



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:33 AM UTC

PDB ID : 6JWQ / pdb_00006jwq
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS wild type
Authors : Chitnumsub, P.; Jaruwat, A.; Yuthavong, Y.
Deposited on : 2019-04-21
Resolution : 2.50 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

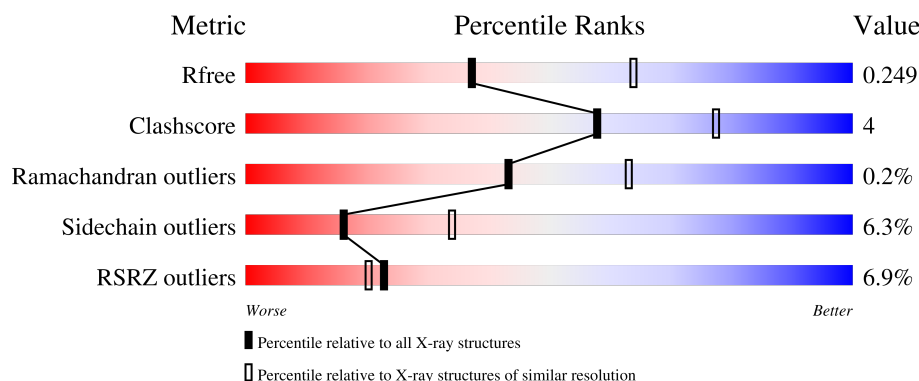
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	728	5% 63% 11% 25%
1	B	728	6% 68% 12% 19%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9605 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 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4544	2923	753	845	23			
1	B	590	Total	C	N	O	S	0	0	0
			4866	3132	801	907	26			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	UNP Q25704
A	714	VAL	-	expression tag	UNP Q25704
A	715	ASP	-	expression tag	UNP Q25704
A	716	LYS	-	expression tag	UNP Q25704
A	717	LEU	-	expression tag	UNP Q25704
A	718	ALA	-	expression tag	UNP Q25704
A	719	ALA	-	expression tag	UNP Q25704
A	720	ALA	-	expression tag	UNP Q25704
A	721	LEU	-	expression tag	UNP Q25704
A	722	GLU	-	expression tag	UNP Q25704
A	723	HIS	-	expression tag	UNP Q25704
A	724	HIS	-	expression tag	UNP Q25704
A	725	HIS	-	expression tag	UNP Q25704
A	726	HIS	-	expression tag	UNP Q25704
A	727	HIS	-	expression tag	UNP Q25704
A	728	HIS	-	expression tag	UNP Q25704
B	707	LYS	-	expression tag	UNP Q25704
B	708	ASP	-	expression tag	UNP Q25704

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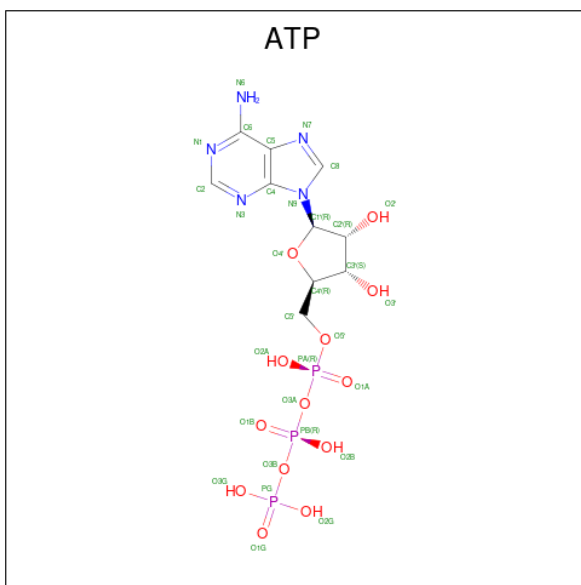
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Chain	Residue	Modelled	Actual	Comment	Reference
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	UNP Q25704
B	716	LYS	-	expression tag	UNP Q25704
B	717	LEU	-	expression tag	UNP Q25704
B	718	ALA	-	expression tag	UNP Q25704
B	719	ALA	-	expression tag	UNP Q25704
B	720	ALA	-	expression tag	UNP Q25704
B	721	LEU	-	expression tag	UNP Q25704
B	722	GLU	-	expression tag	UNP Q25704
B	723	HIS	-	expression tag	UNP Q25704
B	724	HIS	-	expression tag	UNP Q25704
B	725	HIS	-	expression tag	UNP Q25704
B	726	HIS	-	expression tag	UNP Q25704
B	727	HIS	-	expression tag	UNP Q25704
B	728	HIS	-	expression tag	UNP Q25704

