



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:55 AM GMT

PDB ID : 2GWK  
Title : SpvB ADP-ribosylated actin: orthorhombic crystal form  
Authors : Stebbins, C.E.; Margarit, S.M.  
Deposited on : 2006-05-04  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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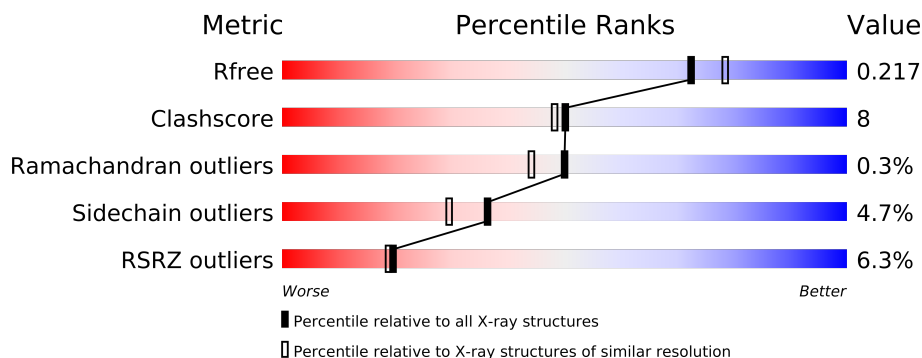
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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))
$R_{free}$	66092	4888 (2.00-2.00)
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	371	
1	B	371	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	1401	-	X
2	CA	B	1501	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6392 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	1	0
			2841	1801	478	542	20			
1	B	366	Total	C	N	O	S	0	1	0
			2869	1818	483	547	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135
B	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is water.

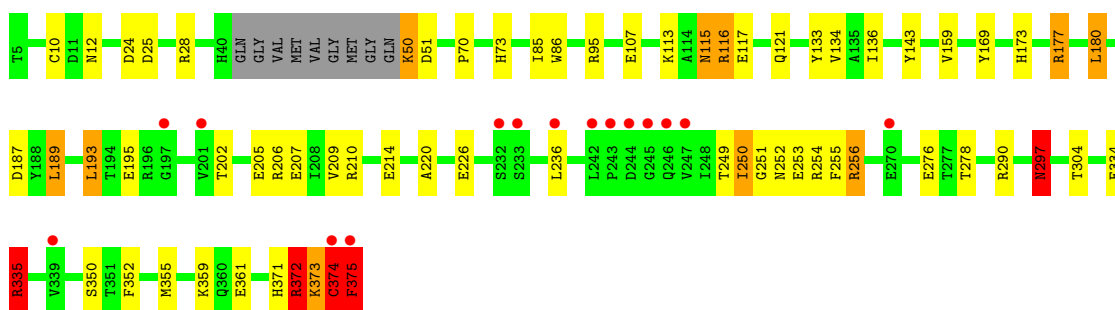
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	371	Total	O	0	0
			371	371		
4	B	247	Total	O	0	0
			247	247		

### 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.

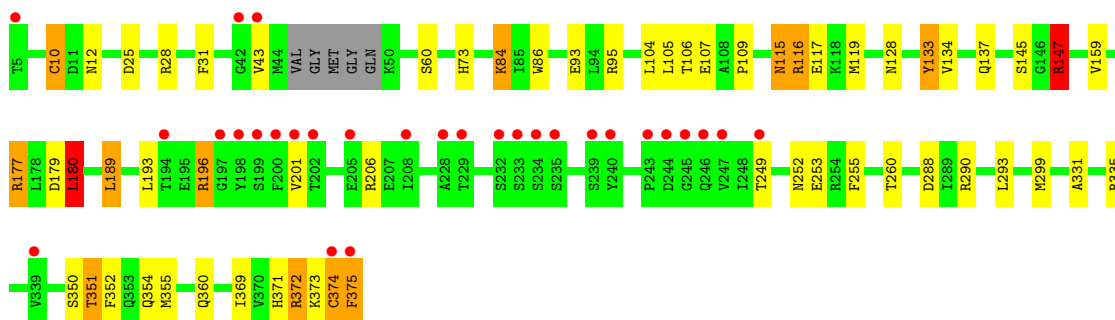
- Molecule 1: Actin, alpha skeletal muscle

Chain A: 



