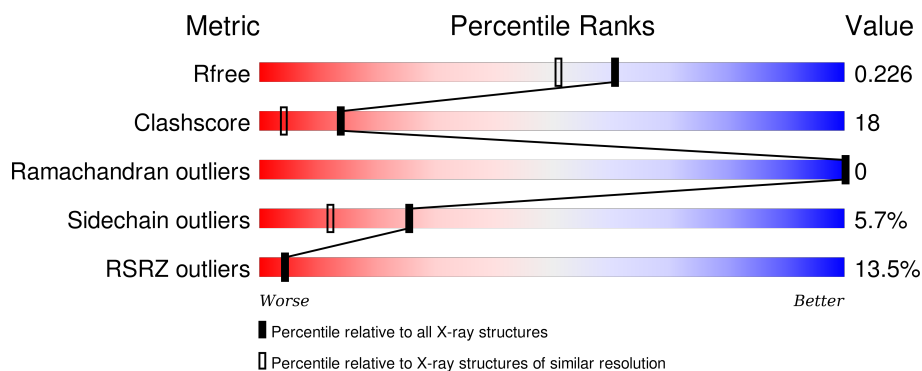
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	306	
1	B	306	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4670 atoms, of which 0 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 Serine/threonine-protein kinase PAK 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2218	1408	371	422	17			
1	B	279	Total	C	N	O	S	0	0	0
			2188	1389	367	417	15			

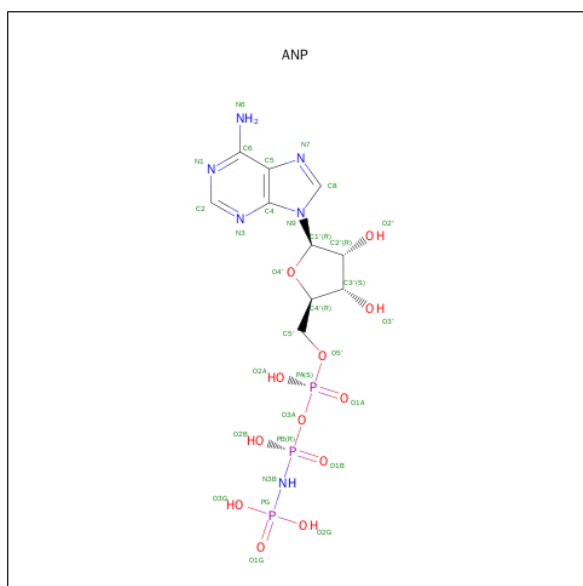
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	259	ILE	SER	ENGINEERED MUTATION	UNP Q13153
A	299	ARG	LYS	ENGINEERED MUTATION	UNP Q13153
A	389	ASN	ASP	ENGINEERED MUTATION	UNP Q13153
A	516	ILE	LEU	ENGINEERED MUTATION	UNP Q13153
A	546	LEU	-	EXPRESSION TAG	UNP Q13153
A	547	GLU	-	EXPRESSION TAG	UNP Q13153
A	548	HIS	-	EXPRESSION TAG	UNP Q13153
A	549	HIS	-	EXPRESSION TAG	UNP Q13153
A	550	HIS	-	EXPRESSION TAG	UNP Q13153
A	551	HIS	-	EXPRESSION TAG	UNP Q13153
A	552	HIS	-	EXPRESSION TAG	UNP Q13153
A	553	HIS	-	EXPRESSION TAG	UNP Q13153
B	259	ILE	SER	ENGINEERED MUTATION	UNP Q13153
B	299	ARG	LYS	ENGINEERED MUTATION	UNP Q13153
B	389	ASN	ASP	ENGINEERED MUTATION	UNP Q13153
B	516	ILE	LEU	ENGINEERED MUTATION	UNP Q13153
B	546	LEU	-	EXPRESSION TAG	UNP Q13153
B	547	GLU	-	EXPRESSION TAG	UNP Q13153
B	548	HIS	-	EXPRESSION TAG	UNP Q13153
B	549	HIS	-	EXPRESSION TAG	UNP Q13153
B	550	HIS	-	EXPRESSION TAG	UNP Q13153
B	551	HIS	-	EXPRESSION TAG	UNP Q13153
B	552	HIS	-	EXPRESSION TAG	UNP Q13153
B	553	HIS	-	EXPRESSION TAG	UNP Q13153

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

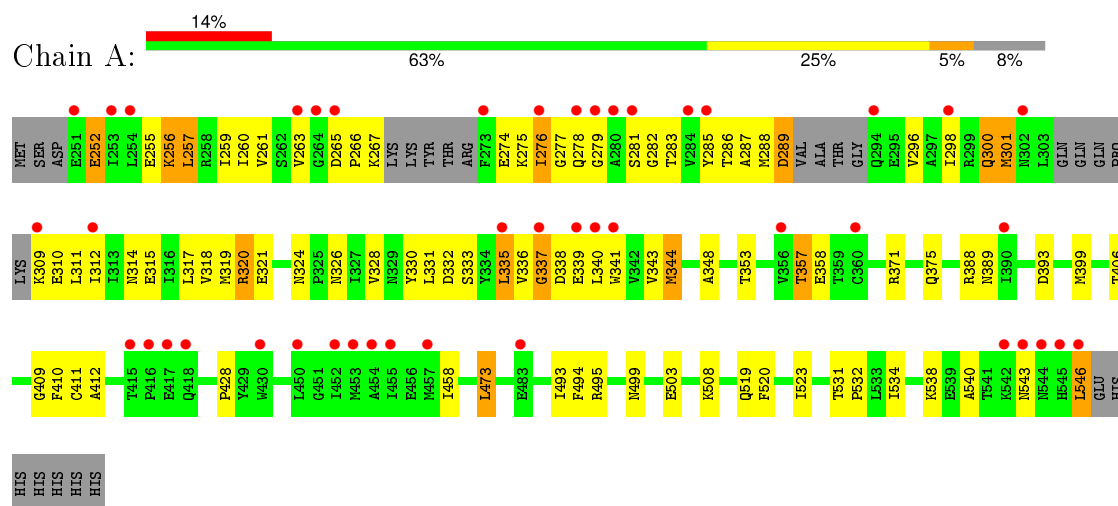
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



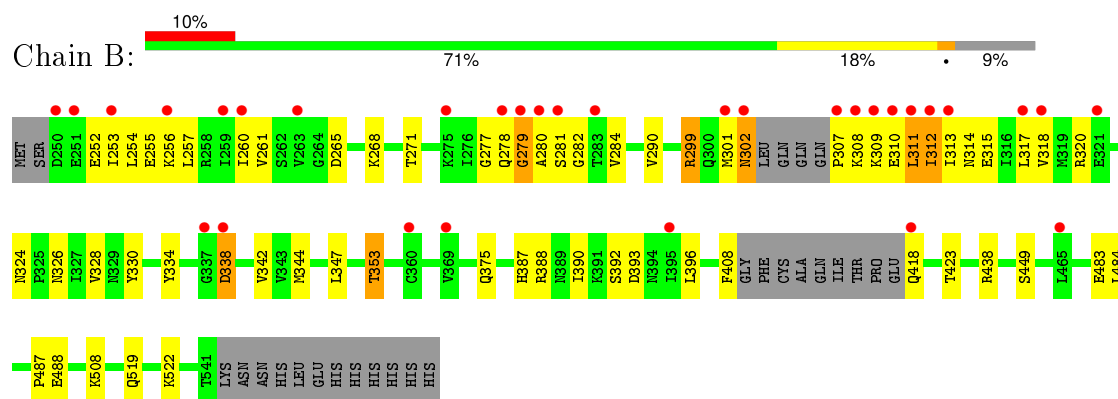
### 3 Residue-property plots

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: Serine/threonine-protein kinase PAK 1



#### • Molecule 1: Serine/threonine-protein kinase PAK 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.99 Å   80.00 Å   65.66 Å 90.00°   107.51°   90.00°	Depositor
Resolution (Å)	31.99 – 1.89 31.99 – 1.89	Depositor EDS