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

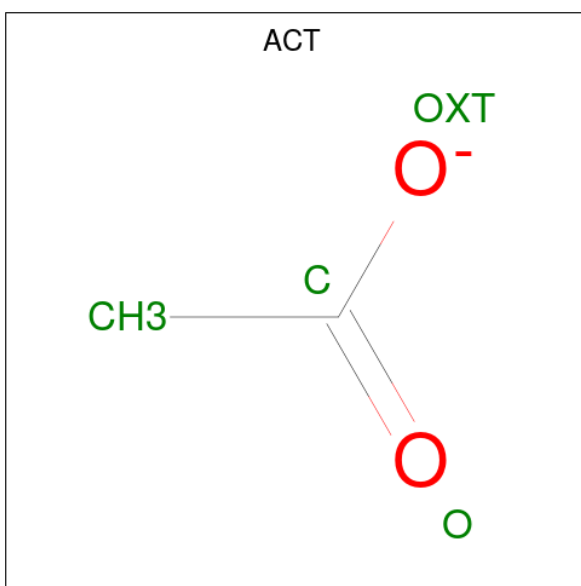


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

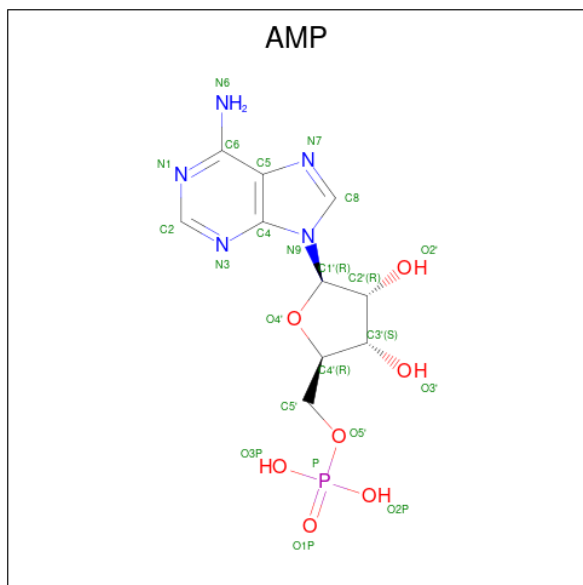
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O P 23 10 5 7 1	0	0

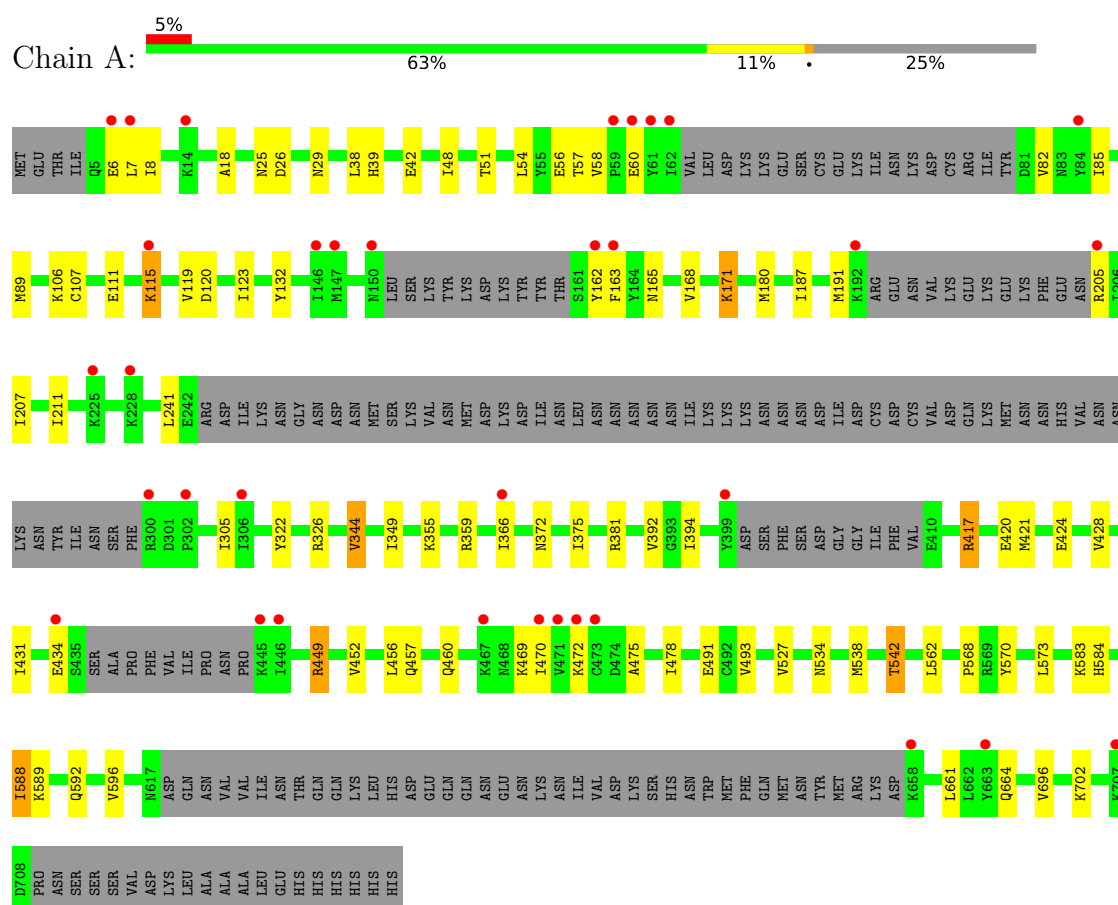
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	70	Total O 70 70	0	0
7	B	60	Total O 60 60	0	0

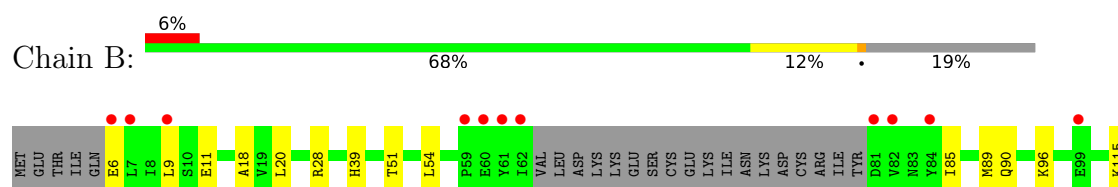
3 Residue-property plots [i](#)

