



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:00 AM BST

PDB ID : 6JWX  
Title : Crystal structure of Plasmodium falciparum HPPK-DHPS wild type with SDX-DHP  
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](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 : 2.13  
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) : 2.13

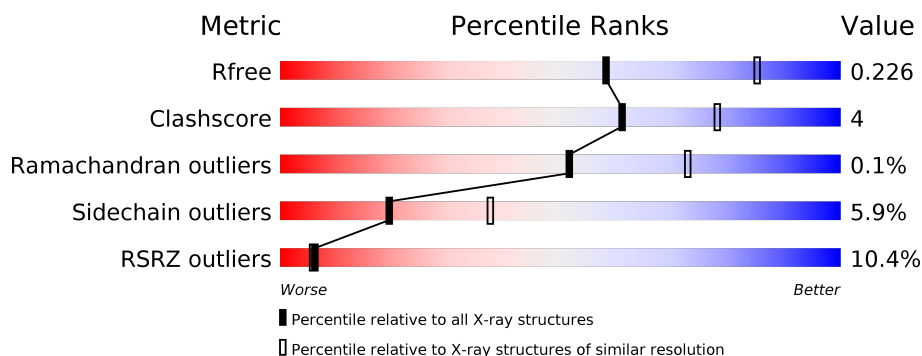
# 1 Overall quality at a glance

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))
$R_{free}$	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 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	728	
1	B	728	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9288 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	544	Total	C	N	O	S	0	0	0
			4504	2904	744	833	23			
1	B	526	Total	C	N	O	S	0	0	0
			4341	2796	720	804	21			

There are 44 discrepancies between the modelled and reference sequences:

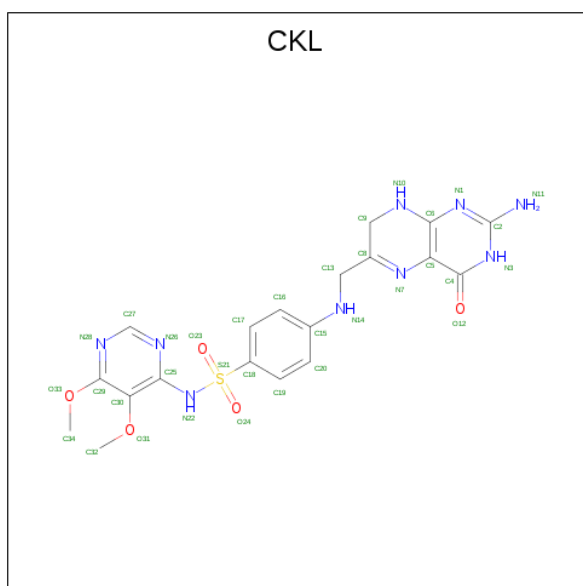
Chain	Residue	Modelled	Actual	Comment	Reference
A	707	LYS	-	expression tag	UNP Q25704
A	708	ASP	-	expression tag	UNP Q25704
A	709	PRO	-	expression tag	UNP Q25704
A	710	ASN	-	expression tag	UNP Q25704
A	711	SER	-	expression tag	UNP Q25704
A	712	SER	-	expression tag	UNP Q25704
A	713	SER	-	expression tag	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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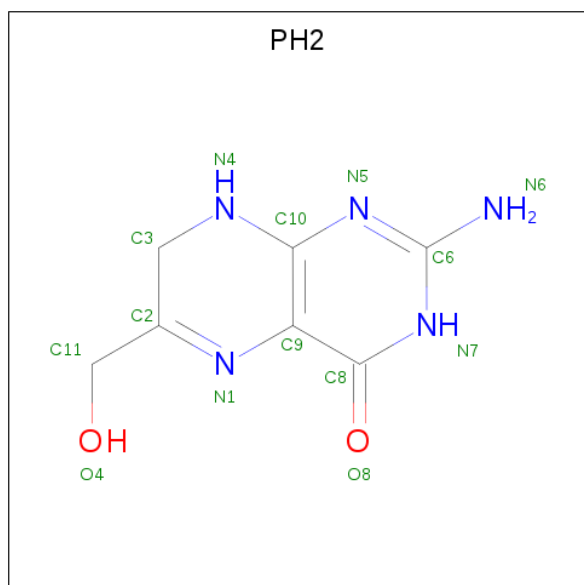
Chain	Residue	Modelled	Actual	Comment	Reference
B	709	PRO	-	expression tag	UNP Q25704
B	710	ASN	-	expression tag	UNP Q25704
B	711	SER	-	expression tag	UNP Q25704
B	712	SER	-	expression tag	UNP Q25704
B	713	SER	-	expression tag	UNP Q25704
B	714	VAL	-	expression tag	UNP Q25704
B	715	ASP	-	expression tag	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 4-[(2-azanyl-4-oxidanylidene-7,8-dihydro-3 {H}-pteridin-6-yl)methylamino]-{N}-(5,6-dimethoxypyrimidin-4-yl)benzenesulfonamide (three-letter code: CKL) (formula: C<sub>19</sub>H<sub>21</sub>N<sub>9</sub>O<sub>5</sub>S).



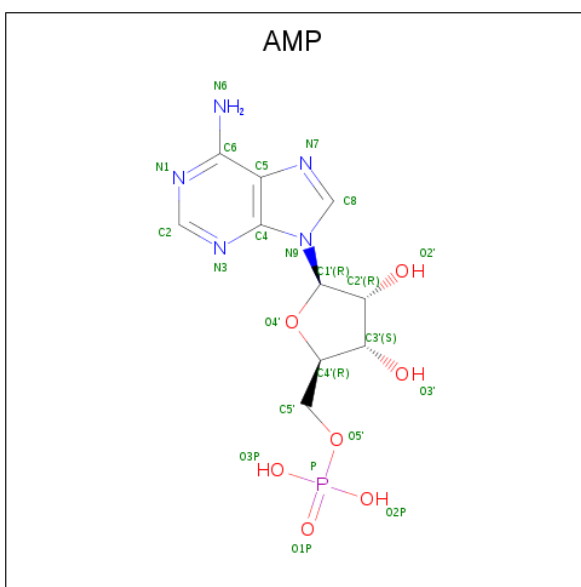
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	19	9	5	1		
2	B	1	Total	C	N	O	S	0	0
			34	19	9	5	1		

- Molecule 3 is 2-AMINO-6-HYDROXYMETHYL-7,8-DIHYDRO-3H-PTERIDIN-4-ONE (three-letter code: PH2) (formula: C<sub>7</sub>H<sub>9</sub>N<sub>5</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	7	5	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