% Data completeness (in resolution range)	49.6 (31.99-1.89) 97.5 (31.99-1.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.89 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.184 , 0.231 0.182 , 0.226	Depositor DCC
$R_{free}$ test set	2466 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.6	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 56.7	EDS
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 48798 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4670	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: MG, ANP

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	0/2252	0.55	1/3043 (0.0%)
1	B	0.44	0/2222	0.57	1/3002 (0.0%)
All	All	0.44	0/4474	0.56	2/6045 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	GLY	N-CA-C	-6.66	96.44	113.10
1	B	279	GLY	N-CA-C	-6.05	97.97	113.10

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	2218	0	2248	90	0
1	B	2188	0	2230	74	0
2	A	1	0	0	0	0
3	A	31	0	13	5	0
4	A	95	0	0	2	0
4	B	137	0	0	0	0
All	All	4670	0	4491	164	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 (164) 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:279:GLY:HA3	1:B:282:GLY:O	1.33	1.25
1:B:310:GLU:CB	1:B:312:ILE:HG23	1.83	1.08
1:B:277:GLY:HA2	1:B:278:GLN:HB2	1.13	1.07
1:A:309:LYS:HG2	1:A:310:GLU:H	1.20	1.07
1:B:310:GLU:HB3	1:B:312:ILE:HG23	1.36	1.03
1:A:546:LEU:HD23	1:A:546:LEU:C	1.81	1.00
1:B:353:THR:HG21	1:B:393:ASP:OD1	1.65	0.95
1:B:301:MET:O	1:B:302:ASN:HB2	1.64	0.94
1:A:276:ILE:HD11	3:A:800:ANP:O4'	1.69	0.92
1:B:309:LYS:HB3	1:B:309:LYS:NZ	1.86	0.91
1:A:276:ILE:HG22	1:A:286:THR:OG1	1.71	0.89
1:A:336:VAL:HG22	1:A:336:VAL:O	1.72	0.89
1:B:277:GLY:CA	1:B:278:GLN:HB2	2.02	0.88
1:B:310:GLU:OE1	1:B:312:ILE:HG22	1.72	0.88
1:B:277:GLY:HA2	1:B:278:GLN:CB	2.03	0.88
1:A:546:LEU:CD2	1:A:546:LEU:C	2.42	0.88
1:A:287:ALA:HB3	1:A:298:ILE:HD13	1.59	0.82
1:B:309:LYS:O	1:B:310:GLU:HG3	1.79	0.82
1:A:256:LYS:O	1:A:259:ILE:HG13	1.79	0.82
1:B:308:LYS:O	1:B:309:LYS:HG2	1.77	0.81