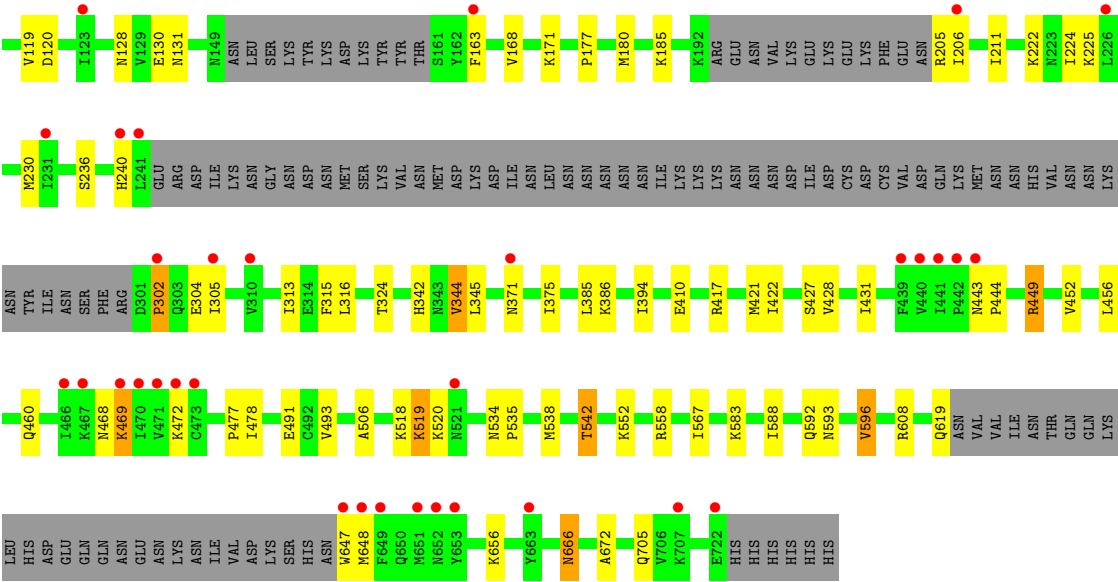
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase



- Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.17Å 137.22Å 139.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.50) 97.1 (30.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.205 , 0.257 0.199 , 0.249	Depositor DCC
R_{free} test set	6645 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9605	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.67	0/4613	1.02	2/6217 (0.0%)
1	B	0.68	0/4948	1.03	3/6677 (0.0%)
All	All	0.67	0/9561	1.02	5/12894 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	LYS	N-CA-C	7.37	119.00	110.97
1	B	115	LYS	N-CA-C	6.40	118.79	111.11
1	B	222	LYS	N-CA-C	5.52	117.16	111.03
1	A	60	GLU	N-CA-C	5.29	117.74	111.33
1	B	538	MET	N-CA-C	5.28	118.50	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	4544	0	4645	44	0
1	B	4866	0	4950	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	12	0	0
4	A	1	0	0	0	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	23	0	12	0	0
7	A	70	0	0	0	0
7	B	60	0	0	0	0
All	All	9605	0	9625	86	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 4.

