



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:12 AM UTC

PDB ID : 6I4G / pdb_00006i4g
Title : Crystal Structure of Plasmodium falciparum actin I (H74Q) in the Mg-K-ATP state
Authors : Kumpula, E.-P.; Lopez, A.J.; Tajedin, L.; Han, H.; Kursula, I.
Deposited on : 2018-11-09
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

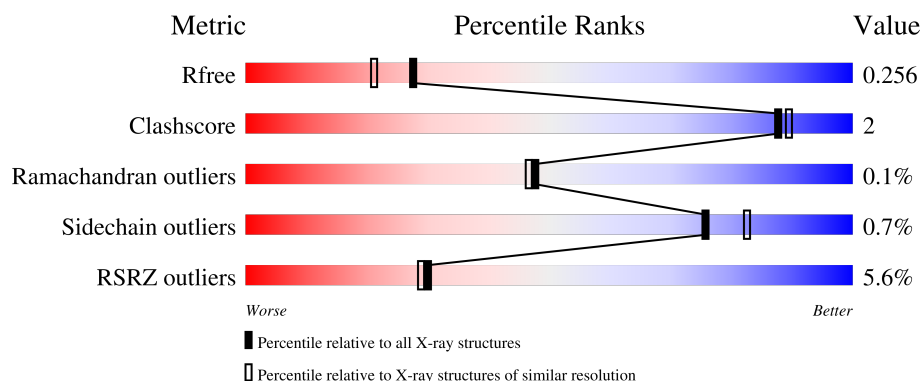
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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 $\leq 5\%$. 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	378	 7% 89% 5% • 6%
1	B	378	 4% 90% • 6%
2	G	127	 5% 92% • 5%
2	H	127	 3% 94% ...

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 15581 atoms, of which 7515 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-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	356	Total	C	H	N	O	S	0	8	0
			5633	1787	2814	474	545	13			
1	B	356	Total	C	H	N	O	S	0	5	0
			5596	1778	2788	472	545	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8I4X0
A	0	ALA	-	expression tag	UNP Q8I4X0
A	74	GLN	HIS	engineered mutation	UNP Q8I4X0
B	-1	GLY	-	expression tag	UNP Q8I4X0
B	0	ALA	-	expression tag	UNP Q8I4X0
B	74	GLN	HIS	engineered mutation	UNP Q8I4X0

- Molecule 2 is a protein called Gelsolin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	121	Total	C	H	N	O	S	0	1	0
			1886	624	922	157	182	1			
2	H	124	Total	C	H	N	O	S	0	1	0
			1942	640	951	164	186	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP P13020
G	0	PRO	-	expression tag	UNP P13020
H	-1	GLY	-	expression tag	UNP P13020
H	0	PRO	-	expression tag	UNP P13020

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		
3	B	1	Total	C	H	N	O	P	0	0
			42	10	11	5	13	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	K	0	0
			1	1		
5	B	1	Total	K	0	0
			1	1		

- Molecule 6 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	G	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	H	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	Ca	0	0
			2	2		
7	H	2	Total	Ca	0	0
			2	2		

- Molecule 8 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).

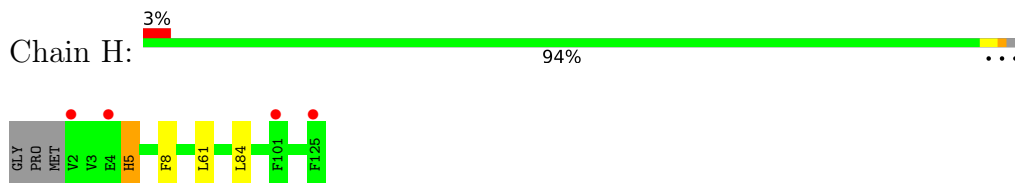
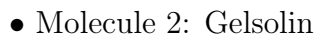


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	G	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	139	Total	O	0	0
			139	139		
9	B	140	Total	O	0	0
			140	140		
9	G	59	Total	O	0	0
			59	59		
9	H	61	Total	O	0	0
			61	61		

- Molecule 1: Actin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.61Å 110.62Å 138.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.00 48.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.80-2.00) 95.1 (48.80-2.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.216 , 0.257 0.217 , 0.256	Depositor DCC
R_{free} test set	1395 reflections (1.03%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15581	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9298e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, SCN, CA, K, BME, 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	0.23	0/2908	0.33	0/3937
1	B	0.25	0/2877	0.34	0/3894
2	G	0.25	0/993	0.34	0/1341
2	H	0.26	0/1021	0.34	0/1380
All	All	0.24	0/7799	0.33	0/10552

There are no bond length outliers.