1:B:308:LYS:O	1:B:309:LYS:CG	2.30	0.80
1:B:310:GLU:OE1	1:B:312:ILE:CG2	2.30	0.79
1:A:309:LYS:HG2	1:A:310:GLU:N	1.99	0.77
1:B:309:LYS:HZ3	1:B:309:LYS:HB3	1.46	0.76
1:B:312:ILE:HG12	1:B:313:ILE:N	2.01	0.76
1:B:310:GLU:HB2	1:B:312:ILE:HD12	1.68	0.76
1:A:353:THR:O	1:A:357:THR:HB	1.86	0.75
1:B:310:GLU:HB2	1:B:312:ILE:HG23	1.70	0.72
1:B:310:GLU:HB3	1:B:312:ILE:H	1.55	0.72
1:A:357:THR:HG22	1:A:358:GLU:HG2	1.72	0.71
1:B:254:LEU:HA	1:B:257:LEU:HD12	1.73	0.71
1:A:309:LYS:CG	1:A:310:GLU:H	2.01	0.68
1:A:260:ILE:HG23	1:A:320:ARG:HH21	1.59	0.67
1:A:288:MET:HG2	1:A:289:ASP:N	2.09	0.66
1:A:300:GLN:C	1:A:301:MET:HG3	2.15	0.66
1:B:309:LYS:O	1:B:310:GLU:CG	2.44	0.66
1:A:276:ILE:HG13	1:A:277:GLY:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ILE:HD11	1:A:519:GLN:C	2.16	0.65
1:A:336:VAL:C	1:A:337:GLY:O	2.33	0.63
1:A:337:GLY:O	1:A:338:ASP:C	2.34	0.63
1:B:256:LYS:HB2	1:B:313:ILE:HG21	1.80	0.63
1:A:340:LEU:HD23	1:A:341:TRP:N	2.13	0.63
1:B:347:LEU:HB2	1:B:396:LEU:HG	1.79	0.62
1:B:312:ILE:HG12	1:B:313:ILE:HG13	1.79	0.62
1:A:301:MET:O	1:A:340:LEU:N	2.29	0.62
1:A:318:VAL:HG21	1:A:411:CYS:SG	2.40	0.62
1:B:353:THR:HG22	1:B:392:SER:C	2.20	0.61
1:A:503:GLU:HG2	1:A:508:LYS:HB2	1.81	0.61
1:A:315:GLU:O	1:A:319:MET:HG3	1.99	0.61
1:A:337:GLY:O	1:A:339:GLU:N	2.32	0.61
1:B:387:HIS:CD2	1:B:408:PHE:HB3	2.35	0.61
1:A:336:VAL:O	1:A:336:VAL:CG2	2.47	0.61
1:B:347:LEU:H	1:B:396:LEU:HD21	1.65	0.60
1:A:324:ASN:ND2	1:A:326:ASN:H	2.00	0.59
1:A:255:GLU:O	1:A:259:ILE:HG23	2.02	0.59
1:A:281:SER:N	1:A:282:GLY:HA2	2.17	0.59
1:B:314:ASN:O	1:B:318:VAL:HG23	2.03	0.58
1:A:324:ASN:HD22	1:A:326:ASN:H	1.52	0.58
1:A:256:LYS:HD2	1:A:256:LYS:N	2.20	0.57
1:A:296:VAL:HG12	1:A:298:ILE:HD11	1.87	0.57
1:A:298:ILE:HG13	1:A:343:VAL:HG22	1.87	0.56
1:B:302:ASN:ND2	1:B:307:PRO:HB3	2.20	0.56
1:B:253:ILE:O	1:B:257:LEU:HG	2.05	0.56
1:B:309:LYS:CB	1:B:309:LYS:NZ	2.67	0.56
1:B:252:GLU:O	1:B:256:LYS:HG2	2.06	0.55
1:A:337:GLY:O	1:A:338:ASP:CB	2.51	0.55
1:A:310:GLU:OE2	1:A:314:ASN:HB2	2.06	0.55
1:A:340:LEU:HD23	1:A:341:TRP:H	1.71	0.55