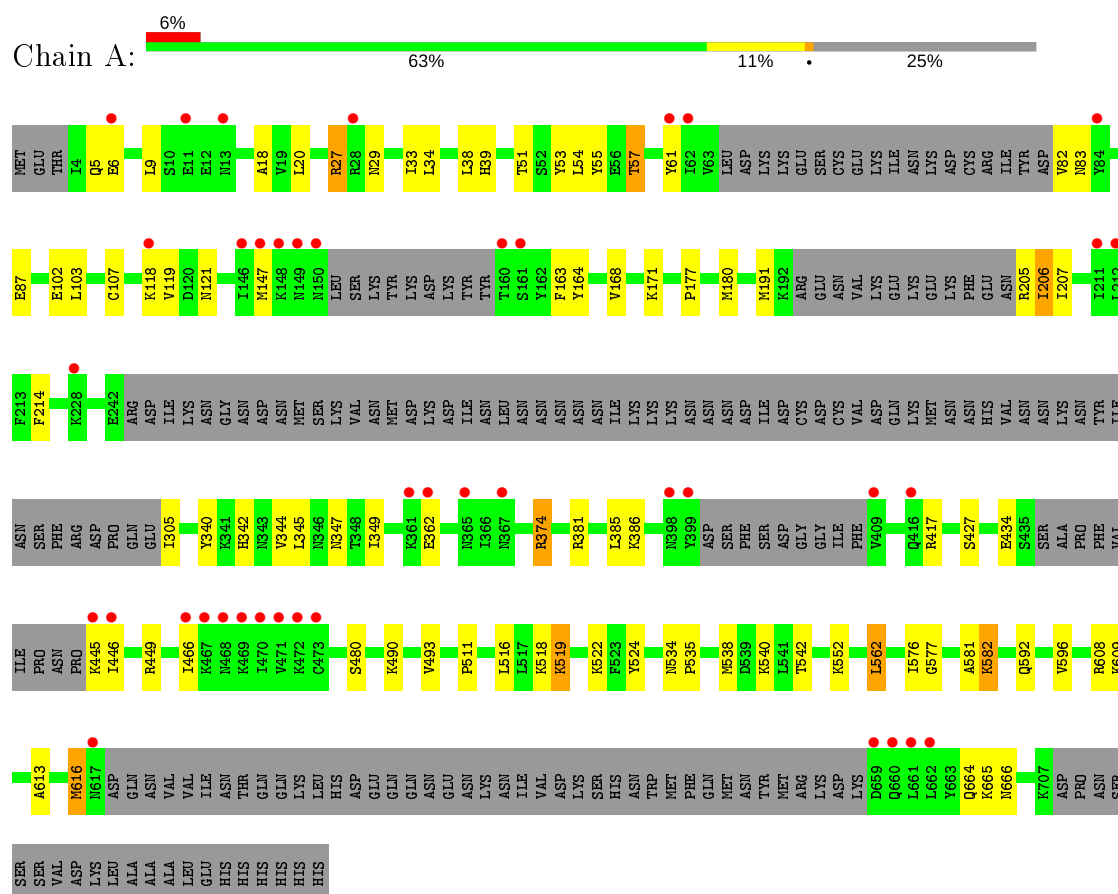
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	185	Total O 185 185	0	0
8	B	106	Total O 106 106	0	0

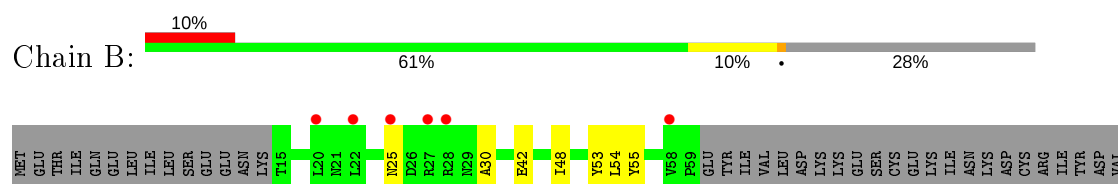
### 3 Residue-property plots [i](#)

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.

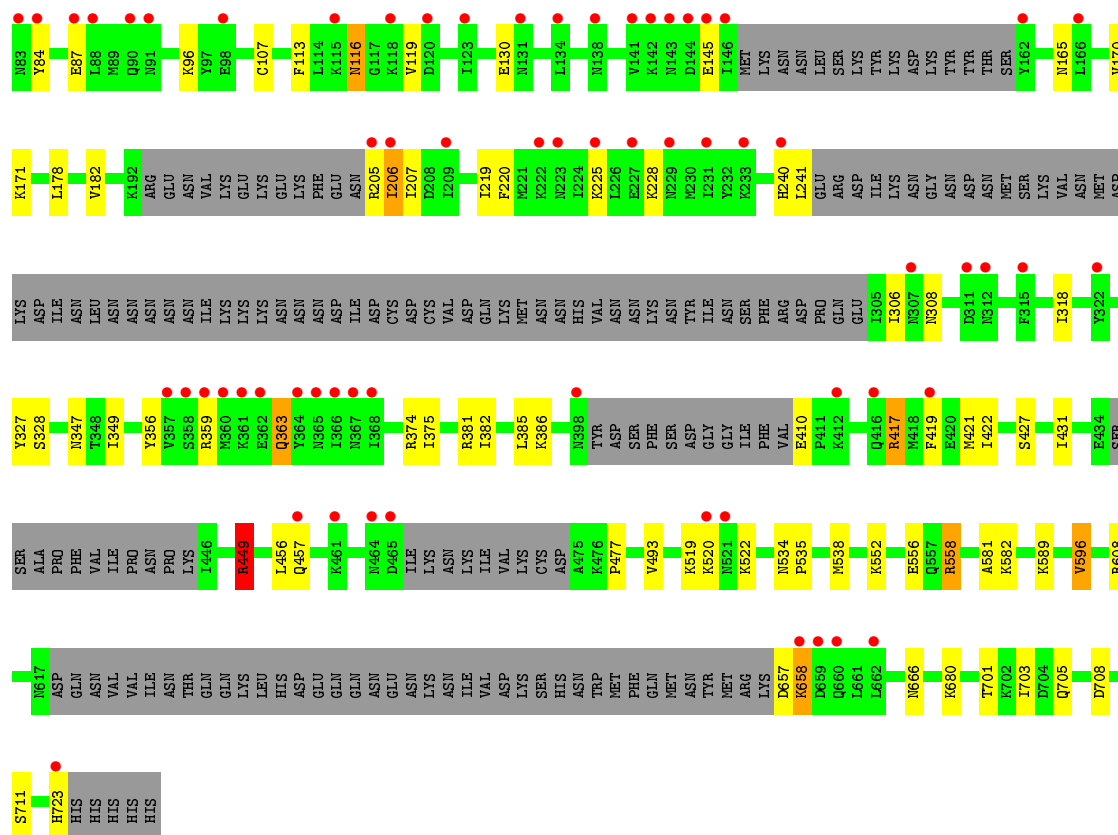
- Molecule 1: 7,8-dihydro-6-hydroxymethylpterin pyrophosphokinase-dihydropteroate synthase