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:B:443:ASN:HB3	1:B:444:PRO:HD3	1.58	0.84
1:A:449:ARG:HH11	1:A:449:ARG:HG3	1.49	0.77
1:A:51:THR:HG22	1:A:168:VAL:HG12	1.67	0.74
1:B:608:ARG:HA	1:B:666:ASN:ND2	2.01	0.74
1:B:449:ARG:HH11	1:B:449:ARG:HG3	1.53	0.74
1:A:18:ALA:HB1	1:A:180:MET:HE1	1.70	0.74
1:B:608:ARG:HA	1:B:666:ASN:HD21	1.57	0.68
1:A:18:ALA:CB	1:A:180:MET:HE1	2.29	0.63
1:B:51:THR:HG22	1:B:168:VAL:HG12	1.81	0.62
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.82	0.60
1:B:177:PRO:HB2	1:B:316:LEU:HD21	1.84	0.59
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.75	0.57
1:A:584:HIS:O	1:A:588:ILE:HD12	2.04	0.57
1:A:111:GLU:O	1:A:115:LYS:HG2	2.05	0.57
1:B:39:HIS:HD2	1:B:89:MET:HE1	1.69	0.57
1:A:42:GLU:HG2	1:A:48:ILE:HG13	1.87	0.57
1:A:469:LYS:HB3	1:A:472:LYS:HG2	1.89	0.54
1:A:39:HIS:HD2	1:A:89:MET:HE1	1.72	0.54
1:A:449:ARG:NE	1:A:491:GLU:OE1	2.40	0.54
1:B:394:ILE:O	1:B:421:MET:HE1	2.08	0.54
1:A:58:VAL:HG22	1:A:162:TYR:CE1	2.43	0.53
1:A:191:MET:HE3	1:A:207:ILE:HG21	1.89	0.53
1:A:417:ARG:O	1:A:417:ARG:HD2	2.09	0.53
1:A:542:THR:HG21	1:A:583:LYS:HE2	1.92	0.52
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.92	0.52
1:A:394:ILE:O	1:A:421:MET:HE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:HIS:CD2	1:A:89:MET:HE1	2.45	0.51
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.41	0.51
1:B:302:PRO:HA	1:B:305:ILE:HD12	1.93	0.51
1:B:344:VAL:HG12	1:B:345:LEU:HD23	1.92	0.51
1:A:449:ARG:HH11	1:A:449:ARG:CG	2.19	0.51
1:B:449:ARG:HD3	1:B:491:GLU:OE1	2.10	0.51
1:A:449:ARG:HE	1:A:491:GLU:CD	2.18	0.50
1:B:18:ALA:HB1	1:B:180:MET:HE1	1.94	0.50
1:B:443:ASN:HB3	1:B:444:PRO:CD	2.35	0.50
1:A:58:VAL:HG22	1:A:162:TYR:HE1	1.77	0.50
1:A:428:VAL:HG22	1:A:478:ILE:HB	1.94	0.50
1:B:542:THR:HG21	1:B:583:LYS:HE2	1.94	0.50
1:A:355:LYS:O	1:A:359:ARG:HB2	2.13	0.49
1:B:324:THR:HG21	1:B:345:LEU:HD22	1.95	0.49
1:B:342:HIS:HB3	1:B:345:LEU:HG	1.95	0.49
1:B:518:LYS:HD2	1:B:567:ILE:HD13	1.95	0.48
1:B:469:LYS:H	1:B:469:LYS:HD2	1.78	0.48
1:A:534:ASN:O	1:A:538:MET:HB2	2.13	0.48
1:B:449:ARG:CD	1:B:491:GLU:OE1	2.62	0.48
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.95	0.47
1:A:119:VAL:HG12	1:A:120:ASP:H	1.79	0.47
1:B:128:ASN:HD21	1:B:131:ASN:HD22	1.61	0.47
1:A:54:LEU:HB3	1:A:375:ILE:HB	1.96	0.46
1:B:119:VAL:HG12	1:B:120:ASP:H	1.79	0.46
1:A:26:ASP:OD2	1:A:29:ASN:HB2	2.16	0.46
1:A:392:VAL:HG22	1:A:428:VAL:HB	1.97	0.46
1:B:385:LEU:HG	1:B:386:LYS:HG2	1.98	0.46
1:A:132:TYR:CD2	1:A:344:VAL:HG21	2.52	0.45
1:A:664:GLN:HE22	1:B:648:MET:HG3	1.82	0.45
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.99	0.44
1:B:20:LEU:HB2	1:B:168:VAL:CG2	2.48	0.43
1:B:96:LYS:HG2	1:B:240:HIS:CD2	2.52	0.43
1:B:593:ASN:O	1:B:596:VAL:HB	2.18	0.43
1:A:56:GLU:O	1:A:372:ASN:HA	2.19	0.43
1:B:185:LYS:HG3	1:B:313:ILE:HD11	2.00	0.43
1:B:519:LYS:HB3	1:B:520:LYS:H	1.70	0.43
1:A:472:LYS:HB2	1:A:475:ALA:HB3	2.00	0.43
1:B:506:ALA:HB1	1:B:558:ARG:HG3	2.00	0.43
1:A:420:GLU:HG2	1:A:424:GLU:OE2	2.19	0.43
1:A:696:VAL:HA	1:B:672:ALA:HB2	2.00	0.43
1:B:20:LEU:HB2	1:B:168:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HG21	1:A:456:LEU:HD21	2.01	0.42
1:A:588:ILE:O	1:A:592:GLN:HG3	2.19	0.42
1:B:224:ILE:HD12	1:B:315:PHE:HA	2.00	0.42
1:A:568:PRO:HB3	1:A:570:TYR:CE2	2.54	0.42
1:A:107:CYS:SG	1:A:171:LYS:HE3	2.60	0.42
1:B:449:ARG:HE	1:B:491:GLU:CD	2.27	0.42
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.50	0.42
1:A:180:MET:HE3	1:A:211:ILE:HG12	2.01	0.42
1:A:322:TYR:HB3	1:A:326:ARG:HG3	2.02	0.42
1:A:542:THR:HG21	1:A:583:LYS:HG2	2.02	0.41
1:B:180:MET:HE3	1:B:211:ILE:HG12	2.01	0.41
1:B:588:ILE:O	1:B:592:GLN:HG3	2.21	0.41
1:A:449:ARG:HG3	1:A:449:ARG:NH1	2.24	0.41
1:B:18:ALA:CB	1:B:180:MET:HE1	2.50	0.41
1:B:422:ILE:HG12	1:B:477:PRO:HG3	2.03	0.41
1:A:527:VAL:HG22	1:A:573:LEU:HD12	2.03	0.41
1:B:119:VAL:HG12	1:B:120:ASP:N	2.35	0.40
1:A:187:ILE:HG22	1:A:191:MET:HE2	2.03	0.40
1:B:428:VAL:HG22	1:B:478:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

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	532/728 (73%)	510 (96%)	21 (4%)	1 (0%)	43 63
1	B	578/728 (79%)	552 (96%)	25 (4%)	1 (0%)	43 63
All	All	1110/1456 (76%)	1062 (96%)	46 (4%)	2 (0%)	43 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	302	PRO