- Molecule 1: Actin, alpha skeletal muscle

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.39Å 102.35Å 123.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.00 – 2.00 32.12 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (32.00-2.00) 92.5 (32.12-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.171 , 0.211 0.182 , 0.217	Depositor DCC
$R_{free}$ test set	4084 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 63.7	EDS
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 84622 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HIC, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.04	12/2895 (0.4%)	1.06	20/3920 (0.5%)
1	B	0.86	5/2923 (0.2%)	0.98	19/3957 (0.5%)
All	All	0.96	17/5818 (0.3%)	1.02	39/7877 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	GLU	CD-OE2	9.87	1.36	1.25
1	A	334	GLU	CB-CG	9.35	1.70	1.52
1	A	334	GLU	CG-CD	8.51	1.64	1.51
1	A	195	GLU	CD-OE2	8.37	1.34	1.25
1	A	374	CYS	CB-SG	-7.81	1.69	1.82
1	A	195	GLU	CD-OE1	7.44	1.33	1.25
1	B	10[A]	CYS	CB-SG	-7.07	1.70	1.82
1	B	10[B]	CYS	CB-SG	-7.07	1.70	1.82
1	A	297	ASN	CG-OD1	6.64	1.38	1.24
1	A	350	SER	CB-OG	-5.48	1.35	1.42
1	A	335	ARG	CD-NE	-5.30	1.37	1.46
1	B	116	ARG	CD-NE	-5.26	1.37	1.46
1	B	133	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	143	TYR	CD2-CE2	5.13	1.47	1.39
1	A	375	PHE	CE2-CZ	-5.07	1.27	1.37
1	B	84	LYS	CD-CE	5.03	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	116	ARG	CD-NE	-5.02	1.38	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ARG	NE-CZ-NH2	-20.85	109.88	120.30
1	A	335	ARG	NE-CZ-NH1	16.51	128.55	120.30
1	B	335	ARG	NE-CZ-NH2	-14.76	112.92	120.30
1	B	335	ARG	NE-CZ-NH1	13.62	127.11	120.30
1	B	116	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	A	372	ARG	NE-CZ-NH2	-8.65	115.98	120.30
1	B	116	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	116	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	A	25	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	180	LEU	CA-CB-CG	8.26	134.29	115.30
1	A	335	ARG	CD-NE-CZ	8.18	135.05	123.60
1	B	288	ASP	CB-CG-OD1	7.58	125.12	118.30
1	B	109	PRO	C-N-CA	-7.54	102.85	121.70
1	A	290	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	374	CYS	N-CA-C	-7.21	91.53	111.00
1	B	180	LEU	CA-CB-CG	7.03	131.46	115.30
1	A	116	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	335	ARG	CG-CD-NE	-6.90	97.31	111.80
1	A	256	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	95	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	147	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	84	LYS	CD-CE-NZ	6.46	126.57	111.70
1	B	372	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	25	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	177	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	B	335	ARG	CD-NE-CZ	6.04	132.06	123.60
1	A	372	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	374	CYS	N-CA-C	-5.80	95.34	111.00
1	A	25	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	256	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	290	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	109	PRO	O-C-N	-5.70	113.58	122.70
1	A	375	PHE	CB-CG-CD1	5.35	124.55	120.80
1	B	177	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	95	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	95	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	95	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	25	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	290	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2841	0	2811	52	0
1	B	2869	0	2840	37	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
4	A	371	0	0	14	1
4	B	247	0	0	5	0
All	All	6392	0	5675	86	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (86) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:LYS:HB3	4:A:1613:HOH:O	1.52	1.07