- 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, $\alpha$ , $\beta$ , $\gamma$	99.11Å 137.17Å 137.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 33.26 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.7 (30.00-2.50) 87.8 (33.26-2.50)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.206 , 0.231 0.201 , 0.226	Depositor DCC
$R_{free}$ test set	5594 reflections (9.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: MG, CKL, CA, ACT, PH2, AMP

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	0.54	1/4572 (0.0%)	0.72	2/6164 (0.0%)
1	B	0.49	0/4408	0.69	2/5945 (0.0%)
All	All	0.52	1/8980 (0.0%)	0.71	4/12109 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	GLU	CD-OE2	11.42	1.38	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	LEU	CA-CB-CG	6.48	130.21	115.30
1	A	374	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	B	449	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	449	ARG	NE-CZ-NH1	5.78	123.19	120.30

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	4504	0	4622	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4341	0	4435	38	0
2	A	34	0	0	1	0
2	B	34	0	0	0	0
3	A	14	0	9	4	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	6	0	0
6	B	12	0	9	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	185	0	0	1	0
8	B	106	0	0	0	0
All	All	9288	0	9105	81	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 (81) 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:57:THR:CG2	3:A:802:PH2:HN62	1.87	0.87
1:A:519:LYS:NZ	1:A:524:TYR:OH	2.21	0.74
1:B:658:LYS:H	1:B:658:LYS:HD2	1.57	0.70
1:A:191:MET:HE1	1:A:207:ILE:HG12	1.75	0.69
1:B:534:ASN:HB2	1:B:535:PRO:CD	2.22	0.68
1:B:708:ASP:HB3	1:B:711:SER:HB3	1.78	0.65
1:B:608:ARG:HA	1:B:666:ASN:OD1	1.98	0.63
1:A:538:MET:HG2	1:A:581:ALA:H	1.64	0.62
1:A:29:ASN:O	1:A:33:ILE:HG12	2.00	0.62
1:A:51:THR:HG22	1:A:168:VAL:HG12	1.82	0.61
1:A:27:ARG:HG3	1:A:164:TYR:OH	1.99	0.61
1:A:608:ARG:HA	1:A:666:ASN:ND2	2.16	0.61
1:B:55:TYR:OH	1:B:374:ARG:NH1	2.33	0.61
1:B:552:LYS:HD2	1:B:596:VAL:HG13	1.83	0.60
1:B:54:LEU:HB3	1:B:375:ILE:HB	1.86	0.57
1:A:53:TYR:CD2	1:A:374:ARG:HD3	2.40	0.57
1:B:534:ASN:HB2	1:B:535:PRO:HD2	1.86	0.57
1:A:107:CYS:SG	1:A:171:LYS:NZ	2.76	0.56
1:B:417:ARG:HH11	1:B:421:MET:HG3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:TYR:CG	1:A:374:ARG:HD3	2.41	0.56
1:A:342:HIS:HD2	1:A:344:VAL:H	1.54	0.55
1:A:82:VAL:HG13	1:A:83:ASN:H	1.71	0.55
1:A:39:HIS:HB2	8:A:914:HOH:O	2.09	0.52
1:A:57:THR:HG23	3:A:802:PH2:HN62	1.72	0.52
1:A:55:TYR:OH	1:A:374:ARG:NH1	2.42	0.51
1:B:113:PHE:O	1:B:116:ASN:HB3	2.09	0.51
1:A:57:THR:HG22	1:A:163:PHE:HB2	1.93	0.51
1:B:519:LYS:HB2	1:B:522:LYS:HB2	1.93	0.51
1:A:38:LEU:CD2	1:A:168:VAL:HG11	2.41	0.50
1:B:53:TYR:CG	1:B:374:ARG:HD3	2.46	0.50
1:A:552:LYS:HD2	1:A:596:VAL:HG13	1.94	0.50
1:A:57:THR:CG2	3:A:802:PH2:N6	2.68	0.49
1:A:5:GLN:HG2	1:A:9:LEU:HD12	1.95	0.49
1:A:445:LYS:HG3	1:A:446:ILE:H	1.77	0.49
1:A:206:ILE:HG23	1:A:207:ILE:HG22	1.95	0.48
1:B:228:LYS:HE2	1:B:306:ILE:HB	1.95	0.48
1:A:18:ALA:CB	1:A:180:MET:HE1	2.43	0.48
1:B:165:ASN:HD22	1:B:328:SER:HB2	1.79	0.48
1:B:552:LYS:HE2	1:B:556:GLU:OE2	2.13	0.48
1:A:609:LYS:NZ	2:A:801:CKL:O12	2.47	0.47
1:B:25:ASN:HD21	1:B:205:ARG:HB2	1.78	0.47
1:B:419:PHE:HA	1:B:422:ILE:HD12	1.97	0.47
1:B:701:THR:O	1:B:705:GLN:HG2	2.14	0.47
1:B:178:LEU:O	1:B:182:VAL:HG23	2.14	0.47
1:A:103:LEU:CD1	1:A:511:PRO:HB2	2.45	0.47
1:A:61:TYR:HB3	1:A:147:MET:HG2	1.97	0.46
1:B:96:LYS:HG2	1:B:240:HIS:CE1	2.49	0.46
1:A:342:HIS:HB3	1:A:345:LEU:HG	1.99	0.45
1:B:116:ASN:OD1	1:B:116:ASN:N	2.48	0.45
1:A:592:GLN:HG2	1:B:703:ILE:O	2.16	0.45
1:B:449:ARG:HG3	1:B:449:ARG:HH11	1.82	0.45
1:A:534:ASN:HB2	1:A:535:PRO:CD	2.46	0.45
1:B:219:ILE:HB	1:B:318:ILE:HB	1.98	0.45
1:A:57:THR:HG21	3:A:802:PH2:HN62	1.76	0.45
1:B:431:ILE:HG21	1:B:456:LEU:HD21	1.99	0.45
1:B:42:GLU:HG2	1:B:48:ILE:HD12	1.99	0.45
1:A:340:TYR:HD2	1:A:349:ILE:CD1	2.30	0.44
1:B:327:TYR:HB2	1:B:356:TYR:CZ	2.52	0.44
1:B:558:ARG:HD2	1:B:558:ARG:HA	1.66	0.44
1:A:107:CYS:SG	1:A:171:LYS:HE3	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:CD1	1:A:54:LEU:HD11	2.48	0.43
1:B:538:MET:O	1:B:581:ALA:HA	2.18	0.43
1:B:30:ALA:HB3	1:B:382:ILE:HD11	2.01	0.43
1:B:385:LEU:HG	1:B:386:LYS:HG2	2.01	0.43
1:A:613:ALA:HA	1:A:616:MET:HE2	2.01	0.42
1:B:422:ILE:HD11	1:B:477:PRO:HG3	2.02	0.42
1:A:103:LEU:HD13	1:A:511:PRO:HB2	2.01	0.42
1:B:680:LYS:HD3	1:B:680:LYS:HA	1.88	0.42
1:A:18:ALA:HB1	1:A:180:MET:HE1	2.01	0.41
1:B:107:CYS:SG	1:B:171:LYS:HE2	2.60	0.41
1:A:107:CYS:SG	1:A:171:LYS:CE	3.09	0.41
1:B:359:ARG:O	1:B:363:GLN:HB2	2.20	0.41
1:A:490:LYS:HD3	1:A:516:LEU:HD22	2.03	0.41
1:A:342:HIS:CD2	1:A:344:VAL:H	2.36	0.41
1:B:55:TYR:CE1	1:B:374:ARG:HG3	2.55	0.41
1:B:206:ILE:HG23	1:B:207:ILE:HG22	2.01	0.41
1:A:385:LEU:HG	1:A:386:LYS:HG2	2.04	0.40
1:A:577:GLY:O	1:A:582:LYS:HE2	2.21	0.40
1:B:449:ARG:HH11	1:B:449:ARG:CG	2.34	0.40
1:A:20:LEU:HB2	1:A:168:VAL:HG22	2.03	0.40
1:A:177:PRO:HD3	1:A:214:PHE:CD1	2.57	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	528/728 (72%)	510 (97%)	17 (3%)	1 (0%)	47	68
1	B	508/728 (70%)	488 (96%)	20 (4%)	0	100	100
All	All	1036/1456 (71%)	998 (96%)	37 (4%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	LYS