There are no bond angle outliers.

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	2819	2814	2801	13	0
1	B	2808	2788	2784	13	0
2	G	964	922	920	4	0
2	H	991	951	951	2	0
3	A	31	11	12	0	0
3	B	31	11	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	B	4	6	6	0	0
6	G	4	6	6	0	0
6	H	4	6	6	0	0
7	G	2	0	0	0	0
7	H	2	0	0	0	0
8	G	3	0	0	0	0
9	A	139	0	0	4	0
9	B	140	0	0	4	0
9	G	59	0	0	3	0
9	H	61	0	0	0	0
All	All	8066	7515	7498	31	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 2.

All (31) 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:66:LEU:O	9:B:501:HOH:O	1.98	0.82
1:A:29:ARG:NH2	9:A:504:HOH:O	2.18	0.75
1:B:64:GLY:O	1:B:66:LEU:N	2.19	0.75
1:B:335[A]:GLU:OE2	9:B:502:HOH:O	2.05	0.72
1:A:223:ASN:OD1	9:A:501:HOH:O	2.10	0.70
2:G:55:GLY:N	9:G:302:HOH:O	2.23	0.70
1:B:35:ILE:HD11	1:B:70:TYR:CZ	2.28	0.69
1:A:287:ASP:OD2	9:A:502:HOH:O	2.11	0.68
1:A:155[B]:ASP:OD1	9:A:503:HOH:O	2.16	0.61
2:G:7:GLU:OE2	9:G:301:HOH:O	2.16	0.60
1:B:100:GLU:OE1	9:B:503:HOH:O	2.16	0.60
1:B:335[B]:GLU:N	1:B:335[B]:GLU:OE1	2.31	0.59
1:A:202:SER:N	1:A:206:GLU:OE1	2.35	0.56
1:A:325[B]:THR:CG2	1:A:326:MET:HE2	2.38	0.54
2:G:111:LYS:N	9:G:304:HOH:O	2.42	0.53
1:A:304:THR:O	1:A:304:THR:HG22	2.10	0.50
1:B:304:THR:HG22	1:B:304:THR:O	2.12	0.49
1:B:222:LEU:O	1:B:316:ARG:NH2	2.47	0.48
1:B:184:ARG:NH1	9:B:508:HOH:O	2.48	0.46
1:B:352:THR:HB	2:G:3:VAL:HG11	1.97	0.46
1:A:105:LEU:C	1:A:105:LEU:HD23	2.42	0.45
1:A:347:LEU:HD11	1:A:356:MET:HE1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:GLU:OE1	1:A:312:GLU:N	2.43	0.45
1:B:35:ILE:HD11	1:B:70:TYR:CE1	2.52	0.44
2:H:5:HIS:O	2:H:8:PHE:N	2.48	0.44
1:B:312:GLU:OE1	1:B:312:GLU:N	2.41	0.44
1:A:60:GLN:O	1:A:63:ARG:HG2	2.19	0.43
1:B:263:PHE:CZ	1:B:275:ILE:HD11	2.55	0.42
2:H:61:LEU:HD21	2:H:84:LEU:HD23	2.02	0.41
1:A:181:LEU:HD23	1:A:182:ALA:N	2.36	0.41

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	360/378 (95%)	353 (98%)	7 (2%)	0	100	100
1	B	355/378 (94%)	349 (98%)	6 (2%)	0	100	100
2	G	118/127 (93%)	116 (98%)	2 (2%)	0	100	100
2	H	123/127 (97%)	121 (98%)	1 (1%)	1 (1%)	16	11
All	All	956/1010 (95%)	939 (98%)	16 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	5	HIS

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	313/322 (97%)	307 (98%)	6 (2%)	50	56
1	B	310/322 (96%)	309 (100%)	1 (0%)	86	91
2	G	101/105 (96%)	101 (100%)	0	100	100
2	H	104/105 (99%)	104 (100%)	0	100	100
All	All	828/854 (97%)	821 (99%)	7 (1%)	76	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	65	ILE
1	A	179	LEU
1	A	195	HIS
1	A	325[A]	THR
1	A	325[B]	THR
1	B	372	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	HIS
1	B	7	GLN
1	B	89	HIS
2	H	89	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	B	401	5,4	32,33,33	3.78	6 (18%)	48,52,52	1.95	8 (16%)
6	BME	G	203	-	3,3,3	0.26	0	2,2,2	0.14	0
6	BME	B	404	-	3,3,3	0.34	0	2,2,2	0.14	0
8	SCN	G	204	-	1,2,2	1.00	0	0,1,1	-	-
6	BME	H	203	-	3,3,3	0.28	0	2,2,2	0.15	0
3	ATP	A	401	5,4	32,33,33	3.40	4 (12%)	48,52,52	1.85	10 (20%)