1:A:50:LYS:N	4:A:1759:HOH:O	1.98	0.96
1:B:73:HIC:ND1	4:B:1617:HOH:O	1.99	0.95
1:B:134:VAL:O	1:B:373:LYS:HE2	1.74	0.87
1:A:276:GLU:CD	4:A:1507:HOH:O	2.21	0.78
1:B:299:MET:HE2	1:B:331:ALA:HB2	1.66	0.77
1:B:10[B]:CYS:SG	4:B:1598:HOH:O	2.43	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10[B]:CYS:SG	4:A:1490:HOH:O	2.45	0.74
1:B:117:GLU:OE1	1:B:371:HIS:HE1	1.71	0.72
1:A:50:LYS:HG3	1:A:51:ASP:H	1.55	0.71
1:A:115:ASN:ND2	4:A:1667:HOH:O	2.24	0.69
1:B:299:MET:CE	1:B:331:ALA:HB2	2.23	0.69
1:B:115:ASN:ND2	4:B:1725:HOH:O	2.25	0.69
1:B:375:PHE:HD1	1:B:375:PHE:N	1.90	0.68
1:B:193:LEU:HD13	1:B:253:GLU:HG3	1.75	0.68
1:B:375:PHE:CD1	1:B:375:PHE:N	2.64	0.66
1:A:173:HIS:ND1	4:A:1730:HOH:O	2.29	0.64
1:A:117:GLU:OE1	1:A:371:HIS:HE1	1.80	0.64
1:A:304:THR:OG1	1:A:335:ARG:HD2	1.98	0.64
1:A:116:ARG:HE	1:A:371:HIS:HD2	1.45	0.63
1:B:352:PHE:HA	1:B:355:MET:HG3	1.80	0.63
1:A:202:THR:HG23	1:A:205:GLU:H	1.65	0.62
1:A:220:ALA:HB1	1:A:226:GLU:HG3	1.82	0.62
1:B:189:LEU:O	1:B:193:LEU:HB2	2.00	0.61
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.84	0.60
1:A:375:PHE:N	4:A:1758:HOH:O	2.08	0.59
1:A:24:ASP:OD2	1:A:28:ARG:NH2	2.35	0.59
1:A:359:LYS:HE3	4:A:1436:HOH:O	2.02	0.59
1:A:359:LYS:HD2	4:A:1553:HOH:O	2.04	0.57
1:A:352:PHE:HA	1:A:355:MET:HG3	1.87	0.57
1:A:133:TYR:OH	1:A:374:CYS:O	2.17	0.57
1:A:250:ILE:HD11	1:A:254:ARG:HG2	1.86	0.56
1:A:189:LEU:HD13	1:A:209:VAL:HG13	1.87	0.56
1:B:177:ARG:HD2	1:B:179:ASP:OD2	2.06	0.55
1:B:354:GLN:NE2	4:B:1626:HOH:O	2.36	0.54
1:A:113:LYS:HG3	1:A:371:HIS:CE1	2.41	0.54
1:A:375:PHE:N	1:A:375:PHE:CD1	2.77	0.53
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.58	0.52
1:B:12:ASN:HD21	1:B:86:TRP:HE1	1.56	0.52
1:A:134:VAL:O	1:A:373:LYS:HE3	2.09	0.52
1:B:10[B]:CYS:HB3	1:B:105:LEU:HD23	1.92	0.51
1:A:116:ARG:HH21	1:A:371:HIS:CD2	2.28	0.51
1:A:187:ASP:OD1	1:A:206:ARG:NH1	2.43	0.51
1:B:145:SER:OG	1:B:147:ARG:HG3	2.11	0.50
1:A:73:HIC:HA	1:A:159:VAL:HB	1.94	0.50
4:A:1504:HOH:O	1:B:351:THR:HG22	2.12	0.49
1:B:86:TRP:CH2	1:B:119:MET:HG3	2.47	0.49
1:A:304:THR:OG1	1:A:335:ARG:CD	2.60	0.49
1:A:278:THR:CG2	1:A:297:ASN:HD21	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:10[A]:CYS:HB2	1:B:105:LEU:HD23	1.94	0.49
1:A:189:LEU:HD22	1:A:193:LEU:HD22	1.94	0.49
1:B:31:PHE:CE2	1:B:93:GLU:HG3	2.49	0.48
1:A:134:VAL:O	1:A:373:LYS:CE	2.62	0.48
1:B:180:LEU:HD11	1:B:260:THR:HG22	1.95	0.47
1:A:251:GLY:H	1:A:253:GLU:HG2	1.78	0.47
1:A:250:ILE:HG13	1:A:254:ARG:HG3	1.97	0.47
1:A:12:ASN:ND2	1:A:86:TRP:HE1	2.13	0.46
1:B:107:GLU:OE1	1:B:116:ARG:HD3	2.15	0.46
1:A:133:TYR:HH	1:A:374:CYS:C	2.17	0.46
1:A:107:GLU:OE1	1:A:116:ARG:HD3	2.15	0.46
1:A:372:ARG:HG3	1:B:369:ILE:HD11	1.98	0.46
1:B:73:HIC:HA	1:B:159:VAL:HB	1.97	0.45
1:B:12:ASN:ND2	1:B:86:TRP:HE1	2.14	0.45
1:A:375:PHE:HD1	1:A:375:PHE:N	2.13	0.45
1:B:252:ASN:HA	1:B:255:PHE:CE2	2.53	0.44
1:B:352:PHE:HA	1:B:355:MET:CG	2.48	0.44
1:A:207:GLU:CD	1:A:210:ARG:HH21	2.21	0.44
1:B:106:THR:HB	1:B:137:GLN:HG3	1.98	0.44
1:B:133:TYR:OH	1:B:374:CYS:O	2.27	0.44
1:A:169:TYR:OH	1:B:355:MET:HE1	2.18	0.43
1:A:133:TYR:OH	1:A:374:CYS:C	2.56	0.43
1:B:352:PHE:CD1	1:B:355:MET:HG3	2.54	0.42
1:A:256:ARG:HD2	4:A:1568:HOH:O	2.19	0.42
1:A:121:GLN:NE2	4:A:1647:HOH:O	2.53	0.42
1:A:210:ARG:O	1:A:214:GLU:HG3	2.20	0.41
1:B:43:VAL:HG12	1:B:43:VAL:O	2.20	0.41
1:A:136:ILE:H	1:A:375:PHE:HE2	1.63	0.41
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.56	0.41
1:A:177:ARG:NH2	4:A:1476:HOH:O	2.53	0.41
1:B:116:ARG:HH21	1:B:371:HIS:CD2	2.39	0.41
1:A:361:GLU:CD	4:A:1623:HOH:O	2.59	0.41
1:A:113:LYS:NZ	1:A:117:GLU:OE1	2.54	0.41
1:A:372:ARG:HG3	1:B:369:ILE:CD1	2.51	0.40
1:B:104:LEU:HD23	1:B:104:LEU:C	2.41	0.40
1:A:121:GLN:HB2	1:A:121:GLN:HE21	1.71	0.40
1:B:196:ARG:HG2	4:B:1680:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:1472:HOH:O	4:A:1760:HOH:O[4_456]	2.15	0.05

