



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:09 am BST

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 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

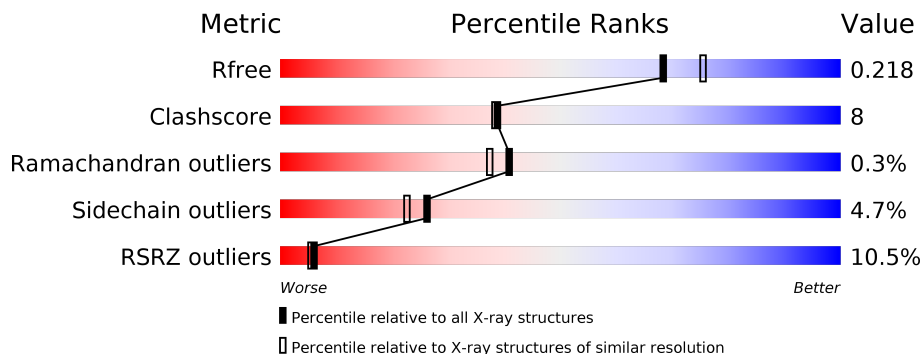
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 respectively. 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	371	 9% 80% 14% ...
1	B	371	 12% 83% 12% ...

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6392 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 Actin, alpha skeletal muscle.

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

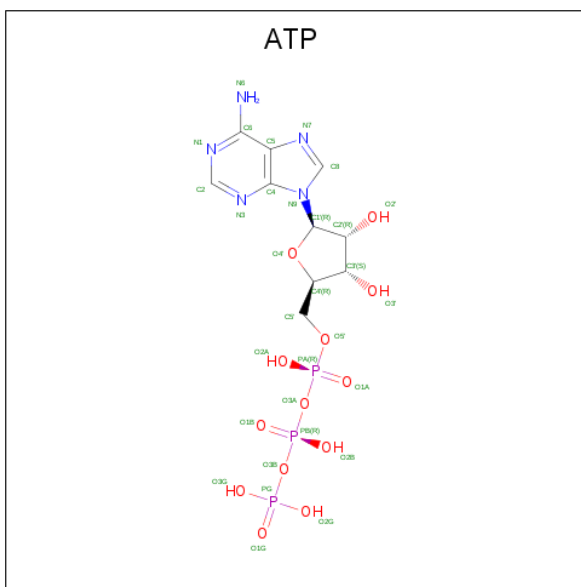
There are 2 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	P		
3	A	1	31	10	5	13	3	0	0
3	B	1	31	10	5	13	3	0	0

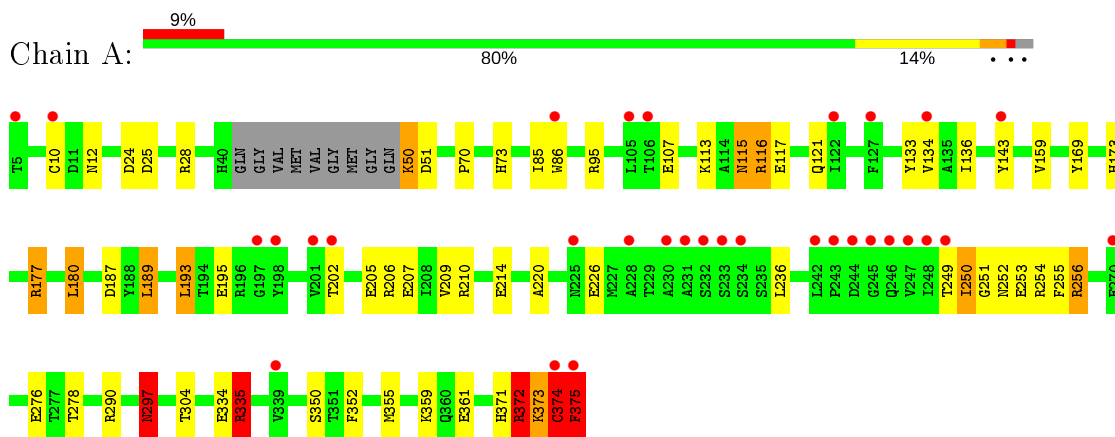
- Molecule 4 is water.