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	B	401	5,4	-	3/22/38/38	0/3/3/3
6	BME	G	203	-	-	0/1/1/1	-
6	BME	B	404	-	-	1/1/1/1	-
6	BME	H	203	-	-	1/1/1/1	-
3	ATP	A	401	5,4	-	2/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	PB-O3A	19.20	1.80	1.59
3	A	401	ATP	PB-O3A	17.28	1.78	1.59
3	B	401	ATP	PA-O5'	5.50	1.80	1.59
3	A	401	ATP	PA-O5'	4.44	1.76	1.59
3	B	401	ATP	C8-N9	3.27	1.43	1.37
3	A	401	ATP	PA-O3A	-2.90	1.56	1.59
3	A	401	ATP	C8-N9	2.87	1.42	1.37
3	B	401	ATP	O2'-C2'	-2.41	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ATP	PA-O3A	-2.36	1.56	1.59
3	B	401	ATP	C4-N3	2.00	1.38	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ATP	O2B-PB-O3B	6.40	124.58	107.27
3	B	401	ATP	O3A-PB-O1B	-5.89	92.99	110.70
3	A	401	ATP	O2B-PB-O3A	-5.41	92.66	107.27
3	B	401	ATP	O2A-PA-O3A	4.87	120.43	107.27
3	A	401	ATP	O3B-PB-O1B	4.51	124.28	110.70
3	A	401	ATP	O3A-PB-O1B	-4.28	97.81	110.70
3	B	401	ATP	O5'-PA-O1A	-3.31	95.81	108.94
3	A	401	ATP	O3A-PA-O1A	3.23	120.41	110.70
3	A	401	ATP	O3G-PG-O2G	3.07	119.32	107.80
3	B	401	ATP	O2B-PB-O3A	-2.96	99.26	107.27
3	B	401	ATP	O2A-PA-O5'	-2.96	94.17	107.57
3	A	401	ATP	O5'-PA-O1A	-2.90	97.44	108.94
3	A	401	ATP	O2A-PA-O5'	-2.67	95.48	107.57
3	A	401	ATP	O3G-PG-O3B	-2.58	95.99	104.64
3	B	401	ATP	O3G-PG-O3B	-2.46	96.40	104.64
3	B	401	ATP	PA-O5'-C5'	-2.31	108.12	121.35
3	A	401	ATP	PA-O5'-C5'	-2.25	108.45	121.35
3	A	401	ATP	O2B-PB-O3B	2.01	112.70	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