### 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	519/696 (75%)	489 (94%)	30 (6%)	20	38
1	B	498/696 (72%)	468 (94%)	30 (6%)	19	37
All	All	1017/1392 (73%)	957 (94%)	60 (6%)	19	37

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	57	THR
1	A	87	GLU
1	A	102	GLU
1	A	119	VAL
1	A	121	ASN
1	A	205	ARG
1	A	206	ILE
1	A	305	ILE
1	A	347	ASN
1	A	362	GLU
1	A	381	ARG
1	A	417	ARG
1	A	427	SER
1	A	434	GLU
1	A	449	ARG
1	A	466	ILE
1	A	480	SER
1	A	493	VAL
1	A	518	LYS
1	A	519	LYS
1	A	522	LYS

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Mol	Chain	Res	Type
1	A	540	LYS
1	A	542	THR
1	A	562	LEU
1	A	576	ILE
1	A	582	LYS
1	A	616	MET
1	A	664	GLN
1	A	665	LYS
1	B	84	TYR
1	B	87	GLU
1	B	116	ASN
1	B	119	VAL
1	B	130	GLU
1	B	145	GLU
1	B	170	VAL
1	B	206	ILE
1	B	220	PHE
1	B	225	LYS
1	B	241	LEU
1	B	308	ASN
1	B	347	ASN
1	B	349	ILE
1	B	363	GLN
1	B	381	ARG
1	B	410	GLU
1	B	417	ARG
1	B	427	SER
1	B	449	ARG
1	B	457	GLN
1	B	493	VAL
1	B	520	LYS
1	B	558	ARG
1	B	582	LYS
1	B	589	LYS
1	B	596	VAL
1	B	657	ASP
1	B	658	LYS
1	B	723	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	5	GLN
1	A	39	HIS
1	A	83	ASN
1	A	342	HIS
1	A	666	ASN
1	B	128	ASN
1	B	165	ASN
1	B	240	HIS
1	B	343	ASN
1	B	557	GLN

### 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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	$\# Z  > 2$
4	AMP	A	803	5	22,25,25	1.12	2 (9%)	25,38,38	1.40	4 (16%)
6	ACT	A	806	-	1,3,3	1.40	0	0,3,3	0.00	-
2	CKL	A	801	-	31,37,37	2.14	5 (16%)	36,53,53	2.71	13 (36%)
2	CKL	B	801	-	31,37,37	2.14	4 (12%)	36,53,53	3.20	19 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ACT	A	805	-	1,3,3	1.00	0	0,3,3	0.00	-
6	ACT	B	806	-	1,3,3	1.71	0	0,3,3	0.00	-
3	PH2	A	802	-	10,15,15	1.13	1 (10%)	10,21,21	2.24	4 (40%)
6	ACT	B	804	-	1,3,3	1.28	0	0,3,3	0.00	-
6	ACT	B	805	-	1,3,3	0.89	0	0,3,3	0.00	-
4	AMP	B	802	5	22,25,25	1.34	3 (13%)	25,38,38	1.36	3 (12%)

