wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 10:17 PM EST

PDB ID	:	3ULE
Title	:	Structure of Bos taurus Arp2/3 complex with bound inhibitor CK-869 and ATP
Authors	:	Nolen, B.J.; Han, M.
Deposited on	:	2011-11-10
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

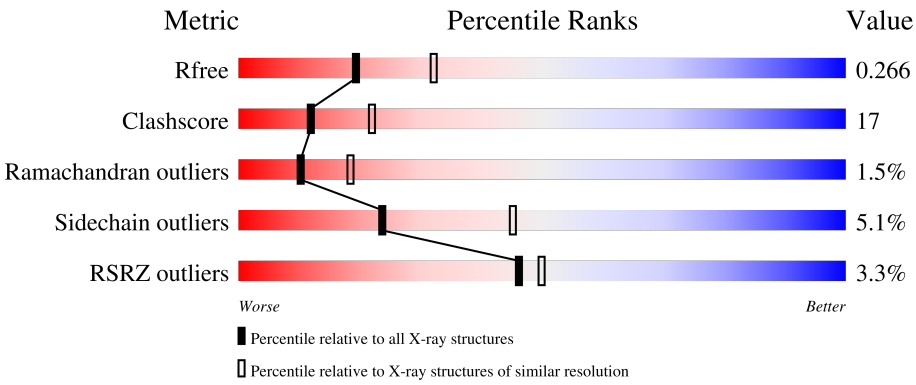
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	418	3% 67% 25% • •
2	B	394	8% 34% 22% • 40%
3	C	372	.% 67% 23% • 8%
4	D	300	.% 69% 23% • 6%
5	E	178	.% 59% 34% 5% •

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Mol	Chain	Length	Quality of chain
6	F	168	% 77% 22% ••
7	G	151	5% 67% 19% 5% 9%

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
9	C69	A	1002	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14186 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-related protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	3198	2055	532	596	15	0	0	0

- Molecule 2 is a protein called Actin-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1835	1181	308	340	6	0	0	0

- Molecule 3 is a protein called Actin-related protein 2/3 complex subunit 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	341	2649	1681	464	485	19	0	0	0

- Molecule 4 is a protein called Actin-related protein 2/3 complex subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	281	2264	1441	393	422	8	0	0	0

- Molecule 5 is a protein called Actin-related protein 2/3 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	174	1412	907	236	260	9	0	0	0

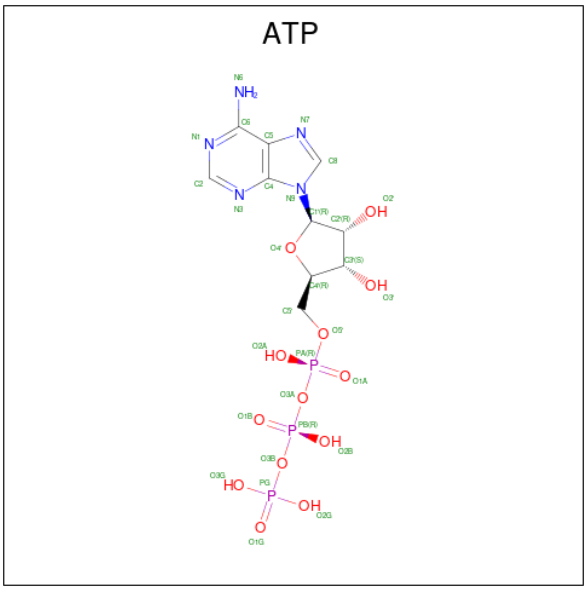
- Molecule 6 is a protein called Actin-related protein 2/3 complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	167	1371	875	239	248	9	0	0	0

- Molecule 7 is a protein called Actin-related protein 2/3 complex subunit 5.

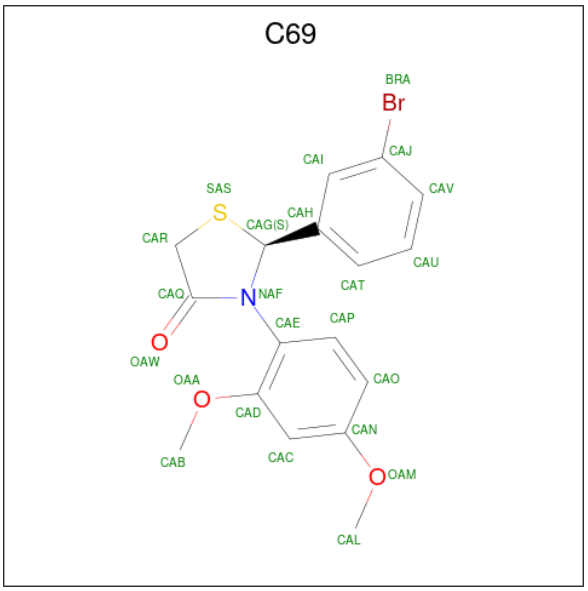
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	137	1045	654	183	205	3	0	0	0