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

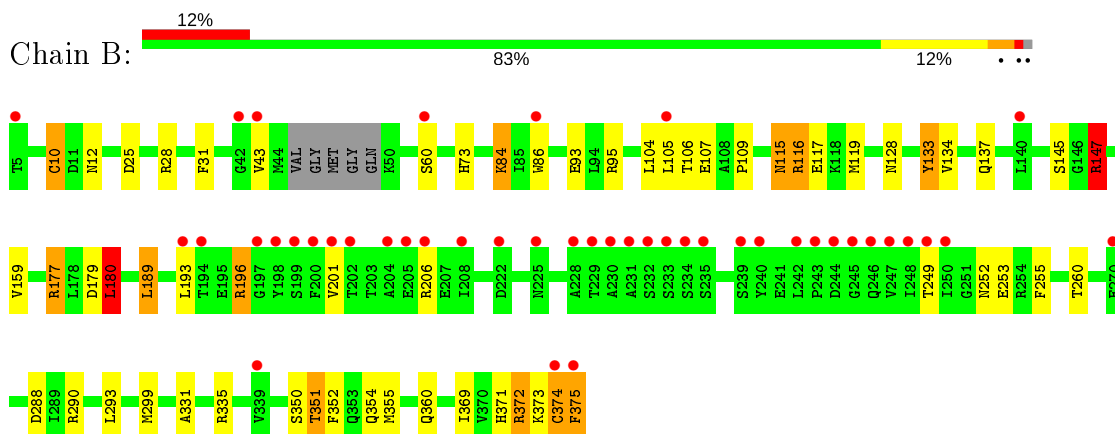
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



- Molecule 1: Actin, alpha skeletal muscle



## 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)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.171 , 0.211 0.182 , 0.218	Depositor DCC
$R_{free}$ test set	4302 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.015 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6392	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage'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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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 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	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

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 8.

All (86) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10[B]:CYS:SG	4:B:1598:HOH:O	2.43	0.76
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:THR:CG2	1:A:297:ASN:HD21	2.26	0.49
1:A:304:THR:OG1	1:A:335:ARG:CD	2.60	0.49
1:A:189:LEU:HD22	1:A:193:LEU:HD22	1.94	0.49
1:B:10[A]:CYS:HB2	1:B:105:LEU:HD23	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:A:133:TYR:HH	1:A:374:CYS:C	2.17	0.46
1:B:107:GLU:OE1	1:B:116:ARG:HD3	2.15	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:A:207:GLU:CD	1:A:210:ARG:HH21	2.21	0.44
1:B:352:PHE:HA	1:B:355:MET:CG	2.48	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:121:GLN:NE2	4:A:1647:HOH:O	2.53	0.42
1:A:256:ARG:HD2	4:A:1568:HOH:O	2.19	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:177:ARG:NH2	4:A:1476:HOH:O	2.53	0.41
1:A:252:ASN:HA	1:A:255:PHE:CE2	2.56	0.41
1:A:361:GLU:CD	4:A:1623:HOH:O	2.59	0.41
1:B:116:ARG:HH21	1:B:371:HIS:CD2	2.39	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.

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

### 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	358/371 (96%)	348 (97%)	9 (2%)	1 (0%)	41	37
1	B	362/371 (98%)	354 (98%)	7 (2%)	1 (0%)	41	37
All	All	720/742 (97%)	702 (98%)	16 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

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

#### 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	308/313 (98%)	296 (96%)	12 (4%)	32	30
1	B	311/313 (99%)	294 (94%)	17 (6%)	21	17
All	All	619/626 (99%)	590 (95%)	29 (5%)	26	22

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 [i](#)

There are no RNA molecules in this entry.