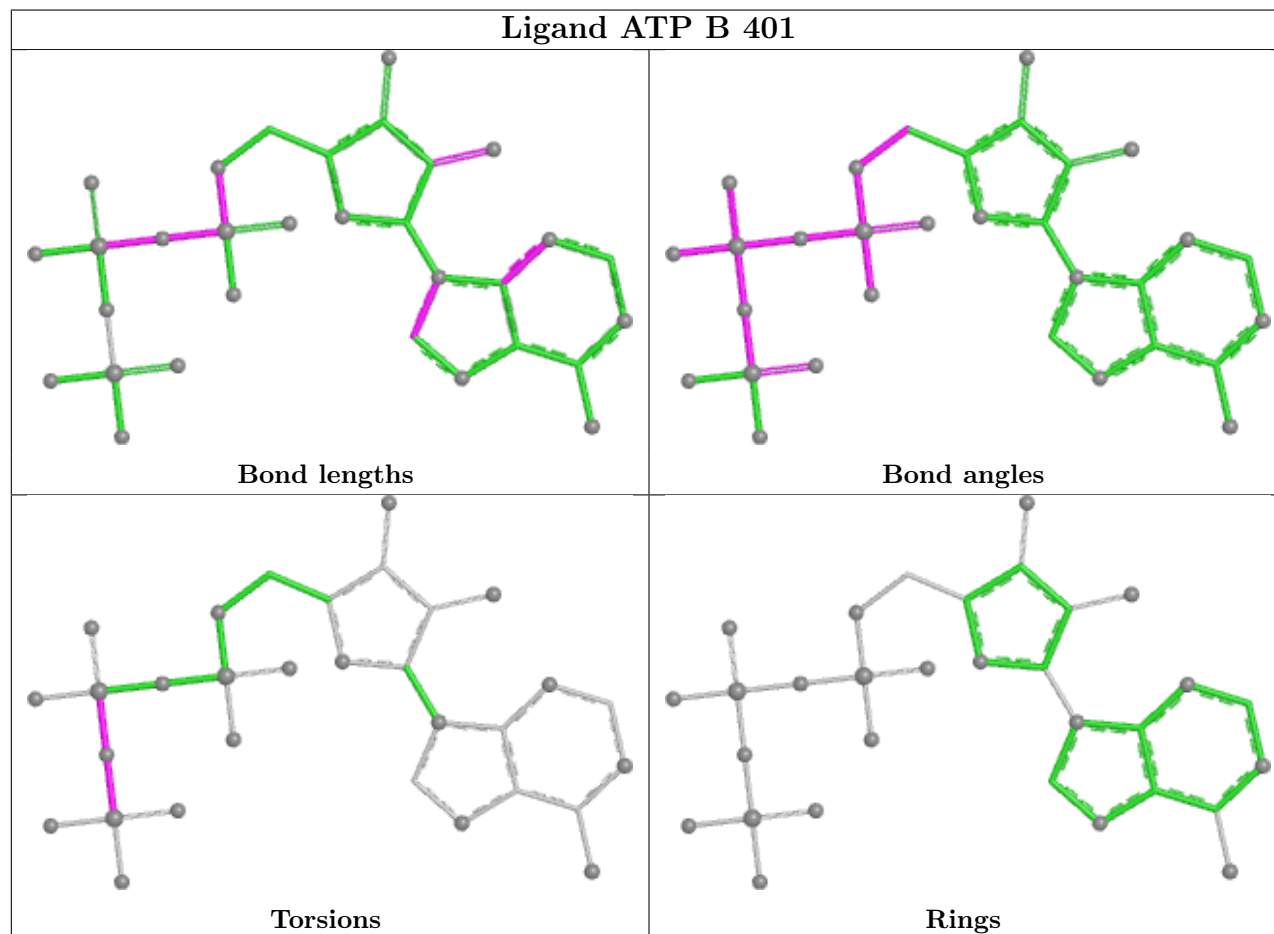
Mol	Chain	Res	Type	Atoms
3	B	401	ATP	PB-O3B-PG-O2G
6	B	404	BME	O1-C1-C2-S2
3	A	401	ATP	PB-O3B-PG-O2G
3	B	401	ATP	PG-O3B-PB-O2B
3	B	401	ATP	PB-O3B-PG-O1G
3	A	401	ATP	PG-O3B-PB-O2B
6	H	203	BME	O1-C1-C2-S2