## 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	358/371 (96%)	348 (97%)	9 (2%)	1 (0%)	50	44
1	B	362/371 (98%)	354 (98%)	7 (2%)	1 (0%)	50	44
All	All	720/742 (97%)	702 (98%)	16 (2%)	2 (0%)	50	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	CYS
1	B	201	VAL

### 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	308/313 (98%)	296 (96%)	12 (4%)	43	38
1	B	311/313 (99%)	294 (94%)	17 (6%)	30	23
All	All	619/626 (99%)	590 (95%)	29 (5%)	36	29

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

Mol	Chain	Res	Type
1	A	50	LYS
1	A	115	ASN
1	A	180	LEU
1	A	189	LEU
1	A	193	LEU
1	A	236	LEU
1	A	249	THR
1	A	250	ILE
1	A	297	ASN
1	A	372	ARG
1	A	373	LYS
1	A	375	PHE
1	B	28	ARG
1	B	60	SER
1	B	84	LYS
1	B	115	ASN
1	B	128	ASN
1	B	147	ARG
1	B	180	LEU
1	B	189	LEU
1	B	196	ARG
1	B	206	ARG
1	B	249	THR
1	B	293	LEU
1	B	350	SER
1	B	351	THR
1	B	360	GLN
1	B	372	ARG
1	B	375	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	115	ASN
1	A	121	GLN
1	A	280	ASN
1	A	297	ASN
1	A	371	HIS
1	B	12	ASN
1	B	115	ASN
1	B	280	ASN
1	B	354	GLN

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Mol	Chain	Res	Type
1	B	371	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	HIC	A	73	1	11,11,12	4.63	1 (9%)	12,14,16	1.31	2 (16%)
1	HIC	B	73	1	11,11,12	5.12	3 (27%)	12,14,16	1.26	1 (8%)

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
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1
1	HIC	B	73	1	-	0/4/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	O-C	16.52	1.22	1.11
1	A	73	HIC	O-C	15.16	1.21	1.11
1	B	73	HIC	CD2-NE2	-2.45	1.34	1.37
1	B	73	HIC	CD2-CG	2.38	1.38	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIC	CG-CB-CA	-3.05	109.67	113.85
1	A	73	HIC	CG-CB-CA	-2.27	110.75	113.85
1	A	73	HIC	ND1-CE1-NE2	-2.21	107.35	112.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ATP	A	1402	2	33,33,33	1.28	2 (6%)	52,52,52	1.40	6 (11%)
3	ATP	B	1502	2	33,33,33	1.20	4 (12%)	52,52,52	1.58	8 (15%)