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

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	8,11,12	0.96	1 (12%)	6,14,16	0.66	0
1	HIC	B	73	1	8,11,12	1.35	1 (12%)	6,14,16	0.56	0

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	-	2/5/6/8	0/1/1/1
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	HIC	CD2-NE2	-2.76	1.34	1.38
1	A	73	HIC	CD2-NE2	-2.29	1.34	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	CA-CB-CG-CD2
1	B	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	1	0
1	B	73	HIC	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	26,33,33	0.96	0	31,52,52	1.20	4 (12%)
3	ATP	B	1502	2	26,33,33	0.92	2 (7%)	31,52,52	1.21	5 (16%)

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	-	2/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ATP	B	1502	2	-	1/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1502	ATP	C5-C4	2.60	1.47	1.40
3	B	1502	ATP	PG-O2G	-2.02	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1502	ATP	N3-C2-N1	-3.43	123.32	128.68
3	A	1402	ATP	C5-C6-N6	-2.51	116.54	120.35
3	A	1402	ATP	N6-C6-N1	2.33	123.40	118.57
3	B	1502	ATP	N6-C6-N1	2.28	123.31	118.57
3	B	1502	ATP	C2-N1-C6	2.27	122.63	118.75
3	B	1502	ATP	O4'-C1'-C2'	-2.26	103.62	106.93
3	A	1402	ATP	C1'-N9-C4	-2.25	122.68	126.64
3	A	1402	ATP	N3-C2-N1	-2.20	125.24	128.68
3	B	1502	ATP	O3G-PG-O2G	2.12	115.75	107.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1402	ATP	PG-O3B-PB-O1B
3	B	1502	ATP	PG-O3B-PB-O1B
3	A	1402	ATP	PG-O3B-PB-O2B

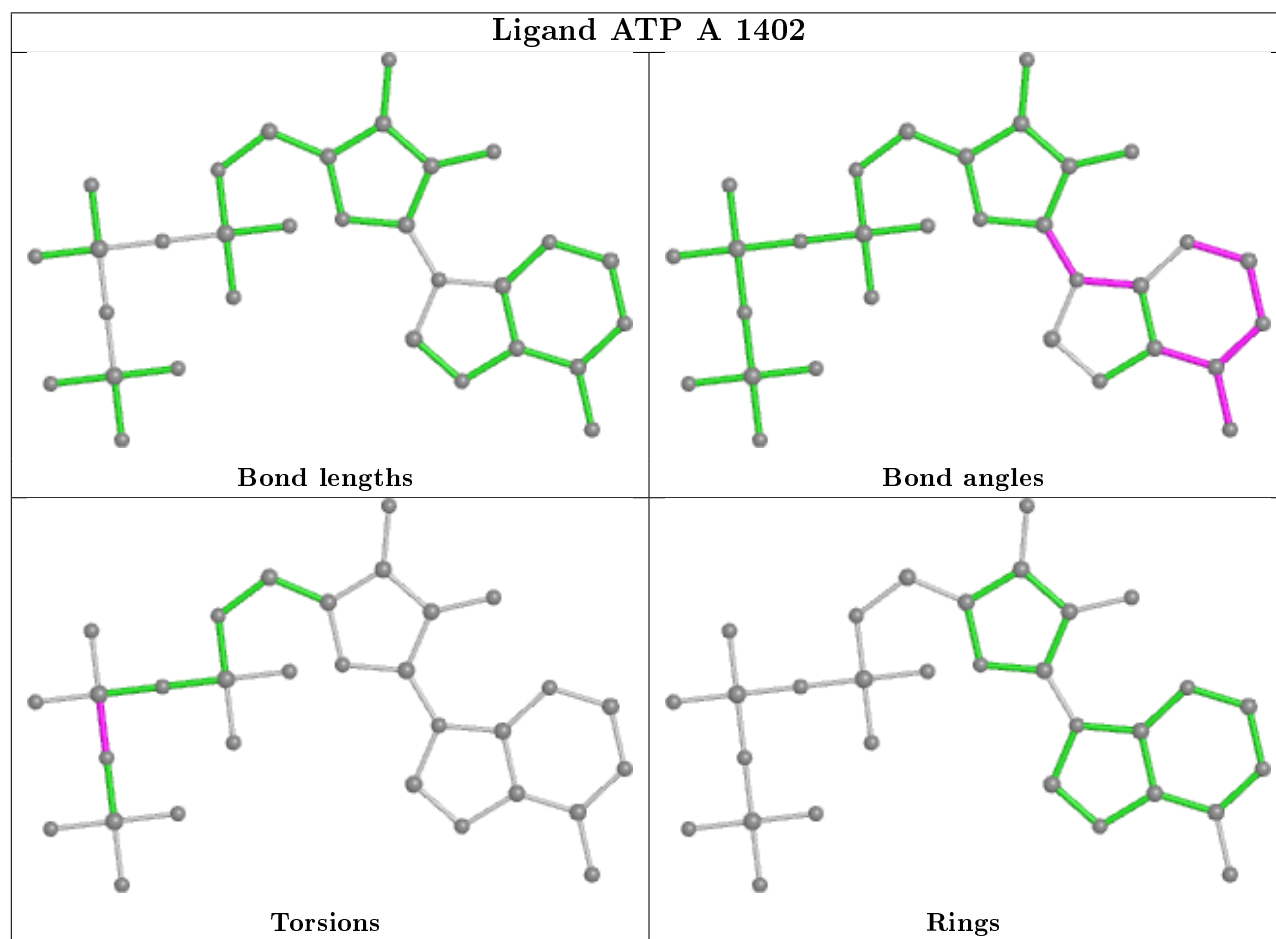
There are no ring outliers.