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	523/696 (75%)	490 (94%)	33 (6%)	16	34
1	B	559/696 (80%)	524 (94%)	35 (6%)	16	34
All	All	1082/1392 (78%)	1014 (94%)	68 (6%)	16	34

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	ILE
1	A	25	ASN
1	A	57	THR
1	A	82	VAL
1	A	85	ILE
1	A	106	LYS
1	A	123	ILE
1	A	163	PHE
1	A	165	ASN
1	A	171	LYS
1	A	205	ARG
1	A	241	LEU
1	A	305	ILE
1	A	344	VAL
1	A	349	ILE
1	A	366	ILE
1	A	381	ARG
1	A	417	ARG
1	A	434	GLU
1	A	449	ARG
1	A	452	VAL

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Mol	Chain	Res	Type
1	A	457	GLN
1	A	460	GLN
1	A	470	ILE
1	A	493	VAL
1	A	542	THR
1	A	562	LEU
1	A	588	ILE
1	A	589	LYS
1	A	596	VAL
1	A	661	LEU
1	A	702	LYS
1	B	6	GLU
1	B	9	LEU
1	B	11	GLU
1	B	28	ARG
1	B	85	ILE
1	B	90	GLN
1	B	130	GLU
1	B	163	PHE
1	B	171	LYS
1	B	205	ARG
1	B	206	ILE
1	B	225	LYS
1	B	230	MET
1	B	236	SER
1	B	304	GLU
1	B	344	VAL
1	B	371	ASN
1	B	410	GLU
1	B	417	ARG
1	B	427	SER
1	B	449	ARG
1	B	452	VAL
1	B	460	GLN
1	B	468	ASN
1	B	469	LYS
1	B	472	LYS
1	B	493	VAL
1	B	519	LYS
1	B	542	THR
1	B	596	VAL
1	B	619	GLN

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Mol	Chain	Res	Type
1	B	647	TRP
1	B	656	LYS
1	B	666	ASN
1	B	705	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	29	ASN
1	A	39	HIS
1	A	100	ASN
1	A	363	GLN
1	A	416	GLN
1	A	592	GLN
1	A	593	ASN
1	A	664	GLN
1	B	29	ASN
1	B	39	HIS
1	B	100	ASN
1	B	131	ASN
1	B	137	ASN
1	B	138	ASN
1	B	240	HIS
1	B	343	ASN
1	B	614	HIS
1	B	617	ASN
1	B	660	GLN
1	B	666	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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
5	ACT	A	804	-	3,3,3	0.67	0	3,3,3	1.33	0
3	ATP	A	802	2	32,33,33	1.68	7 (21%)	48,52,52	1.71	8 (16%)
5	ACT	B	803	-	3,3,3	0.69	0	3,3,3	0.97	0
6	AMP	B	801	2	25,25,25	1.52	4 (16%)	37,38,38	1.89	6 (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	802	2	-	6/22/38/38	0/3/3/3
6	AMP	B	801	2	-	1/10/26/26	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ATP	C5-C4	5.39	1.48	1.39
6	B	801	AMP	C5-C4	5.14	1.48	1.39
3	A	802	ATP	PB-O3A	3.68	1.63	1.59
3	A	802	ATP	PA-O3A	2.95	1.62	1.59
3	A	802	ATP	PB-O3B	2.79	1.62	1.59
6	B	801	AMP	C5-N7	-2.69	1.34	1.39
3	A	802	ATP	C5-C6	2.64	1.48	1.41
3	A	802	ATP	C5-N7	-2.40	1.34	1.39
6	B	801	AMP	C8-N7	2.37	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	801	AMP	C5-C6	2.17	1.47	1.41
3	A	802	ATP	C8-N7	2.13	1.35	1.31

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	801	AMP	C5-C4-N3	-5.68	118.90	126.72
3	A	802	ATP	C5-C4-N3	-5.55	119.07	126.72
6	B	801	AMP	N3-C4-N9	5.07	135.78	127.17
3	A	802	ATP	N3-C4-N9	5.01	135.69	127.17
3	A	802	ATP	C2-N3-C4	3.55	120.50	111.83
6	B	801	AMP	N3-C2-N1	-3.49	123.30	128.58
3	A	802	ATP	N3-C2-N1	-3.45	123.35	128.58
6	B	801	AMP	C2-N3-C4	3.45	120.25	111.83
3	A	802	ATP	C4-N9-C8	2.61	108.47	105.74
3	A	802	ATP	C4-C5-N7	-2.59	107.62	110.58
6	B	801	AMP	C4-N9-C8	2.28	108.13	105.74
3	A	802	ATP	C2-N1-C6	2.24	122.41	118.73
6	B	801	AMP	C4-C5-N7	-2.18	108.08	110.58
3	A	802	ATP	C1'-N9-C8	-2.04	122.57	127.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