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
2	CKL	A	801	-	-	13/18/29/29	0/4/4/4
4	AMP	A	803	5	-	2/6/26/26	0/3/3/3
4	AMP	B	802	5	-	3/6/26/26	0/3/3/3
2	CKL	B	801	-	-	5/18/29/29	0/4/4/4
3	PH2	A	802	-	-	0/0/11/11	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	CKL	C18-S21	-10.18	1.60	1.76
2	A	801	CKL	C18-S21	-10.00	1.61	1.76
4	B	802	AMP	C5-C4	3.17	1.49	1.40
4	B	802	AMP	C2-N3	2.91	1.36	1.32
2	B	801	CKL	C5-C6	2.88	1.49	1.41
3	A	802	PH2	C9-C10	2.77	1.49	1.41
4	B	802	AMP	O4'-C1'	2.68	1.44	1.41
4	A	803	AMP	O4'-C1'	2.56	1.44	1.41
2	A	801	CKL	C29-N28	2.55	1.37	1.32
2	A	801	CKL	C5-C6	2.43	1.48	1.41
2	B	801	CKL	C29-N28	2.31	1.36	1.32
4	A	803	AMP	C5-C4	2.27	1.46	1.40
2	A	801	CKL	C25-N22	-2.27	1.36	1.40
2	B	801	CKL	O33-C29	2.25	1.38	1.35
2	A	801	CKL	O33-C29	2.17	1.38	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CKL	O23-S21-O24	-10.70	106.39	119.55
2	B	801	CKL	O23-S21-O24	-10.19	107.03	119.55
2	B	801	CKL	C25-N22-S21	6.78	136.48	124.16
2	B	801	CKL	N26-C27-N28	-5.81	119.52	128.60
2	A	801	CKL	N26-C27-N28	-5.36	120.21	128.60
2	A	801	CKL	C4-N3-C2	4.68	123.37	115.93
2	B	801	CKL	C34-O33-C29	4.22	121.39	117.21
2	B	801	CKL	O24-S21-C18	4.18	113.12	107.97
2	A	801	CKL	C34-O33-C29	3.93	121.11	117.21
2	B	801	CKL	O24-S21-N22	3.90	116.50	106.73
4	A	803	AMP	N3-C2-N1	-3.85	122.66	128.68
2	A	801	CKL	C5-C4-N3	-3.83	118.19	123.43
3	A	802	PH2	C8-C9-C10	3.83	117.03	114.53
2	B	801	CKL	C17-C18-S21	3.81	123.92	119.77
3	A	802	PH2	C9-C8-N7	-3.61	118.49	123.43
2	B	801	CKL	C4-N3-C2	3.53	121.54	115.93
2	B	801	CKL	O23-S21-C18	3.49	112.26	107.97
4	B	802	AMP	N3-C2-N1	-3.47	123.25	128.68
2	B	801	CKL	C19-C18-S21	-3.43	116.04	119.77
2	A	801	CKL	C27-N28-C29	3.33	121.45	115.88
2	B	801	CKL	C2-N1-C6	3.27	121.88	114.54
3	A	802	PH2	C8-N7-C6	3.21	121.03	115.93
2	B	801	CKL	C27-N28-C29	3.12	121.10	115.88
2	B	801	CKL	C32-O31-C30	3.11	123.30	114.78
3	A	802	PH2	C6-N5-C10	3.10	121.48	114.54
2	B	801	CKL	C5-C4-N3	-3.05	119.26	123.43
2	A	801	CKL	C2-N1-C6	2.80	120.81	114.54
2	A	801	CKL	O24-S21-C18	2.79	111.41	107.97
2	A	801	CKL	O23-S21-N22	2.76	113.64	106.73
2	B	801	CKL	C4-C5-C6	2.61	116.23	114.53
2	A	801	CKL	C32-O31-C30	2.59	121.88	114.78
2	B	801	CKL	C27-N26-C25	2.50	123.66	115.25
4	A	803	AMP	O3P-P-O1P	2.40	120.09	110.68
2	A	801	CKL	C4-C5-C6	2.39	116.09	114.53
4	A	803	AMP	O5'-P-O1P	-2.38	99.79	106.47
2	B	801	CKL	N22-C25-N26	-2.34	114.15	118.66
4	B	802	AMP	C3'-C2'-C1'	2.27	104.39	100.98
4	B	802	AMP	C4-C5-N7	-2.20	107.10	109.40
2	A	801	CKL	N3-C2-N1	-2.18	122.00	125.42
2	A	801	CKL	O23-S21-C18	2.13	110.59	107.97
2	B	801	CKL	O33-C29-C30	2.12	121.06	116.95
4	A	803	AMP	C2-N1-C6	2.08	122.30	118.75
2	B	801	CKL	C18-S21-N22	-2.07	104.23	106.83

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	CKL	C25-N22-S21-O24
2	A	801	CKL	C25-N22-S21-C18
2	A	801	CKL	C30-C29-O33-C34
2	A	801	CKL	N28-C29-O33-C34
2	B	801	CKL	C30-C29-O33-C34
2	B	801	CKL	N28-C29-O33-C34
4	B	802	AMP	C5'-O5'-P-O1P
4	B	802	AMP	C5'-O5'-P-O2P
4	B	802	AMP	C5'-O5'-P-O3P
4	A	803	AMP	C3'-C4'-C5'-O5'
2	A	801	CKL	C25-N22-S21-O23
2	A	801	CKL	C20-C15-N14-C13
2	A	801	CKL	N26-C25-N22-S21
2	B	801	CKL	N26-C25-N22-S21
4	A	803	AMP	O4'-C4'-C5'-O5'
2	A	801	CKL	C19-C18-S21-O24
2	A	801	CKL	C17-C18-S21-O24
2	A	801	CKL	C16-C15-N14-C13
2	B	801	CKL	C8-C13-N14-C15
2	A	801	CKL	C19-C18-S21-N22
2	A	801	CKL	C8-C13-N14-C15
2	A	801	CKL	C17-C18-S21-N22
2	B	801	CKL	C16-C15-N14-C13

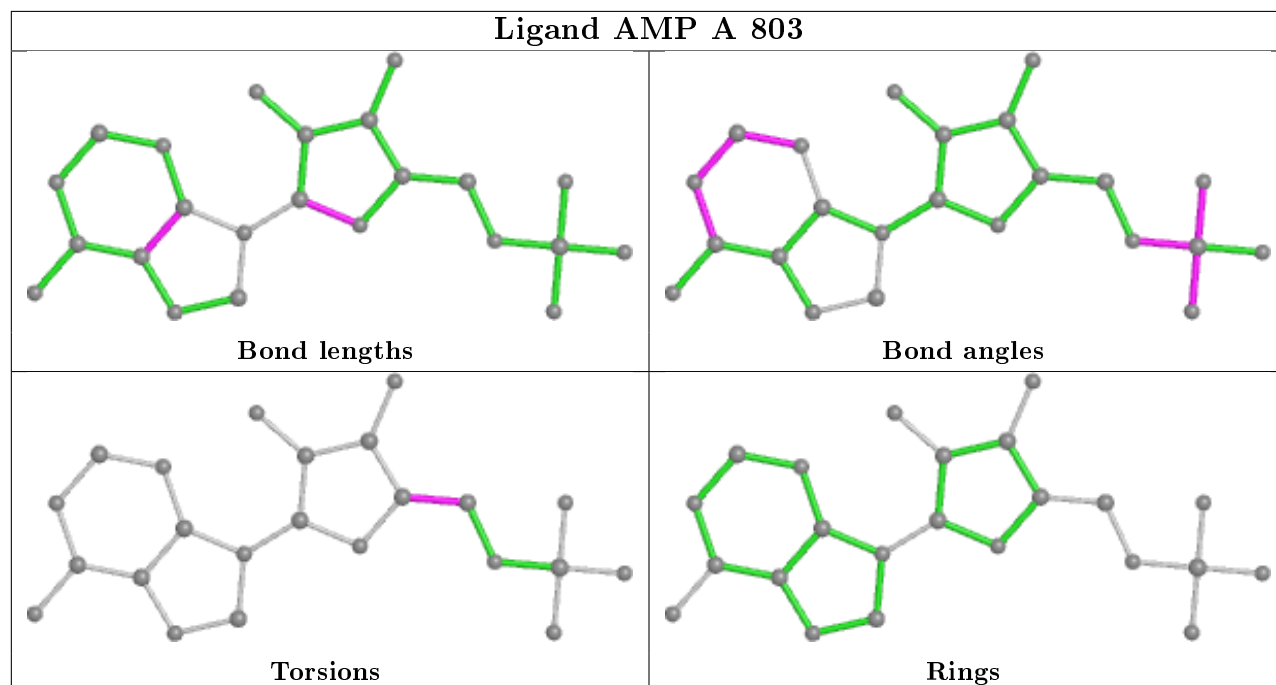
There are no ring outliers.