1:B:519:GLN:OE1	1:B:522:LYS:HE2	2.07	0.55
1:A:340:LEU:C	1:A:341:TRP:HD1	2.10	0.54
1:A:257:LEU:HD11	1:A:340:LEU:HD11	1.88	0.54
1:B:324:ASN:ND2	1:B:326:ASN:H	2.06	0.54
1:B:313:ILE:O	1:B:317:LEU:HG	2.08	0.53
1:A:331:LEU:HB2	1:A:343:VAL:HG12	1.91	0.53
1:B:254:LEU:HD23	1:B:257:LEU:HD12	1.90	0.53
1:A:534:ILE:O	1:A:538:LYS:HG2	2.08	0.53
1:B:312:ILE:CG1	1:B:313:ILE:N	2.72	0.53
1:A:296:VAL:HG12	1:A:298:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:GLY:O	1:A:338:ASP:HB3	2.10	0.52
1:A:274:GLU:CB	1:A:286:THR:HB	2.39	0.52
1:A:263:VAL:O	1:A:263:VAL:HG23	2.09	0.52
1:A:428:PRO:HB3	1:A:473:LEU:HD13	1.91	0.52
1:A:300:GLN:O	1:A:301:MET:HG3	2.09	0.51
1:A:279:GLY:HA2	4:A:175:HOH:O	2.10	0.51
1:A:371:ARG:O	1:A:375:GLN:HG3	2.11	0.51
1:A:276:ILE:CD1	3:A:800:ANP:O4'	2.53	0.51
1:A:520:PHE:O	1:A:523:ILE:HG12	2.11	0.51
1:B:338:ASP:O	1:B:338:ASP:CG	2.49	0.51
1:B:310:GLU:CB	1:B:312:ILE:HD12	2.40	0.50
1:A:276:ILE:HD11	3:A:800:ANP:C4'	2.41	0.50
1:A:357:THR:CG2	1:A:358:GLU:HG2	2.42	0.50
1:B:326:ASN:HD21	1:B:375:GLN:HE21	1.59	0.50
1:A:301:MET:CE	1:A:312:ILE:HD11	2.42	0.50
1:A:266:PRO:O	1:A:267:LYS:HB2	2.12	0.50
1:A:348:ALA:HB3	1:A:399:MET:HG2	1.93	0.50
1:A:275:LYS:HG3	1:A:285:TYR:CD2	2.47	0.50
1:A:276:ILE:CG1	1:A:277:GLY:N	2.76	0.49
1:A:287:ALA:HB3	1:A:298:ILE:CD1	2.36	0.49
1:A:301:MET:HE2	1:A:312:ILE:HD11	1.94	0.49
1:A:286:THR:HG22	1:A:287:ALA:N	2.28	0.49
1:B:308:LYS:O	1:B:309:LYS:HG3	2.11	0.49
1:A:336:VAL:O	1:A:337:GLY:O	2.30	0.49
1:A:274:GLU:HB3	1:A:286:THR:HB	1.93	0.49
1:B:387:HIS:O	1:B:388:ARG:HB2	2.13	0.49
1:B:260:ILE:CG1	1:B:320:ARG:HD2	2.43	0.49
3:A:800:ANP:O2G	3:A:800:ANP:O1B	2.31	0.48
1:A:328:VAL:HG12	1:A:344[B]:MET:HE1	1.95	0.48
1:A:312:ILE:HD13	1:A:340:LEU:HD13	1.95	0.48
1:B:326:ASN:ND2	1:B:375:GLN:HE21	2.12	0.48
1:A:279:GLY:HA3	3:A:800:ANP:O2A	2.14	0.48
1:B:299:ARG:CD	1:B:344:MET:HE1	2.43	0.48
1:A:276:ILE:HD12	1:A:276:ILE:C	2.33	0.48
1:B:488:GLU:H	1:B:488:GLU:CD	2.17	0.48
1:B:284:VAL:HG22	1:B:299:ARG:HB3	1.96	0.47
1:B:338:ASP:O	1:B:338:ASP:OD1	2.31	0.47