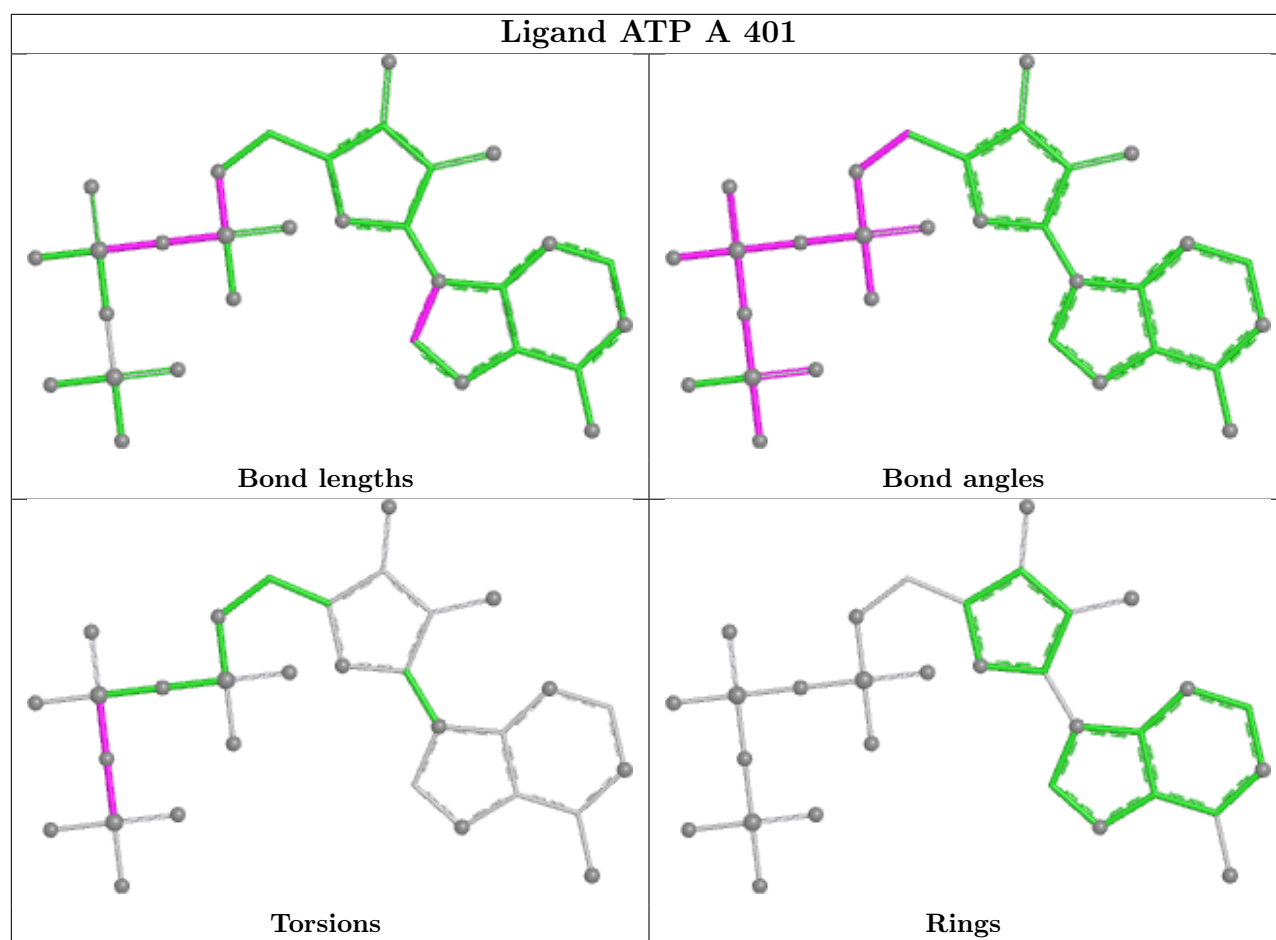
There are no ring outliers.

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](#)

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, 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	356/378 (94%)	0.57	27 (7%)	20 18	16, 43, 90, 132	7 (1%)
1	B	356/378 (94%)	0.43	17 (4%)	35 34	17, 39, 87, 133	5 (1%)
2	G	121/127 (95%)	0.41	6 (4%)	34 33	21, 40, 77, 134	1 (0%)
2	H	124/127 (97%)	0.32	4 (3%)	50 49	21, 39, 72, 157	1 (0%)
All	All	957/1010 (94%)	0.47	54 (5%)	30 29	16, 40, 88, 157	14 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	VAL	5.0
2	H	2	VAL	4.4
1	A	201	PHE	4.1
1	B	39	PRO	4.1
2	G	3	VAL	3.6
1	A	39	PRO	3.6
1	A	180	ASP	3.2
1	B	66	LEU	3.2
1	B	68	LEU	3.2
1	B	357	TRP	3.1
2	G	111	LYS	3.0
1	B	245	ASP	2.9
1	B	29	ARG	2.9
1	B	54	PHE	2.8
2	G	2	VAL	2.8
2	G	112	SER	2.8
2	H	101	PHE	2.7
1	A	70	TYR	2.7
1	B	64	GLY	2.7
1	A	53	ALA	2.6
1	A	170	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	55	GLY	2.6
1	A	365	GLU	2.6
1	B	63	ARG	2.6
1	A	248	ILE	2.6
1	A	357	TRP	2.6
1	A	67	THR	2.6
1	A	63	ARG	2.5
1	B	81	ASP	2.4
2	H	125	PHE	2.4
1	B	179	LEU	2.3
1	A	195	HIS	2.3
1	A	205	ALA	2.3
1	B	269	GLY	2.3
1	A	17	ASN	2.3
1	B	67	THR	2.2
1	B	38	ARG	2.2
1	A	246	GLY	2.2
1	A	247	ASN	2.2
1	A	203	THR	2.2
1	B	233	GLN	2.2
1	A	179	LEU	2.2
2	H	4	GLU	2.1
1	A	181	LEU	2.1
1	A	245	ASP	2.1
1	A	271	GLU	2.1
1	A	65	ILE	2.1
1	B	372	HIS	2.1
1	B	40	LYS	2.1
1	A	157	GLY	2.1
1	A	202	SER	2.0
2	G	114	LEU	2.0
1	A	64	GLY	2.0
1	A	199	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