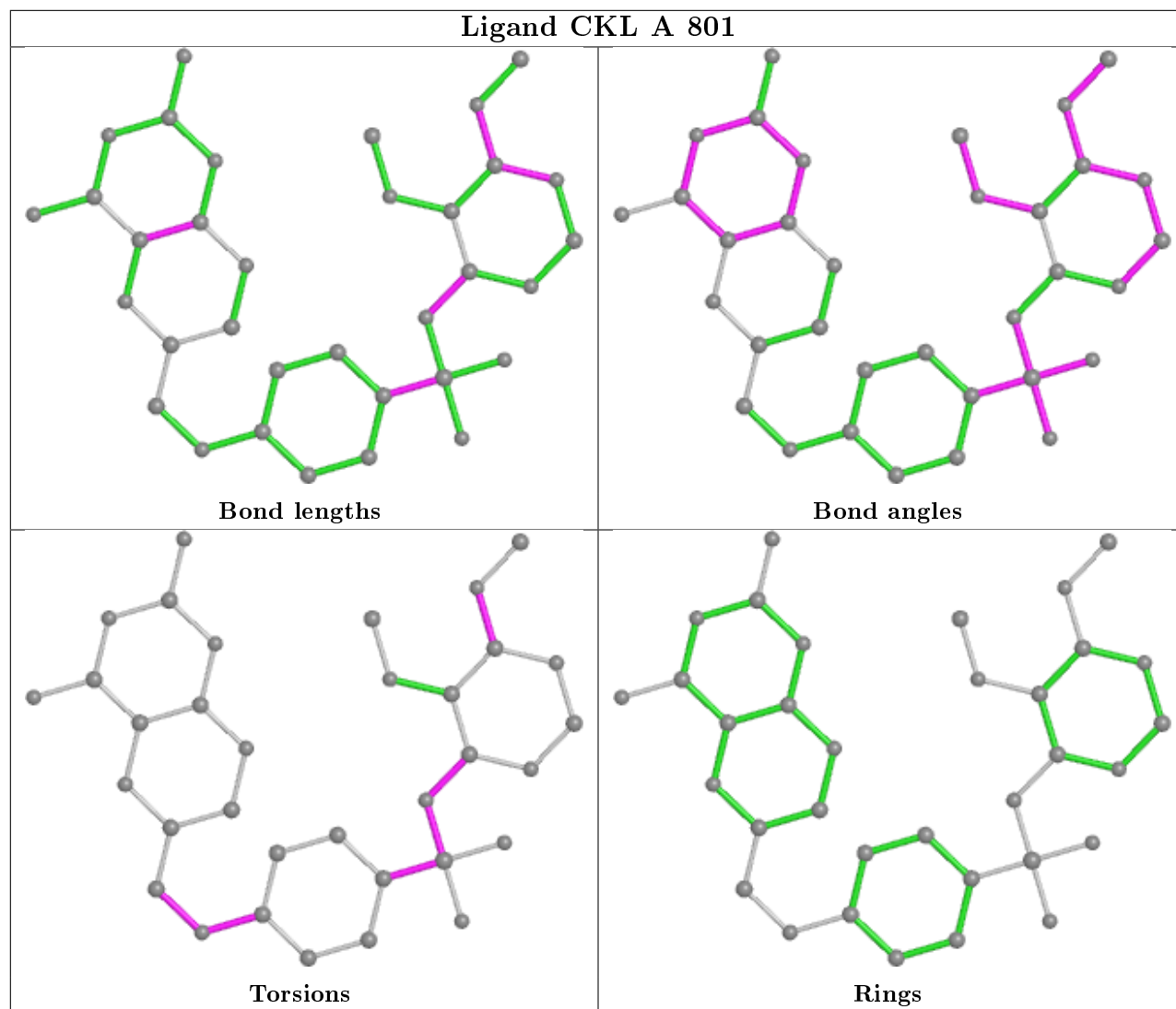
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	CKL	1	0
3	A	802	PH2	4	0

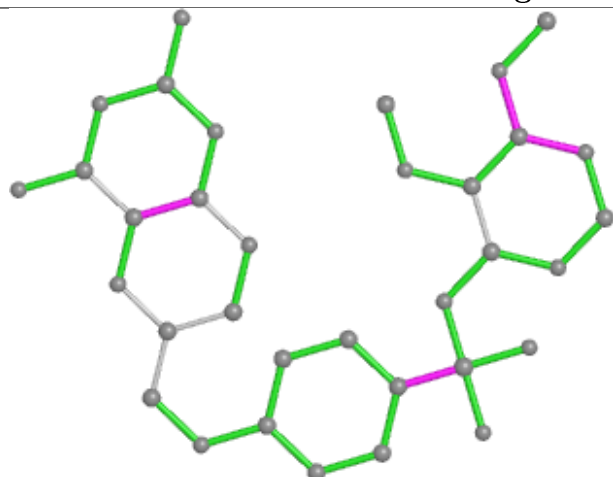
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