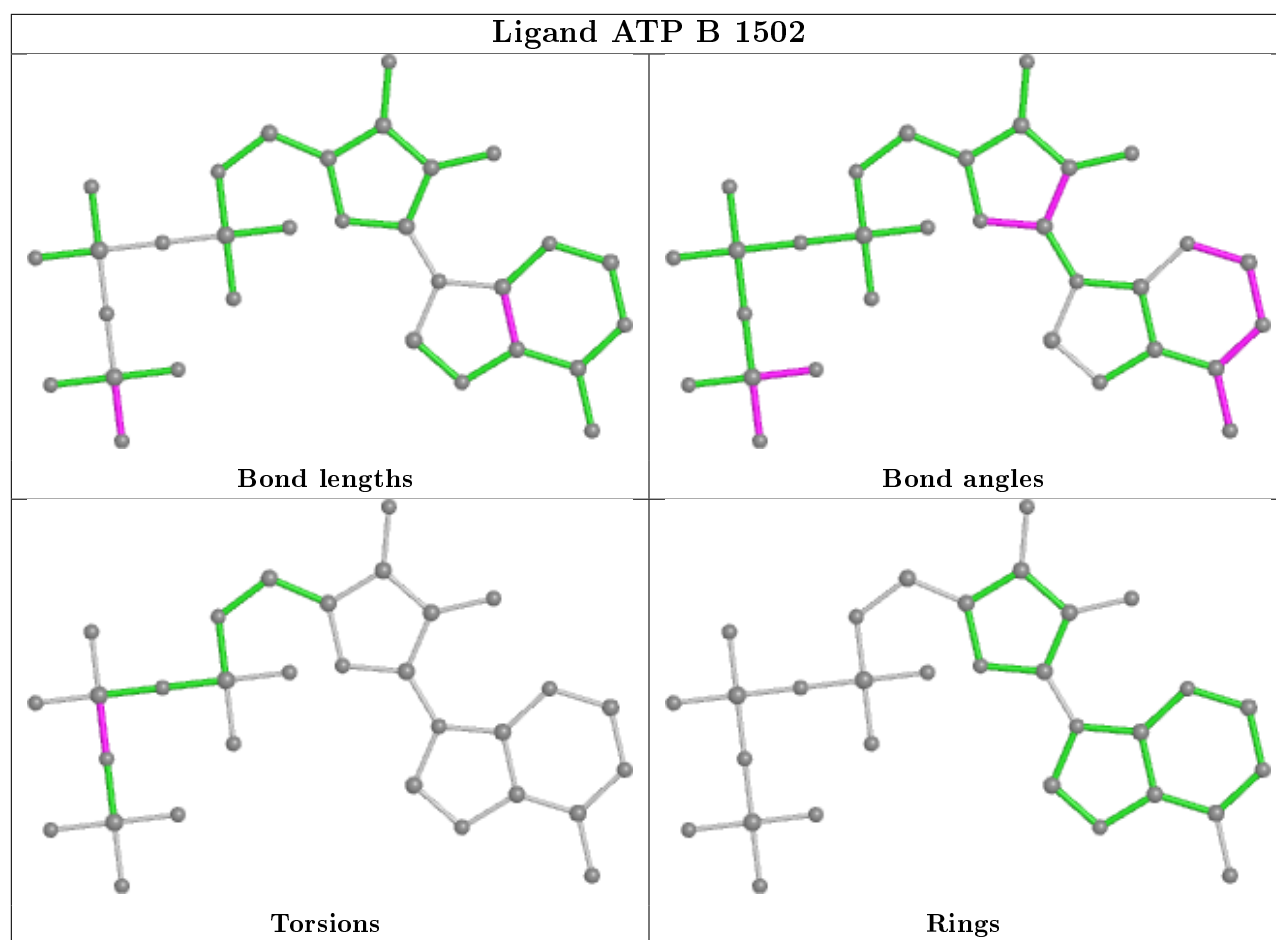
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.