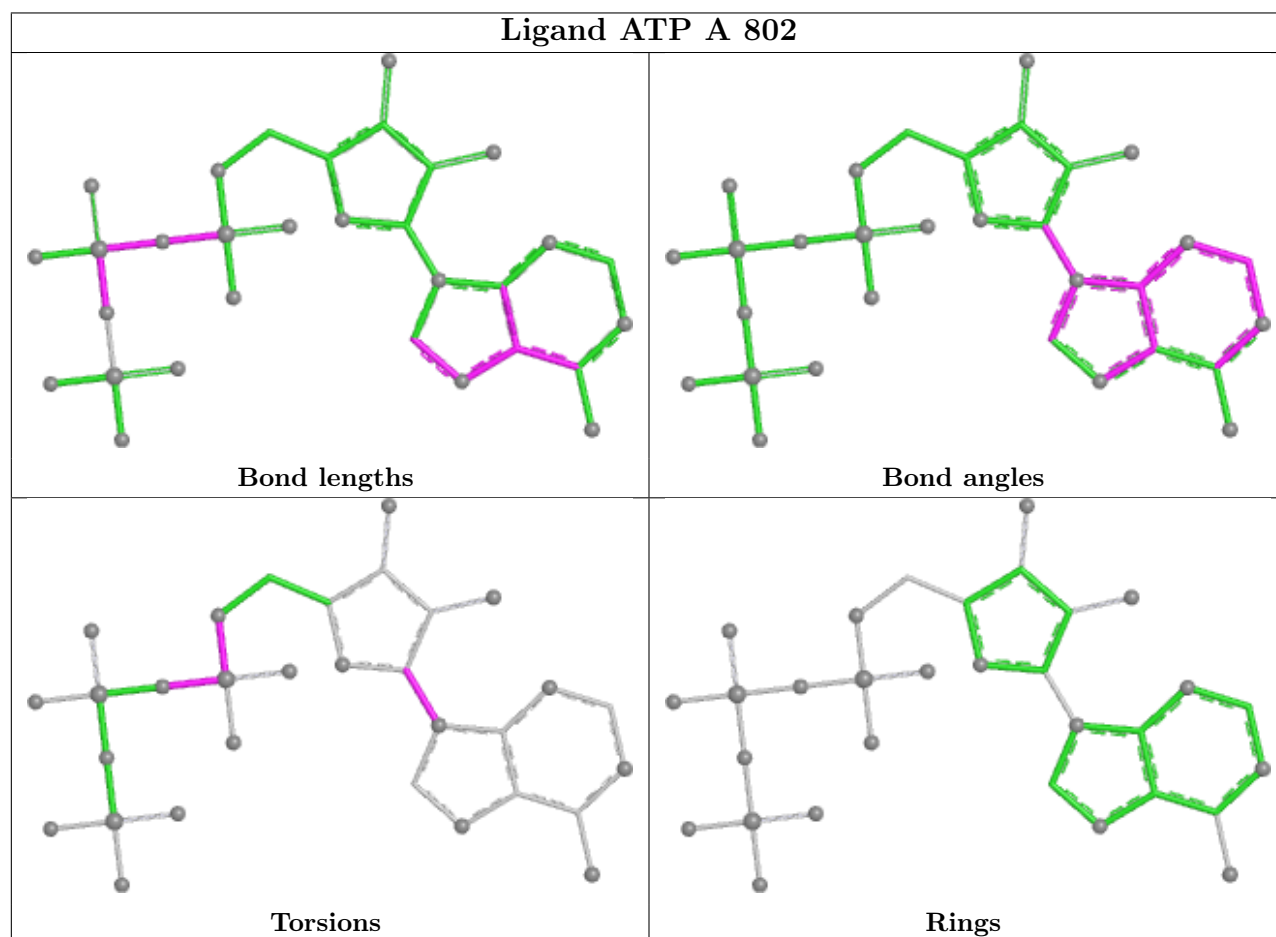
Mol	Chain	Res	Type	Atoms
3	A	802	ATP	C5'-O5'-PA-O1A
3	A	802	ATP	C5'-O5'-PA-O3A
3	A	802	ATP	PB-O3A-PA-O5'
3	A	802	ATP	C5'-O5'-PA-O2A
3	A	802	ATP	O4'-C1'-N9-C8
6	B	801	AMP	O4'-C1'-N9-C8
3	A	802	ATP	C2'-C1'-N9-C8

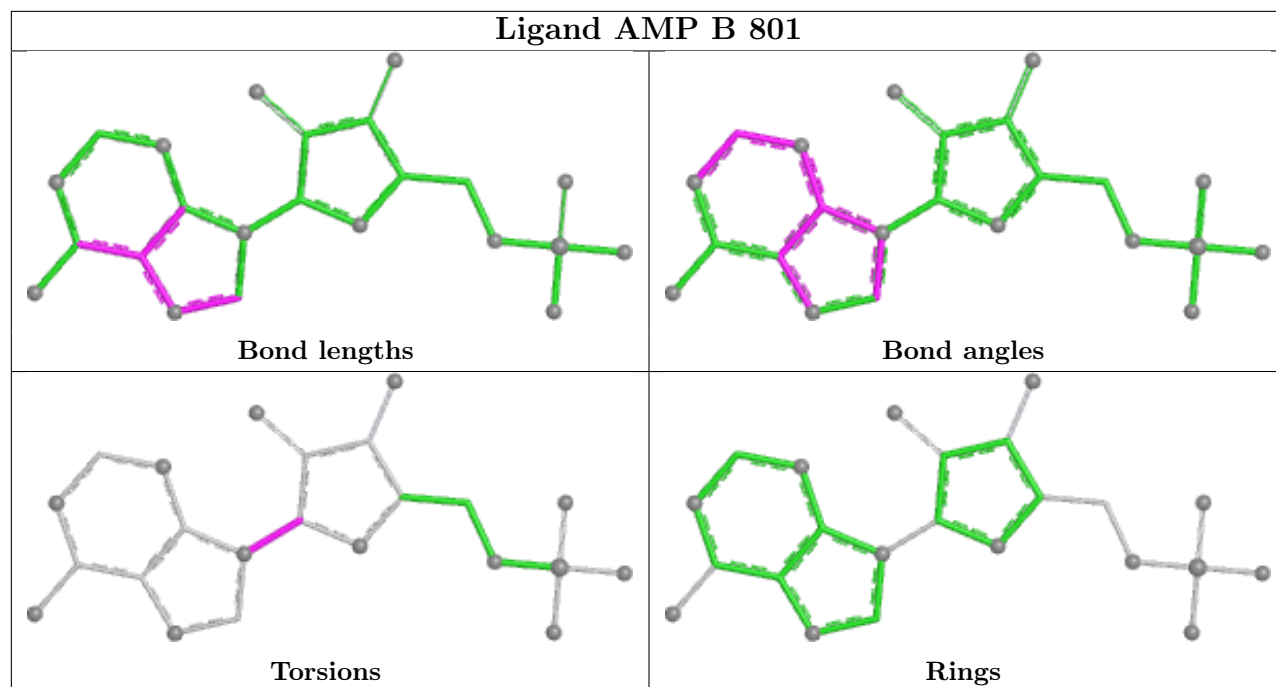
There are no ring outliers.