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 9 is (2S)-2-(3-bromophenyl)-3-(2,4-dimethoxyphenyl)-1,3-thiazolidin-4-one (three-letter code: C69) (formula: $C_{17}H_{16}BrNO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
9	A	1	23	1	17	1	3	1	0	0

- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	57	57	57	0	0
11	B	27	27	27	0	0
11	C	77	77	77	0	0
11	D	72	72	72	0	0
11	E	23	23	23	0	0
11	F	51	51	51	0	0

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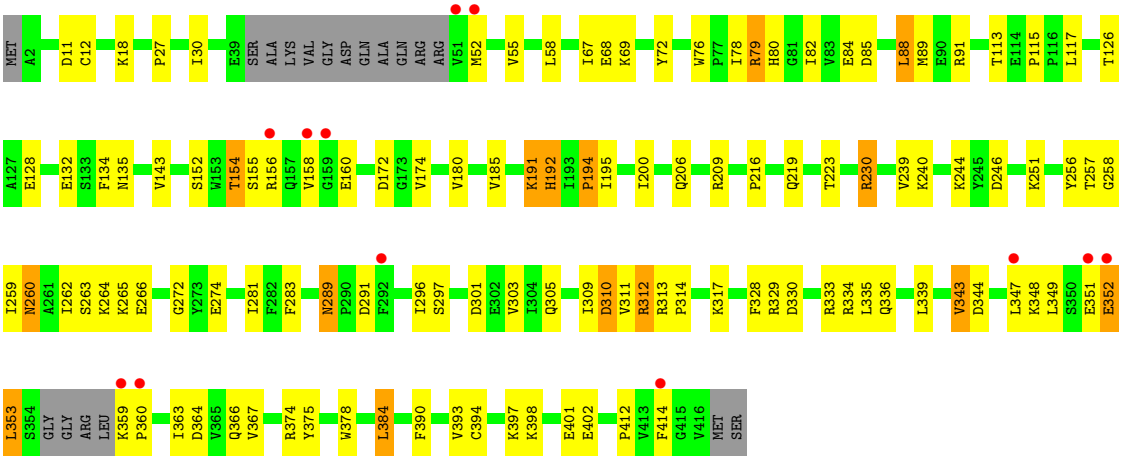
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	G	18	18	18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

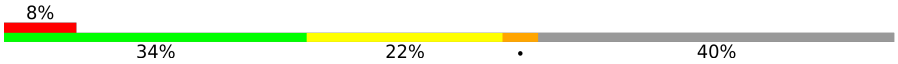
- Molecule 1: Actin-related protein 3

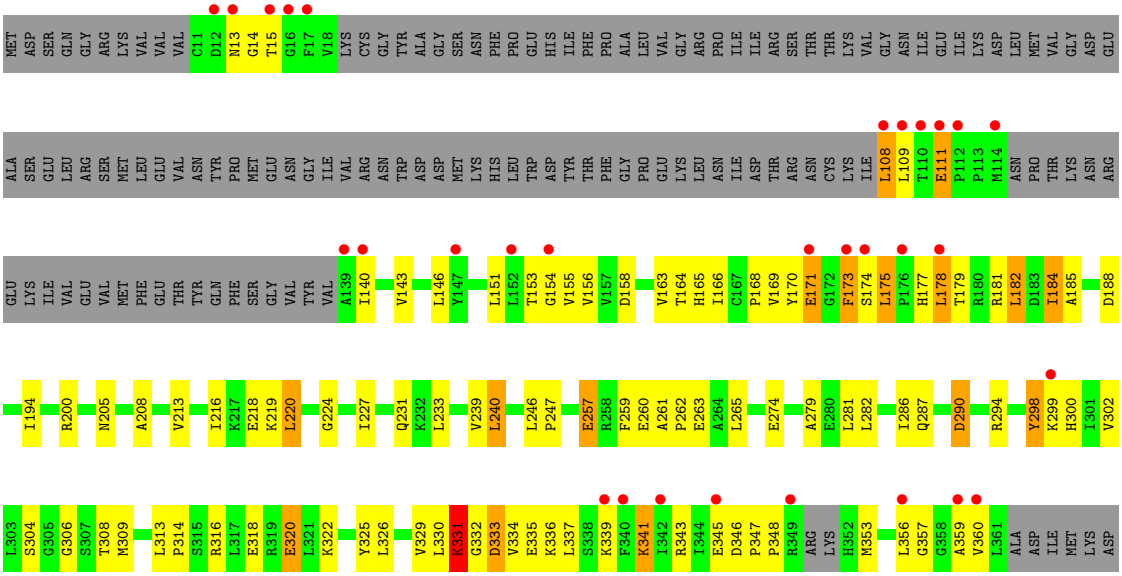
Chain A:



- Molecule 2: Actin-related protein 2

Chain B:





LYS ASP ASN PHE TRP MET THR ARG GLN GLU TYR GLN GLU LYS GLY VAL ARG VAL LEU GLU LYS LEU GLY VAL THR VAL ARG

- Molecule 3: Actin-related protein 2/3 complex subunit 1B

Chain C:

MET A2 L7 V8 E9 P10 H14 A15 W16 N17 K18 D19 R20 T21 Q22 I23 A24 P27 N28 N29 H30 E31 V32 H33 L48 Q54 G57 I58 P62 T69 A76 L81 R84 T85 L90 V91 I92 L93 A98 V102 R103 P106 N107 E108 K109

A112 S115 R118 V119 I120 F125 E126 Q127 D130 W131 K135 H136 I137 P140 T144 H151 P152 N153 S154 V155 L156 L157 R167 I168 K174 E175 E178 R179 P180 T183 P184 W185 F191 E197 S201 C209 D223 A249 V250 T251

T254 E255 S256 D264 C265 R284 V287 P288 LYS GLN SER SER GLN ARG GLY LEU THR ALA ARG GLU ARG PHE GLN ASN LEU ASP LYS LYS ALA SER SER GLU GLY SER ALA ALA ALA GLY A319 Q331 I332 C342 S343 Q344 F345 C346 G352 W357 D358 V359 L366 K367

D368 L369 K370 I371 V372

- Molecule 4: Actin-related protein 2/3 complex subunit 2

Chain D:

M1 V6 L15 D37 V41 I45 T53 K54 V55 M56 L61 K62 K65 E66 L67 Q68 A69 H70 G71 A72 L75 L84 L95 D107 M115 L116 K117 R118 N119 C120 S123 E126 F129 Q130 E134 G135 K136 R141 A142 V143 I144

R147 D148 D149 E150 E155 T167 K170 D171 D172 D173 D174 K186 V198 L199 F200 S201 H202 R203 E204 P205 P206 L207 E208 L209 K210 ASP T212 D213 A214 A215 V216 G217 D218 N219 I220 I223 T224 F228 H231 T232 N233 R237 I241 I244 H245 T246 F247 R248 D249

Y250 K256 C257 S258 I262 H263 M266 K269 R279 A280 R281 P282 ASP ALA GLU LYS LYS GLU MET LYS THR ILE THR GLY LYS THR PHE SER SER ARG

- Molecule 5: Actin-related protein 2/3 complex subunit 3

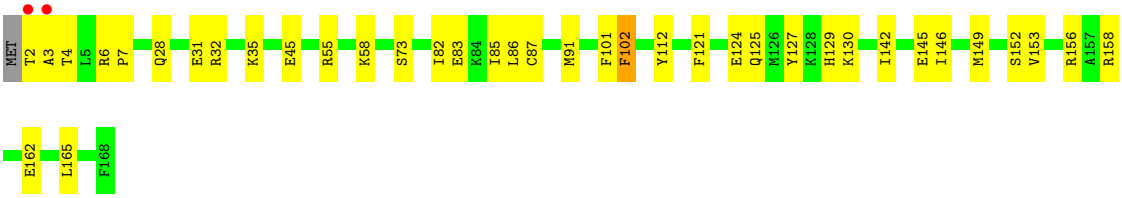
Chain E:

MET P2 A3 Y4 H5 M9 D10 P11 D12 T13 K14 L15 I16 G17 A20 L21 L22 R25 E35 T36 D40 Y48 F49 K50 K56 I60 K61 N62 E63 A64 D65 I69 Y70 I71 Y74 I75 S76 E77 C78 L79 K80 K81 L82 N86 S87 K88 E92

M95 T101 I105 P106 F111 P112 L113 N114 A115 I116 Y117 K123 D126 E127 R130 L133 R137 Q138 G141 L144 C145 E146 F149 D150 P151 Q152 N153 D154 K155 P156 K165 R166 Q167 F168 M169 N170 G175 PRO GLY GLN

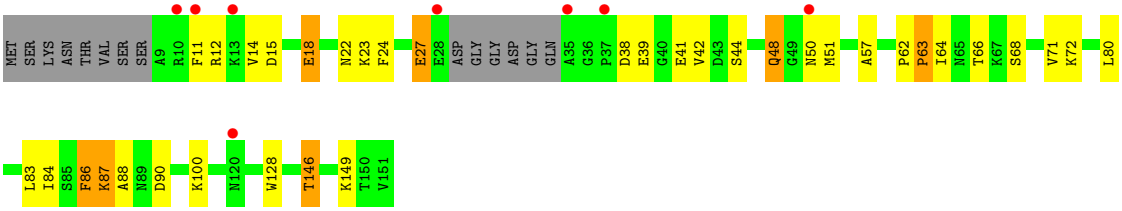
- Molecule 6: Actin-related protein 2/3 complex subunit 4

Chain F:



• Molecule 7: Actin-related protein 2/3 complex subunit 5

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	111.17Å 128.31Å 198.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 49.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 84.6 (49.62-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.274 0.217 , 0.266	Depositor DCC
R_{free} test set	4711 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14186	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, 0.333 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: C69, CA, 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	0.37	0/3279	0.61	0/4450
2	B	0.33	0/1866	0.59	0/2525
3	C	0.37	0/2718	0.65	0/3689
4	D	0.38	0/2312	0.59	0/3121
5	E	0.35	0/1446	0.60	1/1950 (0.1%)
6	F	0.40	0/1393	0.63	0/1868
7	G	0.35	0/1057	0.61	0/1421
All	All	0.37	0/14071	0.61	1/19024 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	17	GLY	N-CA-C	-5.42	99.56	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	3198	0	3143	120	0
2	B	1835	0	1859	102	0
3	C	2649	0	2604	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2264	0	2230	64	0
5	E	1412	0	1414	64	0
6	F	1371	0	1410	26	0
7	G	1045	0	1059	29	0
8	A	31	0	12	3	0
8	B	31	0	12	2	0
9	A	23	0	16	9	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	57	0	0	2	0
11	B	27	0	0	1	0
11	C	77	0	0	6	0
11	D	72	0	0	2	0
11	E	23	0	0	3	0
11	F	51	0	0	1	0
11	G	18	0	0	1	0
All	All	14186	0	13759	478	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 17.

The worst 5 of 478 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)
3:C:17:ASN:HD21	3:C:21:THR:HG22	1.13	1.10
3:C:223:ASP:HB3	7:G:146:THR:HG21	1.44	1.00
6:F:4:THR:HG23	6:F:55:ARG:HE	1.22	1.00
1:A:115:PRO:HD3	9:A:1002:C69:H2	1.45	0.97
3:C:223:ASP:CB	7:G:146:THR:HG21	1.97	0.94

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	394/418 (94%)	367 (93%)	23 (6%)	4 (1%)	15	28
2	B	228/394 (58%)	205 (90%)	18 (8%)	5 (2%)	6	10
3	C	337/372 (91%)	314 (93%)	21 (6%)	2 (1%)	25	43
4	D	277/300 (92%)	266 (96%)	9 (3%)	2 (1%)	22	39
5	E	172/178 (97%)	160 (93%)	6 (4%)	6 (4%)	3	4
6	F	165/168 (98%)	157 (95%)	7 (4%)	1 (1%)	25	43
7	G	133/151 (88%)	117 (88%)	10 (8%)	6 (4%)	2	3
All	All	1706/1981 (86%)	1586 (93%)	94 (6%)	26 (2%)	10	18

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	113	LEU
5	E	153	ASN
1	A	52	MET
2	B	171	GLU
2	B	178	LEU

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	349/363 (96%)	328 (94%)	21 (6%)	19	37
2	B	197/345 (57%)	183 (93%)	14 (7%)	14	28
3	C	290/313 (93%)	277 (96%)	13 (4%)	27	51
4	D	245/264 (93%)	236 (96%)	9 (4%)	34	60
5	E	155/159 (98%)	147 (95%)	8 (5%)	23	44
6	F	154/155 (99%)	150 (97%)	4 (3%)	46	72
7	G	112/123 (91%)	105 (94%)	7 (6%)	18	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1502/1722 (87%)	1426 (95%)	76 (5%)	24 45

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	10	ASP
7	G	39	GLU
5	E	82	LEU
6	F	85	ILE
7	G	146	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	33	HIS
6	F	28	GLN
3	C	65	ASN
7	G	48	GLN
4	D	263	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
8	ATP	A	1001	10	26,33,33	1.17	1 (3%)	31,52,52	1.61	4 (12%)
9	C69	A	1002	-	25,25,25	1.80	3 (12%)	33,35,35	2.54	9 (27%)
8	ATP	B	401	10	26,33,33	1.33	3 (11%)	31,52,52	2.14	11 (35%)

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
8	ATP	A	1001	10	-	7/18/38/38	0/3/3/3
9	C69	A	1002	-	-	8/12/25/25	0/3/3/3
8	ATP	B	401	10	-	2/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1002	C69	CAE-NAF	-7.41	1.34	1.43
8	B	401	ATP	C2-N1	3.54	1.40	1.33
8	A	1001	ATP	C2-N1	3.53	1.40	1.33
9	A	1002	C69	CAQ-NAF	-3.35	1.33	1.37
8	B	401	ATP	PG-O1G	3.31	1.61	1.50

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1002	C69	CAR-CAQ-NAF	7.85	117.51	112.14
9	A	1002	C69	CAQ-CAR-SAS	-6.85	101.74	107.60
8	A	1001	ATP	N3-C2-N1	-5.18	120.58	128.68
8	B	401	ATP	N3-C2-N1	-5.05	120.78	128.68
9	A	1002	C69	CAB-OAA-CAD	-5.04	109.92	117.53