The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	72:GLU	C	73:HIC	N	1.64
1	B	73:HIC	C	74:GLY	N	1.62

## 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	361/371 (97%)	0.47	32 (8%) <b>9</b> <b>8</b>	32, 37, 43, 49	0
1	B	365/371 (98%)	0.67	44 (12%) <b>4</b> <b>3</b>	31, 37, 44, 54	0
All	All	726/742 (97%)	0.57	76 (10%) <b>6</b> <b>5</b>	31, 37, 43, 54	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	CYS	8.0
1	B	247	VAL	6.8
1	B	374	CYS	6.6
1	B	199	SER	6.1
1	B	239	SER	6.1
1	B	201	VAL	5.9
1	B	42	GLY	5.9
1	A	246	GLN	5.5
1	A	247	VAL	5.5
1	A	244	ASP	5.3
1	A	232	SER	5.2
1	B	245	GLY	5.1
1	B	375	PHE	5.0
1	A	201	VAL	4.8
1	B	233	SER	4.6
1	B	240	TYR	4.6
1	B	208	ILE	4.4
1	B	243	PRO	4.4
1	B	198	TYR	4.3
1	B	228	ALA	4.2
1	B	232	SER	4.1
1	A	243	PRO	4.1
1	B	246	GLN	4.0
1	B	202	THR	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	200	PHE	3.8
1	A	242	LEU	3.7
1	A	228	ALA	3.7
1	A	375	PHE	3.5
1	B	242	LEU	3.5
1	A	233	SER	3.4
1	B	339	VAL	3.3
1	A	105	LEU	3.3
1	B	244	ASP	3.3
1	B	234	SER	3.3
1	B	43	VAL	3.3
1	B	231	ALA	3.3
1	A	197	GLY	3.2
1	A	230	ALA	3.1
1	A	339	VAL	3.1
1	B	229	THR	3.1
1	B	235	SER	3.1
1	B	194	THR	2.9
1	B	248	ILE	2.8
1	A	86	TRP	2.8
1	A	202	THR	2.8
1	A	198	TYR	2.7
1	A	106	THR	2.7
1	A	249	THR	2.7
1	A	245	GLY	2.6
1	B	197	GLY	2.6
1	A	270	GLU	2.6
1	B	105	LEU	2.6
1	A	231	ALA	2.6
1	B	230	ALA	2.5
1	A	134	VAL	2.4
1	B	86	TRP	2.4
1	B	205	GLU	2.4
1	A	143	TYR	2.4
1	B	193	LEU	2.4
1	A	248	ILE	2.4
1	B	140	LEU	2.4
1	A	10[A]	CYS	2.3
1	B	206	ARG	2.3
1	B	270	GLU	2.3
1	B	225	ASN	2.3
1	A	127	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	5	THR	2.2
1	B	249	THR	2.2
1	A	234	SER	2.2
1	B	222	ASP	2.2
1	B	250	ILE	2.1
1	A	225	ASN	2.1
1	B	204	ALA	2.1
1	B	60	SER	2.1
1	A	122	ILE	2.0
1	A	5	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	HIC	B	73	11/12	0.91	0.13	35,39,52,53	0
1	HIC	A	73	11/12	0.94	0.11	30,33,42,45	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