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	548/728 (75%)	0.07	34 (6%) 26 23	28, 52, 119, 120	0
1	B	590/728 (81%)	0.21	44 (7%) 20 18	27, 59, 118, 120	0
All	All	1138/1456 (78%)	0.14	78 (6%) 23 20	27, 56, 119, 120	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	470	ILE	5.7
1	B	470	ILE	4.9
1	A	62	ILE	4.4
1	A	7	LEU	4.4
1	A	366	ILE	4.3
1	A	84	TYR	4.2
1	A	467	LYS	4.2
1	B	466	ILE	4.2
1	A	163	PHE	4.0
1	A	225	LYS	4.0
1	A	399	TYR	3.9
1	B	302	PRO	3.9
1	B	84	TYR	3.6
1	A	434	GLU	3.6
1	B	62	ILE	3.5
1	B	206	ILE	3.4
1	A	302	PRO	3.3
1	B	471	VAL	3.3
1	A	471	VAL	3.3
1	B	9	LEU	3.2
1	B	647	TRP	3.1
1	A	658	LYS	3.0
1	B	649	PHE	3.0
1	A	663	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	440	VAL	2.9
1	B	7	LEU	2.9
1	B	241	LEU	2.9
1	B	473	CYS	2.7
1	B	163	PHE	2.7
1	A	192	LYS	2.6
1	A	445	LYS	2.6
1	B	472	LYS	2.6
1	B	59	PRO	2.5
1	B	231	ILE	2.5
1	A	146	ILE	2.5
1	B	467	LYS	2.5
1	B	81	ASP	2.5
1	B	441	ILE	2.5
1	B	442	PRO	2.4
1	B	663	TYR	2.4
1	B	707	LYS	2.4
1	A	228	LYS	2.4
1	A	446	ILE	2.4
1	A	61	TYR	2.3
1	A	150	ASN	2.3
1	A	60	GLU	2.3
1	B	305	ILE	2.3
1	B	469	LYS	2.3
1	B	99	GLU	2.3
1	B	6	GLU	2.3
1	A	115	LYS	2.2
1	A	707	LYS	2.2
1	B	648	MET	2.2
1	B	521	ASN	2.2
1	A	162	TYR	2.2
1	A	205	ARG	2.2
1	B	652	ASN	2.2
1	B	653	TYR	2.2
1	B	310	VAL	2.1
1	B	82	VAL	2.1
1	B	240	HIS	2.1
1	B	443	ASN	2.1
1	B	60	GLU	2.1
1	A	14	LYS	2.1
1	A	147	MET	2.1
1	B	651	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	2.1
1	B	61	TYR	2.1
1	A	59	PRO	2.1
1	B	226	LEU	2.1
1	B	371	ASN	2.1
1	A	306	ILE	2.1
1	A	473	CYS	2.1
1	B	439	PHE	2.0
1	B	722	GLU	2.0
1	A	300	ARG	2.0
1	A	6	GLU	2.0
1	A	472	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