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	ATP	PB-O3B-PG-O2G
8	A	1001	ATP	C5'-O5'-PA-O2A
9	A	1002	C69	CAD-CAE-NAF-CAQ
9	A	1002	C69	CAD-CAE-NAF-CAG
9	A	1002	C69	CAP-CAE-NAF-CAQ

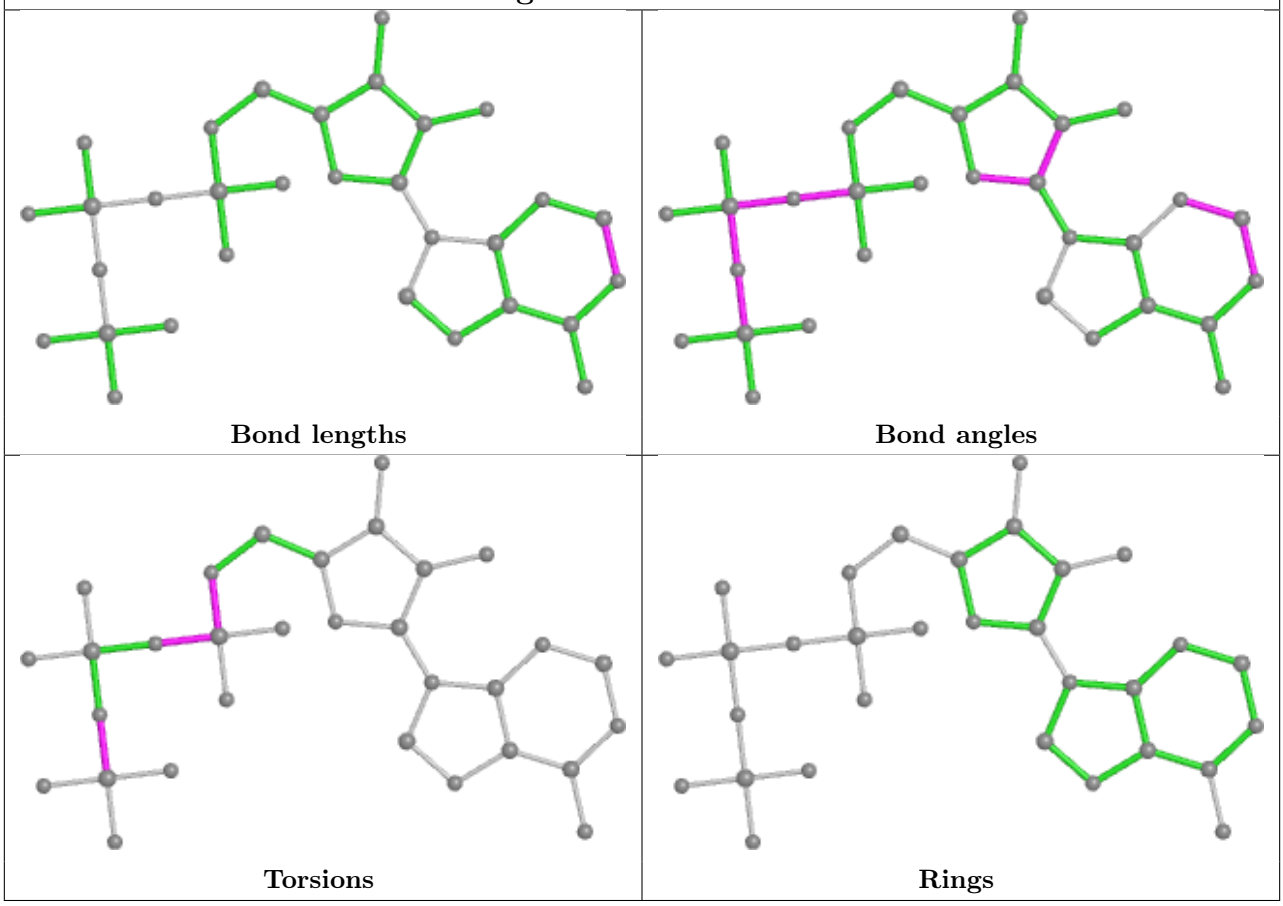
There are no ring outliers.

3 monomers are involved in 14 short contacts:

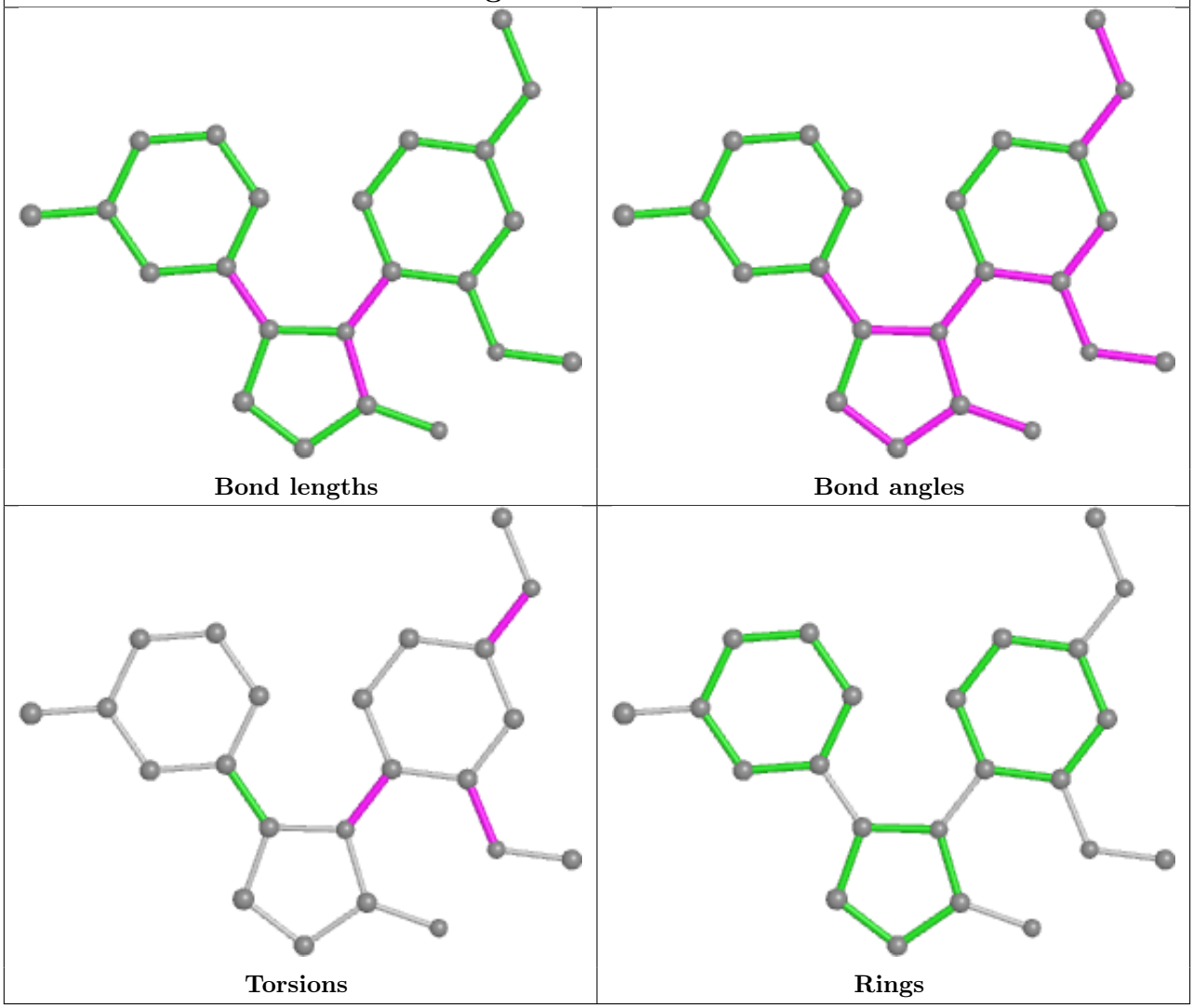
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1001	ATP	3	0
9	A	1002	C69	9	0
8	B	401	ATP	2	0

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 then 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.