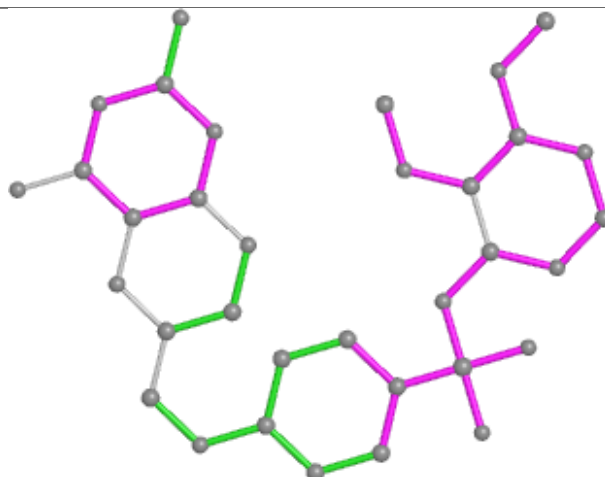




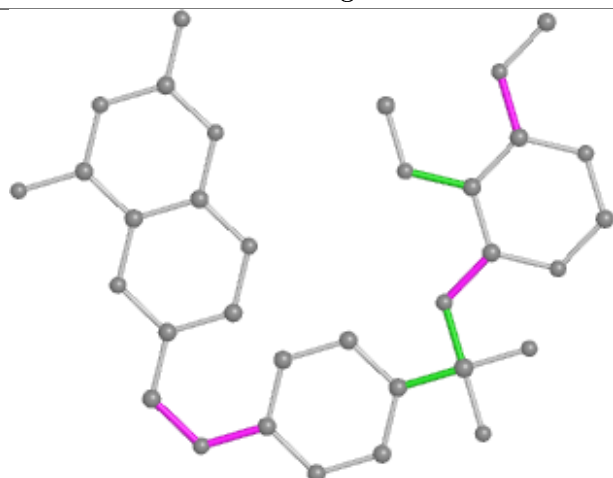
## Ligand CKL B 801



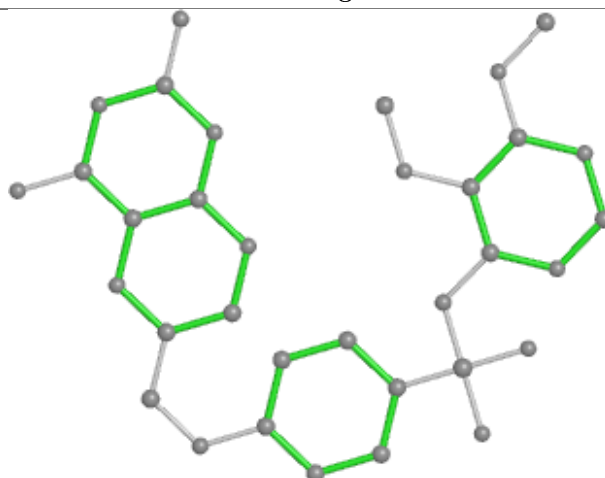
Bond lengths



Bond angles

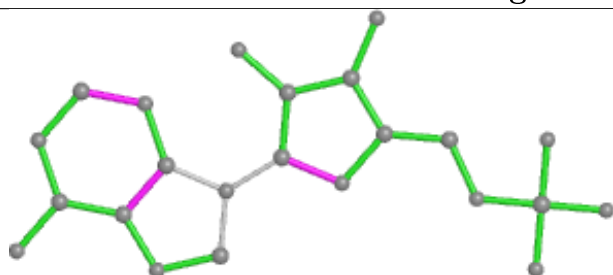


Torsions

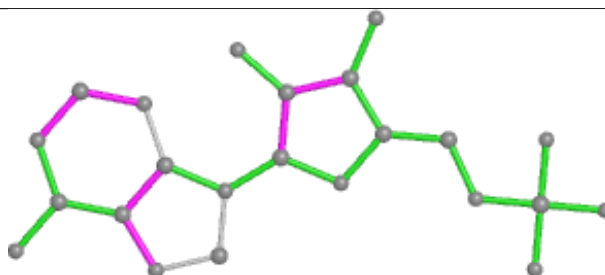


Rings

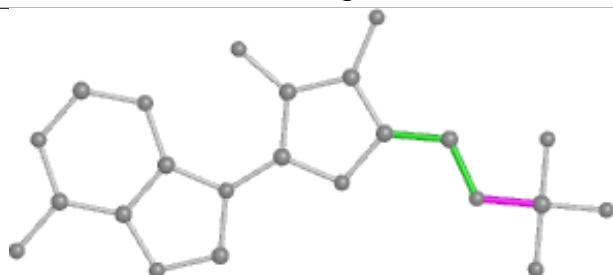
## Ligand AMP B 802



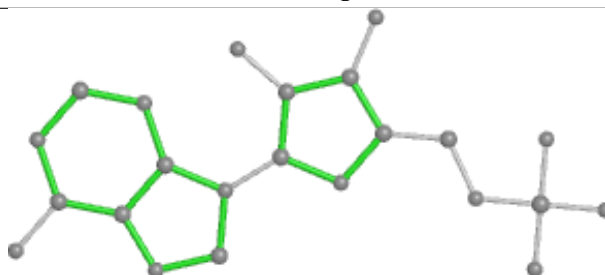
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	544/728 (74%)	0.09	41 (7%) 14 14	8, 24, 85, 120	0
1	B	526/728 (72%)	0.38	70 (13%) 3 2	11, 47, 102, 120	0
All	All	1070/1456 (73%)	0.23	111 (10%) 6 6	8, 33, 95, 120	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	VAL	8.9
1	A	470	ILE	6.2
1	A	467	LYS	5.8
1	A	160	THR	5.7
1	B	366	ILE	5.6
1	B	364	TYR	5.4
1	A	473	CYS	5.1
1	B	58	VAL	5.0
1	A	118	LYS	4.9
1	B	205	ARG	4.8
1	B	84	TYR	4.7
1	B	307	ASN	4.7
1	A	469	LYS	4.6
1	A	468	ASN	4.3
1	A	62	ILE	4.2
1	B	134	LEU	4.2
1	B	87	GLU	4.1
1	B	162	TYR	4.0
1	B	146	ILE	4.0
1	B	367	ASN	3.9
1	B	229	ASN	3.8
1	A	147	MET	3.7
1	B	118	LYS	3.7
1	A	409	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	365	ASN	3.6
1	A	150	ASN	3.6
1	B	361	LYS	3.5
1	B	358	SER	3.5
1	B	83	ASN	3.4
1	B	222	LYS	3.4
1	B	357	VAL	3.3
1	B	231	ILE	3.3
1	B	398	ASN	3.3
1	A	146	ILE	3.3
1	B	28	ARG	3.2
1	A	362	GLU	3.2
1	B	138	ASN	3.2
1	B	322	TYR	3.2
1	B	362	GLU	3.2
1	B	143	ASN	3.2
1	B	141	VAL	3.1
1	A	399	TYR	3.1
1	B	91	ASN	3.1
1	B	227	GLU	3.1
1	A	11	GLU	3.0
1	B	658	LYS	3.0
1	A	661	LEU	3.0
1	A	662	LEU	3.0
1	B	25	ASN	3.0
1	A	617	ASN	2.9
1	A	659	ASP	2.9
1	B	144	ASP	2.8
1	A	61	TYR	2.8
1	A	361	LYS	2.8
1	B	419	PHE	2.8
1	B	461	LYS	2.7
1	B	206	ILE	2.7
1	B	359	ARG	2.7
1	B	662	LEU	2.7
1	B	120	ASP	2.7
1	B	90	GLN	2.7
1	A	149	ASN	2.6
1	B	27	ARG	2.6
1	B	412	LYS	2.6
1	A	365	ASN	2.6
1	B	131	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	472	LYS	2.6
1	A	446	ILE	2.6
1	B	457	GLN	2.6
1	B	20	LEU	2.6
1	A	660	GLN	2.6
1	B	312	ASN	2.6
1	A	28	ARG	2.5
1	A	416	GLN	2.5
1	B	166	LEU	2.4
1	A	211	ILE	2.4
1	A	148	LYS	2.4
1	B	123	ILE	2.4
1	B	416	GLN	2.4
1	B	22	LEU	2.4
1	B	520	LYS	2.4
1	B	311	ASP	2.4
1	B	98	GLU	2.3
1	B	223	ASN	2.3
1	B	233	LYS	2.3
1	B	360	MET	2.3
1	A	466	ILE	2.3
1	B	315	PHE	2.3
1	A	6	GLU	2.3
1	A	367	ASN	2.3
1	B	464	ASN	2.3
1	B	225	LYS	2.3
1	B	115	LYS	2.2
1	B	521	ASN	2.2
1	B	659	ASP	2.2
1	B	88	LEU	2.2
1	A	445	LYS	2.2
1	A	212	LEU	2.2
1	B	660	GLN	2.1
1	A	84	TYR	2.1
1	B	723	HIS	2.1
1	A	13	ASN	2.1
1	B	209	ILE	2.1
1	A	161	SER	2.1
1	B	240	HIS	2.0
1	A	228	LYS	2.0
1	B	142	LYS	2.0
1	B	465	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLU	2.0
1	A	398	ASN	2.0
1	B	368	ILE	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