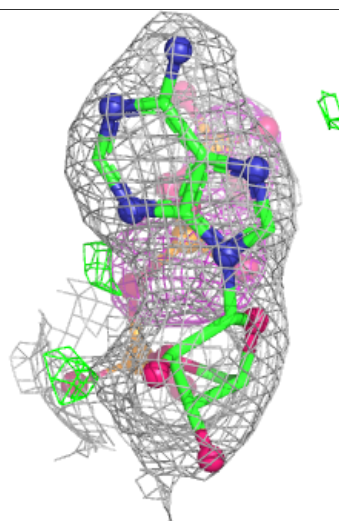
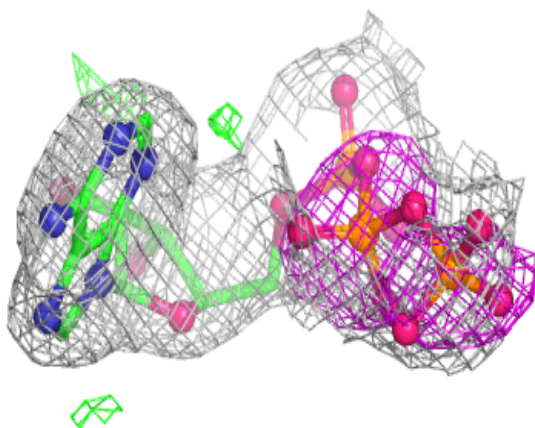
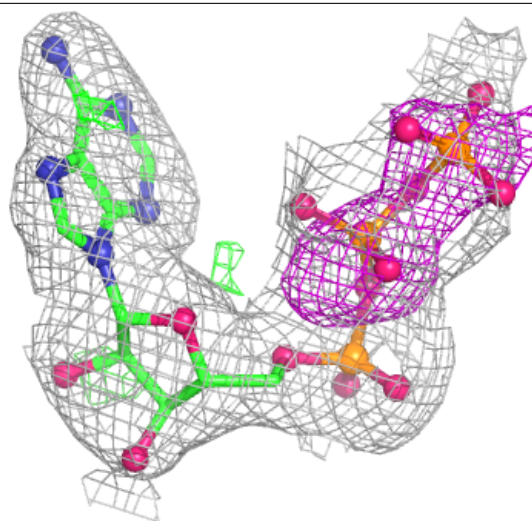
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

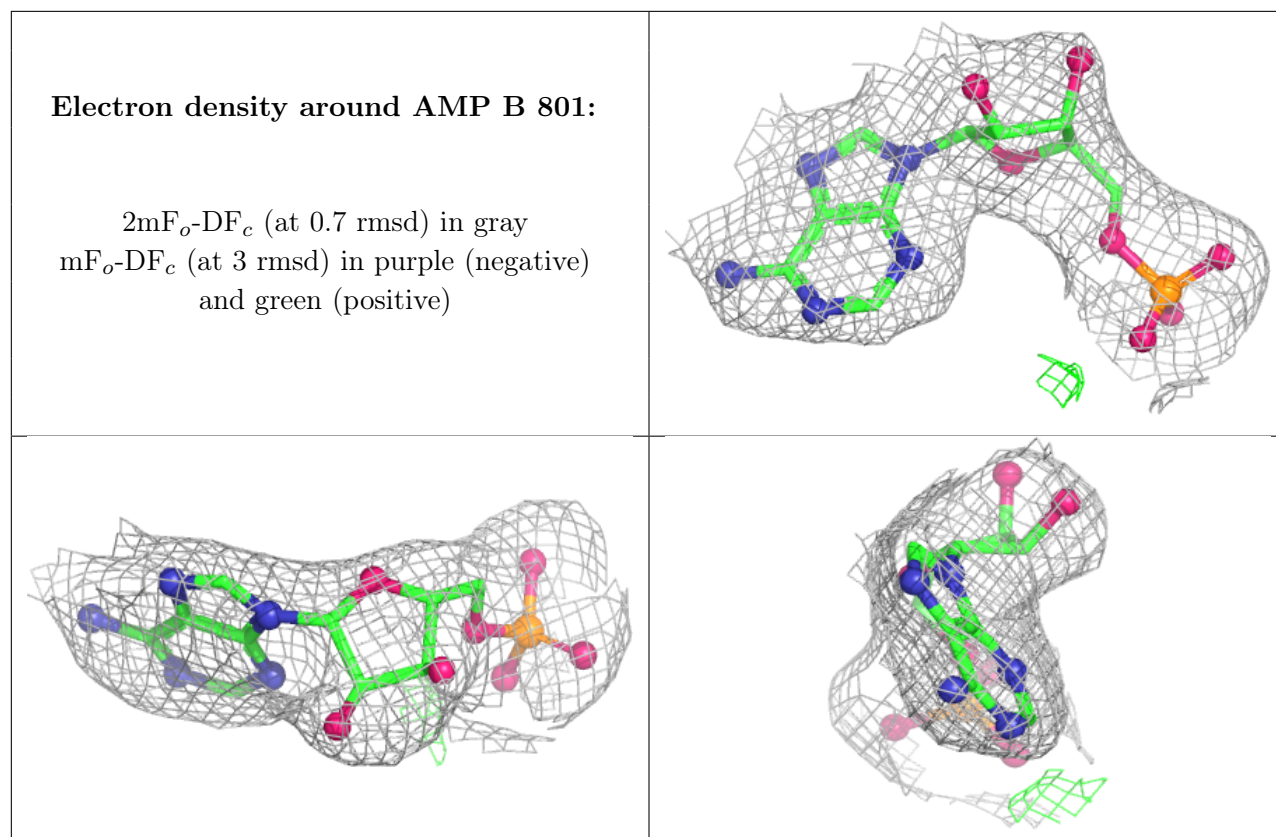
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ATP	A	802	31/31	0.84	0.10	59,91,120,120	0
5	ACT	A	804	4/4	0.90	0.11	38,41,44,48	0
6	AMP	B	801	23/23	0.91	0.08	60,77,107,110	0
2	MG	B	802	1/1	0.92	0.08	64,64,64,64	0
2	MG	A	801	1/1	0.97	0.06	67,67,67,67	0
4	CA	A	803	1/1	0.97	0.05	63,63,63,63	0
5	ACT	B	803	4/4	0.98	0.06	33,37,37,39	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 A 802:

$2mF_o-DF_c$ (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.