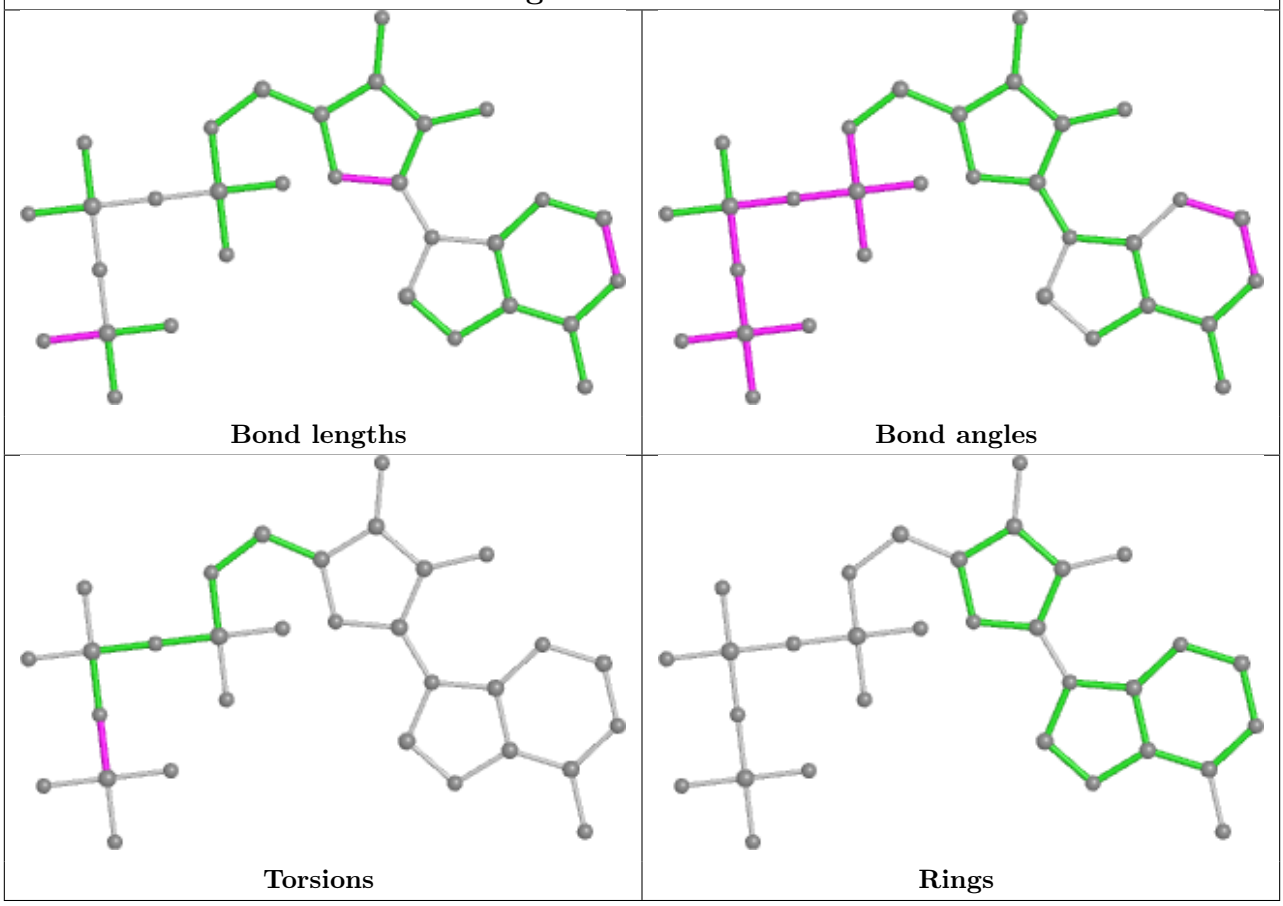
Ligand ATP A 1001



Ligand C69 A 1002



Ligand ATP B 401



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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	400/418 (95%)	0.10	12 (3%) 50 53	20, 40, 74, 93	0
2	B	236/394 (59%)	0.58	30 (12%) 3 3	26, 55, 94, 99	0
3	C	341/372 (91%)	-0.16	2 (0%) 89 90	25, 35, 63, 81	0
4	D	281/300 (93%)	-0.25	3 (1%) 80 82	19, 37, 63, 98	0
5	E	174/178 (97%)	-0.09	1 (0%) 89 90	30, 45, 68, 90	0
6	F	167/168 (99%)	-0.22	2 (1%) 79 80	18, 31, 44, 78	0
7	G	137/151 (90%)	0.20	8 (5%) 23 24	26, 52, 84, 94	0
All	All	1736/1981 (87%)	0.02	58 (3%) 46 50	18, 39, 82, 99	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	VAL	7.6
2	B	114	MET	6.2
1	A	52	MET	5.6
2	B	109	LEU	5.4
2	B	360	VAL	5.1

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 monosaccharides in this entry.

6.4 Ligands (i)

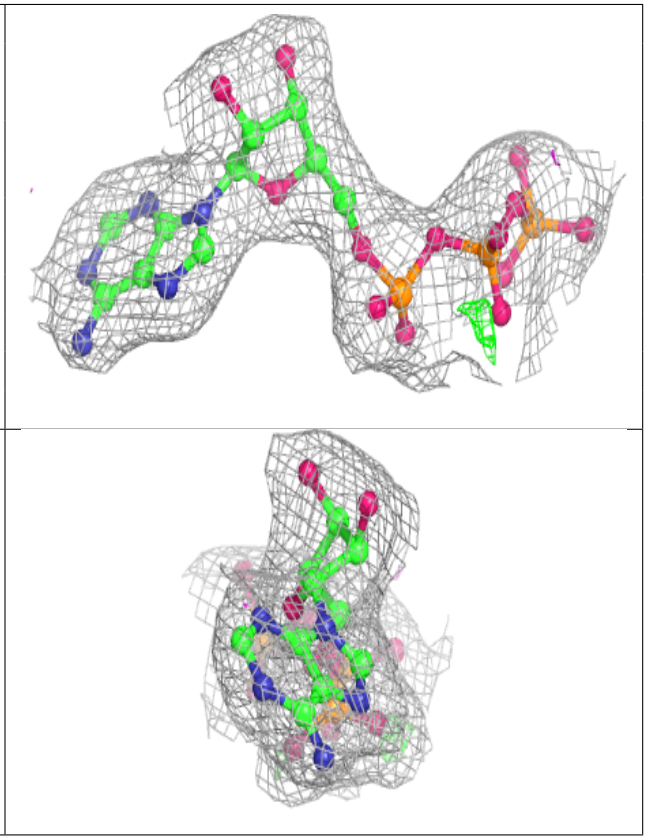
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CA	B	402	1/1	0.88	0.17	70,70,70,70	0
10	CA	A	1003	1/1	0.89	0.29	61,61,61,61	0
8	ATP	B	401	31/31	0.95	0.11	35,39,52,54	0
9	C69	A	1002	23/23	0.95	0.19	44,46,51,52	0
8	ATP	A	1001	31/31	0.97	0.16	31,38,41,43	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.