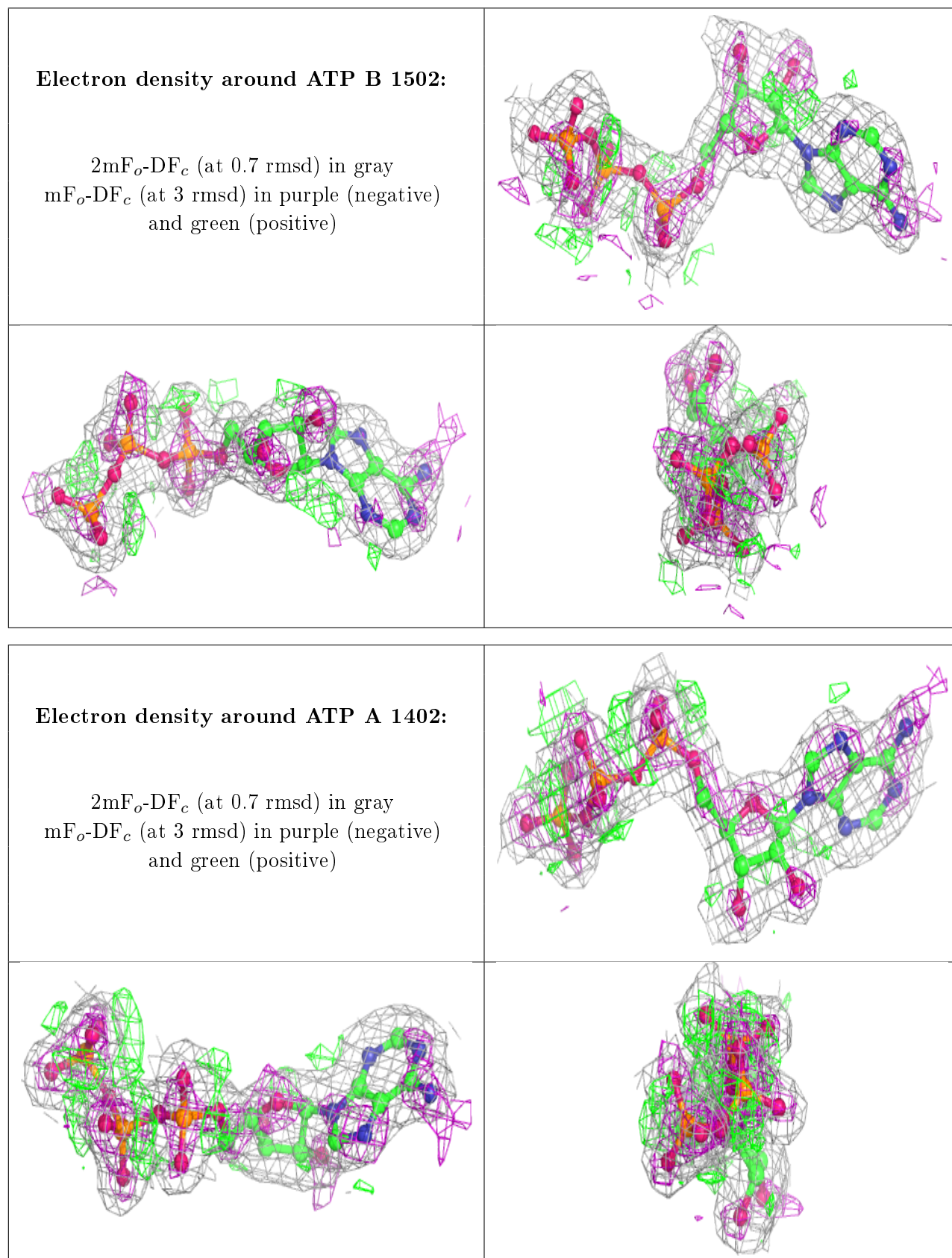
## 6.4 Ligands [i](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	ATP	B	1502	31/31	0.97	0.08	32,35,37,38	0
3	ATP	A	1402	31/31	0.98	0.08	24,30,33,35	0
2	CA	B	1501	1/1	0.98	0.22	35,35,35,35	0
2	CA	A	1401	1/1	0.99	0.19	36,36,36,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers

There are no such residues in this entry.