1:A:259:ILE:C	1:A:259:ILE:HD12	2.35	0.47
1:B:312:ILE:HG12	1:B:313:ILE:H	1.78	0.47
1:B:311:LEU:O	1:B:312:ILE:C	2.53	0.47
1:B:260:ILE:HD11	1:B:320:ARG:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:HD11	1:A:494:PHE:CZ	2.50	0.47
1:A:257:LEU:HD11	1:A:340:LEU:CD1	2.45	0.46
1:A:335:LEU:HG	1:A:337:GLY:H	1.81	0.46
1:B:280:ALA:HB1	1:B:281:SER:OG	2.16	0.46
1:B:265:ASP:HB3	1:B:268:LYS:HE2	1.98	0.46
1:B:487:PRO:HD2	1:B:488:GLU:OE2	2.15	0.46
1:B:310:GLU:CD	1:B:312:ILE:CG2	2.84	0.45
1:B:280:ALA:CB	1:B:281:SER:HA	2.35	0.45
1:B:302:ASN:HD21	1:B:307:PRO:HB3	1.80	0.45
1:A:540:ALA:O	1:A:543:ASN:HB2	2.17	0.45
1:B:390:ILE:HB	1:B:449:SER:HB2	1.99	0.44
1:A:298:ILE:N	1:A:298:ILE:HD12	2.32	0.44
1:B:310:GLU:OE1	1:B:312:ILE:HG23	2.15	0.44
1:B:280:ALA:HA	1:B:281:SER:HA	1.34	0.44
1:A:531:THR:OG1	1:A:532:PRO:HD3	2.17	0.44
1:B:308:LYS:HB3	1:B:308:LYS:HE3	1.68	0.44
1:A:265:ASP:HA	1:A:266:PRO:HD2	1.86	0.44
1:B:253:ILE:CG2	1:B:313:ILE:HD11	2.47	0.43
1:A:335:LEU:HG	1:A:336:VAL:N	2.32	0.43
1:B:279:GLY:HA2	1:B:280:ALA:C	2.39	0.43
1:A:495:ARG:NH1	1:A:499:ASN:OD1	2.52	0.43
1:A:259:ILE:HD12	1:A:260:ILE:N	2.34	0.43
1:B:324:ASN:HD22	1:B:326:ASN:H	1.65	0.43
1:B:312:ILE:HD13	1:B:312:ILE:N	2.35	0.42
1:B:508:LYS:HD2	1:B:508:LYS:O	2.19	0.42
1:A:317:LEU:O	1:A:321:GLU:HG3	2.20	0.42
1:B:308:LYS:C	1:B:309:LYS:CG	2.88	0.42
1:B:320:ARG:HG3	1:B:330:TYR:CE2	2.55	0.42
1:A:260:ILE:HA	4:A:38:HOH:O	2.20	0.41
1:A:388:ARG:CZ	1:A:412:ALA:HB2	2.50	0.41
1:A:335:LEU:HD12	1:A:340:LEU:HG	2.01	0.41
1:A:278:GLN:HB3	1:A:283:THR:CG2	2.50	0.41
1:B:271:THR:HG23	1:B:290:VAL:CG1	2.50	0.41
1:A:309:LYS:CG	1:A:310:GLU:N	2.71	0.41
1:A:332:ASP:OD2	1:A:333:SER:N	2.54	0.41
1:A:319:MET:HE1	1:A:344[B]:MET:HE1	2.03	0.41
1:A:330:TYR:HA	1:A:344[B]:MET:HE3	2.02	0.41
1:A:311:LEU:HD22	1:A:409:GLY:O	2.21	0.41
1:A:266:PRO:O	1:A:267:LYS:CB	2.69	0.41
1:B:418:GLN:O	1:B:438:ARG:NH2	2.53	0.41
1:A:252:GLU:H	1:A:252:GLU:HG3	1.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HG3	1:B:342:VAL:HB	2.03	0.40
1:A:410:PHE:CZ	1:B:423:THR:HG21	2.56	0.40