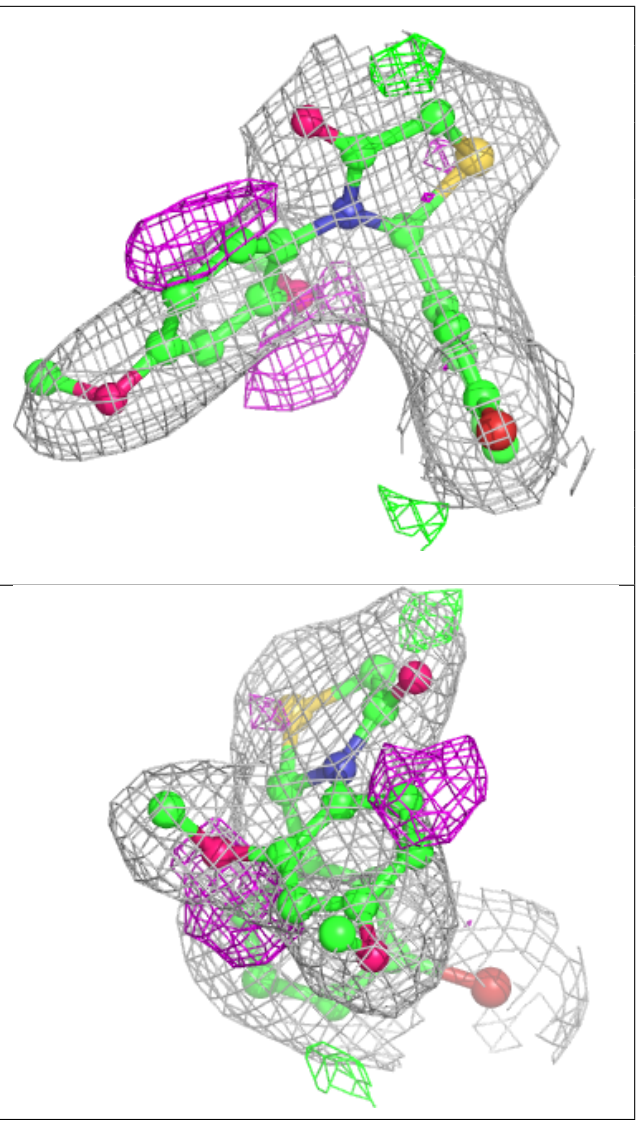
Electron density around ATP B 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



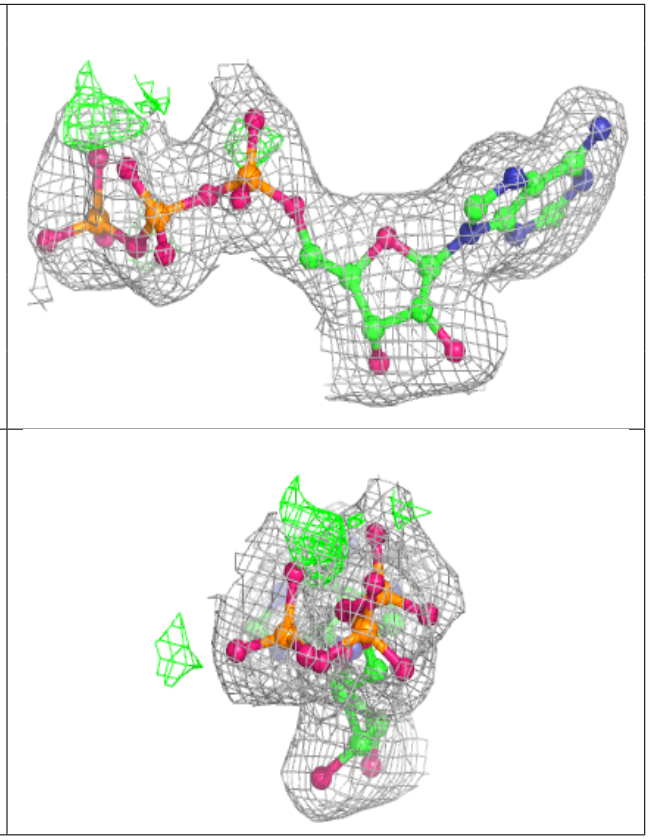
Electron density around C69 A 1002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ATP A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.