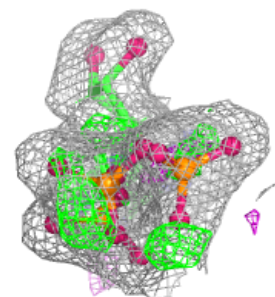
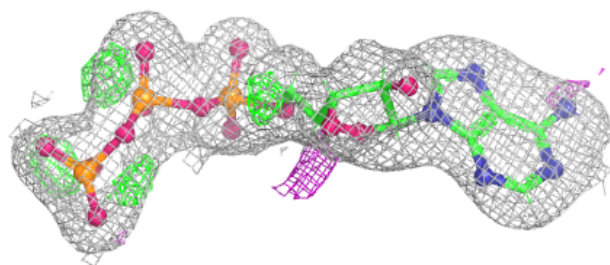
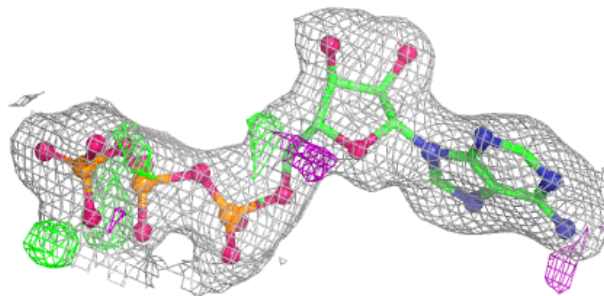
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	BME	H	203	4/4	0.71	0.32	88,107,128,128	0
6	BME	G	203	4/4	0.79	0.32	87,104,117,117	0
8	SCN	G	204	3/3	0.80	0.31	65,65,74,75	0
6	BME	B	404	4/4	0.85	0.15	75,90,92,92	0
3	ATP	A	401	31/31	0.95	0.08	24,30,43,48	0
4	MG	A	402	1/1	0.96	0.05	29,29,29,29	0
5	K	A	403	1/1	0.96	0.10	37,37,37,37	0
7	CA	G	202	1/1	0.96	0.07	51,51,51,51	0
3	ATP	B	401	31/31	0.96	0.07	20,27,33,36	0
7	CA	H	201	1/1	0.97	0.04	25,25,25,25	0
7	CA	G	201	1/1	0.98	0.03	33,33,33,33	0
7	CA	H	202	1/1	0.98	0.09	45,45,45,45	0
4	MG	B	402	1/1	0.98	0.03	22,22,22,22	0
5	K	B	403	1/1	0.99	0.06	23,23,23,23	1

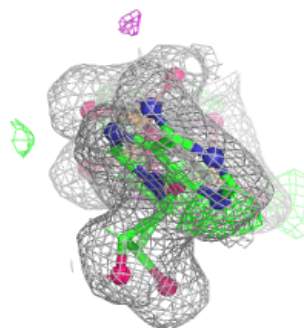
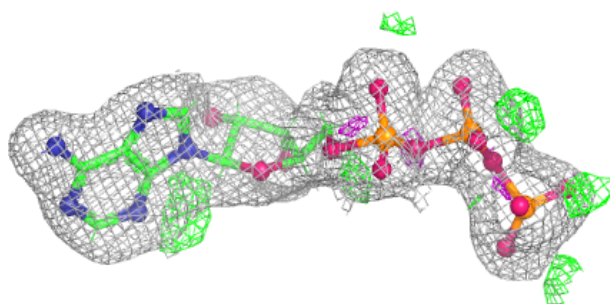
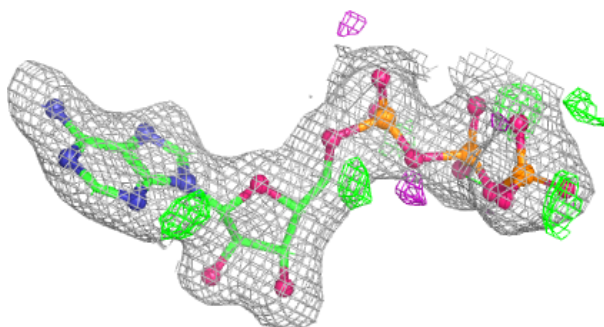
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ATP A 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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.