1:B:261:VAL:HG13	1:B:334:TYR:HA	2.04	0.40
1:B:282:GLY:HA3	1:B:301:MET:HB3	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	275/306 (90%)	266 (97%)	9 (3%)	0	100	100
1	B	273/306 (89%)	264 (97%)	9 (3%)	0	100	100
All	All	548/612 (90%)	530 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/267 (92%)	228 (93%)	18 (7%)	17	6
1	B	242/267 (91%)	231 (96%)	11 (4%)	34	19
All	All	488/534 (91%)	459 (94%)	29 (6%)	25	11

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	GLU
1	A	256	LYS
1	A	257	LEU
1	A	261	VAL
1	A	276	ILE
1	A	289	ASP
1	A	300	GLN
1	A	301	MET
1	A	320	ARG
1	A	335	LEU
1	A	344[A]	MET
1	A	344[B]	MET
1	A	357	THR
1	A	389	ASN
1	A	393	ASP
1	A	406	THR
1	A	473	LEU
1	A	546	LEU
1	B	255	GLU
1	B	299	ARG
1	B	302	ASN
1	B	311	LEU
1	B	312	ILE
1	B	315	GLU
1	B	328	VAL
1	B	338	ASP
1	B	353	THR
1	B	483	GLU
1	B	484	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	324	ASN
1	A	389	ASN
1	B	302	ASN
1	B	324	ASN
1	B	326	ASN
1	B	375	GLN
1	B	468	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ANP	A	800	2	27,33,33	3.56	12 (44%)	30,52,52	3.10	10 (33%)

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
3	ANP	A	800	2	-	0/12/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ANP	C5'-C4'	-3.00	1.41	1.51
3	A	800	ANP	O3'-C3'	-2.44	1.37	1.43
3	A	800	ANP	O2'-C2'	-2.21	1.37	1.43
3	A	800	ANP	PG-O3G	-2.20	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ANP	C3'-C4'	-2.14	1.47	1.53
3	A	800	ANP	PG-N3B	2.08	1.68	1.63
3	A	800	ANP	C6-N6	3.90	1.47	1.34
3	A	800	ANP	PB-O2B	4.36	1.68	1.56
3	A	800	ANP	PB-N3B	5.65	1.78	1.63
3	A	800	ANP	PG-O1G	7.42	1.54	1.46
3	A	800	ANP	PB-O3A	8.08	1.69	1.59
3	A	800	ANP	PB-O1B	10.37	1.58	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	ANP	N3-C2-N1	-9.23	121.83	128.89
3	A	800	ANP	O1B-PB-N3B	-7.77	99.98	111.90
3	A	800	ANP	O2B-PB-O1B	-7.62	94.10	110.00
3	A	800	ANP	PA-O3A-PB	-3.82	119.86	132.67
3	A	800	ANP	C4-C5-N7	-2.89	106.82	109.48
3	A	800	ANP	C1'-N9-C4	-2.04	123.86	126.94
3	A	800	ANP	C2'-C1'-N9	2.16	117.60	114.29