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	ATP	A	1402	2	-	0/22/38/38	0/1/3/3
3	ATP	B	1502	2	-	0/22/38/38	0/1/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1402	ATP	PG-O3B	3.84	1.66	1.60
3	B	1502	ATP	C4-N9	-3.76	1.32	1.37
3	B	1502	ATP	C5-C4	3.24	1.47	1.40
3	A	1402	ATP	C4-N9	-3.17	1.33	1.37
3	B	1502	ATP	PG-O2G	-2.09	1.47	1.54
3	B	1502	ATP	PB-O3A	2.09	1.63	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	ATP	N3-C2-N1	-6.45	123.32	128.71
3	B	1502	ATP	N3-C4-N9	5.07	134.58	125.43
3	A	1402	ATP	N3-C4-N9	4.41	133.39	125.43
3	A	1402	ATP	N3-C2-N1	-4.15	125.24	128.71
3	B	1502	ATP	C8-N9-C4	3.06	109.24	106.90
3	A	1402	ATP	C8-N9-C4	2.80	109.04	106.90
3	B	1502	ATP	C5-C4-N3	-2.36	120.55	125.70
3	A	1402	ATP	C1'-N9-C4	-2.29	122.68	126.64
3	B	1502	ATP	C2-N1-C6	2.14	122.63	118.77
3	B	1502	ATP	O3G-PG-O2G	2.09	115.75	107.61
3	B	1502	ATP	O4'-C1'-C2'	-2.06	103.62	106.77
3	A	1402	ATP	N6-C6-N1	2.06	123.40	119.36
3	A	1402	ATP	C5-C4-N3	-2.01	121.32	125.70
3	B	1502	ATP	N6-C6-N1	2.01	123.31	119.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	362/371 (97%)	-0.06	15 (4%) 35 35	32, 37, 43, 49	0
1	B	366/371 (98%)	0.18	29 (7%) 13 12	31, 37, 44, 54	0
All	All	728/742 (98%)	0.06	44 (6%) 19 20	31, 37, 43, 54	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	GLY	5.9
1	A	374	CYS	5.4
1	B	239	SER	5.0
1	B	374	CYS	4.7
1	B	232	SER	4.7
1	B	199	SER	4.5
1	B	201	VAL	4.2
1	B	245	GLY	3.8
1	A	201	VAL	3.8
1	A	244	ASP	3.8
1	B	247	VAL	3.7
1	B	200	PHE	3.6
1	A	246	GLN	3.3
1	A	243	PRO	3.3
1	A	247	VAL	3.2
1	B	243	PRO	3.2
1	B	375	PHE	3.2
1	B	246	GLN	3.2
1	B	233	SER	3.1
1	A	375	PHE	3.0
1	B	194	THR	3.0
1	A	232	SER	3.0
1	B	235	SER	2.8
1	A	197	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	240	TYR	2.8
1	B	339	VAL	2.7
1	A	233	SER	2.7
1	B	202	THR	2.7
1	B	197	GLY	2.7
1	B	244	ASP	2.6
1	B	229	THR	2.6
1	B	43	VAL	2.6
1	B	228	ALA	2.6
1	B	208	ILE	2.6
1	A	242	LEU	2.6
1	A	245	GLY	2.5
1	B	198	TYR	2.5
1	A	339	VAL	2.4
1	B	5	THR	2.2
1	B	234	SER	2.2
1	B	249	THR	2.1
1	A	270	GLU	2.1
1	A	236	LEU	2.0
1	B	205	GLU	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	HIC	B	73	11/12	0.14	2.52	35,39,52,53	0
1	HIC	A	73	11/12	0.10	-0.65	30,33,42,45	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	B	1501	1/1	0.22	5.86	35,35,35,35	0
2	CA	A	1401	1/1	0.25	3.86	36,36,36,36	0
3	ATP	B	1502	31/31	0.14	0.68	32,35,37,38	0
3	ATP	A	1402	31/31	0.12	-0.03	24,30,33,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.