3	A	800	ANP	O5'-C5'-C4'	2.72	119.16	109.12
3	A	800	ANP	O2B-PB-O3A	2.93	118.39	105.09
3	A	800	ANP	O3A-PB-N3B	3.99	117.42	106.44

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
3	A	800	ANP	5	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, 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	282/306 (92%)	0.78	44 (15%)	3 3	27, 50, 152, 268	0
1	B	279/306 (91%)	0.35	32 (11%)	6 7	27, 46, 143, 297	0
All	All	561/612 (91%)	0.57	76 (13%)	4 4	27, 48, 147, 297	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ALA	9.9
1	A	276	ILE	9.0
1	B	253	ILE	8.8
1	B	278	GLN	7.5
1	A	253	ILE	7.0
1	A	337	GLY	6.9
1	A	254	LEU	6.7
1	B	259	ILE	6.6
1	A	416	PRO	6.3
1	A	273	PHE	6.1
1	A	264	GLY	6.1
1	A	279	GLY	5.1
1	B	260	ILE	5.1
1	A	545	HIS	5.0
1	B	309	LYS	4.9
1	B	251	GLU	4.8
1	B	338	ASP	4.8
1	A	390	ILE	4.7
1	A	281	SER	4.6
1	A	335	LEU	4.5
1	B	281	SER	4.1
1	B	308	LYS	4.1
1	B	263	VAL	3.9
1	B	418	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	311	LEU	3.8
1	A	251	GLU	3.8
1	A	294	GLN	3.8
1	A	450	LEU	3.7
1	B	307	PRO	3.6
1	A	360	CYS	3.6
1	A	417	GLU	3.6
1	A	546	LEU	3.5
1	B	313	ILE	3.5
1	A	285	TYR	3.4
1	B	250	ASP	3.4
1	A	278	GLN	3.3
1	A	263	VAL	3.2
1	A	542	LYS	3.2
1	A	543	ASN	3.2
1	A	339	GLU	3.2
1	A	302	ASN	3.1
1	B	310	GLU	3.1
1	B	360	CYS	3.1
1	A	418	GLN	3.0
1	A	452	ILE	3.0
1	A	284	VAL	3.0
1	A	544	ASN	3.0
1	A	415	THR	3.0
1	A	453	MET	2.9
1	B	465	LEU	2.7
1	B	279	GLY	2.6
1	B	283	THR	2.6
1	B	321	GLU	2.5
1	A	430	TRP	2.4
1	B	317	LEU	2.4
1	A	457	MET	2.4
1	A	341	TRP	2.3
1	B	275	LYS	2.3
1	B	318	VAL	2.3
1	A	280	ALA	2.2
1	B	256	LYS	2.2
1	A	309	LYS	2.2
1	A	454	ALA	2.2
1	B	369	VAL	2.2
1	A	298	ILE	2.1
1	A	483	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	455	ILE	2.1
1	B	312	ILE	2.1
1	A	340	LEU	2.1
1	A	356	VAL	2.1
1	B	301	MET	2.1
1	A	312	ILE	2.0
1	B	337	GLY	2.0
1	B	302	ASN	2.0
1	A	265	ASP	2.0
1	B	395	ILE	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
3	ANP	A	800	31/31	0.89	0.14	-0.39	49,83,110,116	0
2	MG	A	1	1/1	0.95	0.14	-	69,69,69,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.