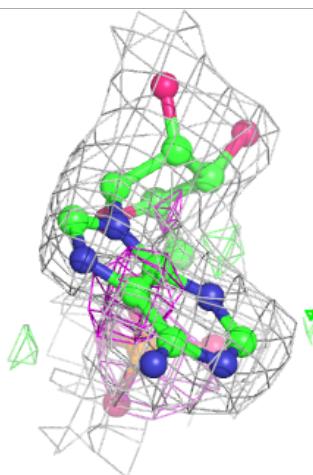
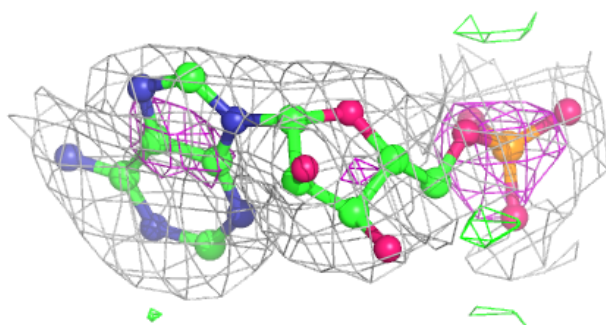
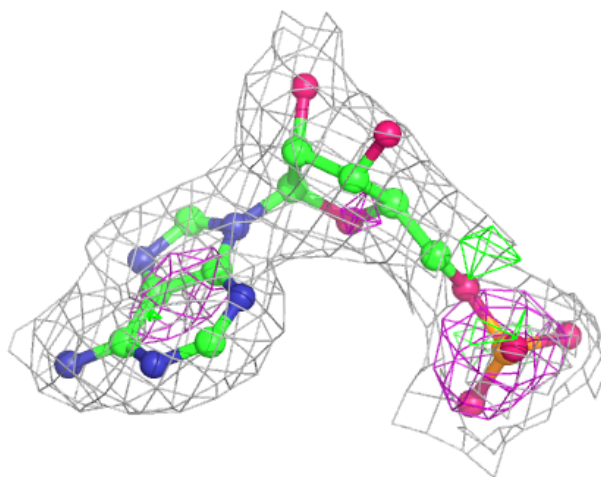
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MG	B	803	1/1	0.68	0.18	43,43,43,43	0
4	AMP	B	802	23/23	0.86	0.20	43,46,51,53	0
2	CKL	A	801	34/34	0.88	0.22	13,32,97,104	0
2	CKL	B	801	34/34	0.91	0.19	14,31,85,87	0
4	AMP	A	803	23/23	0.92	0.16	25,29,39,41	0
3	PH2	A	802	14/14	0.92	0.16	47,51,58,59	0
6	ACT	A	806	4/4	0.94	0.22	32,35,36,36	0
7	CA	B	807	1/1	0.96	0.07	54,54,54,54	0
5	MG	A	804	1/1	0.96	0.25	21,21,21,21	0
6	ACT	B	805	4/4	0.96	0.18	31,32,33,34	0
6	ACT	B	806	4/4	0.96	0.13	42,42,45,46	0
6	ACT	B	804	4/4	0.97	0.10	13,13,13,13	0
6	ACT	A	805	4/4	0.97	0.15	22,23,23,25	0
7	CA	A	807	1/1	0.98	0.12	23,23,23,23	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.

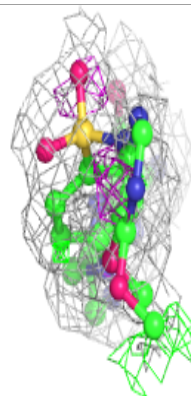
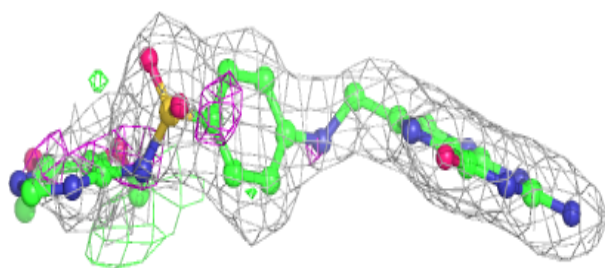
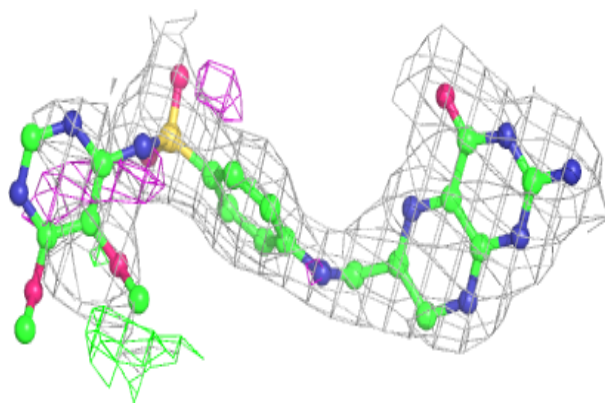
**Electron density around AMP B 802:**

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

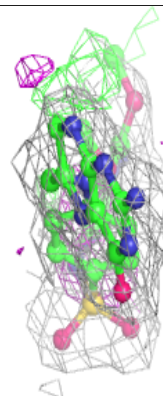
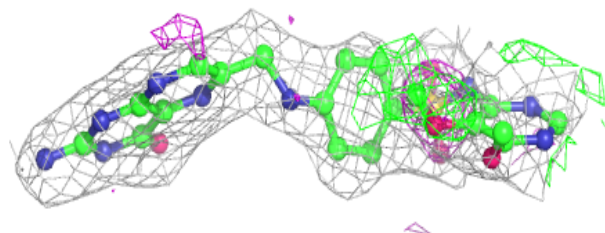
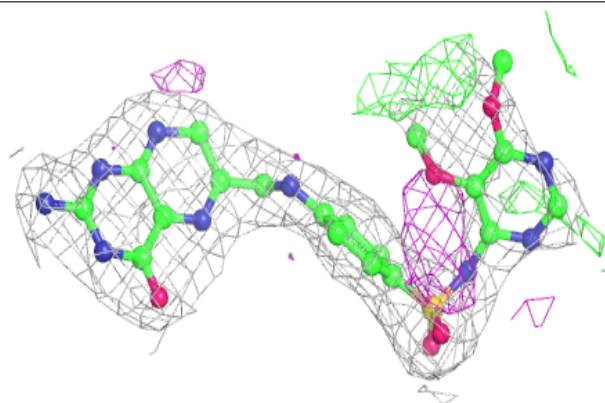


**Electron density around CKL A 801:**

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

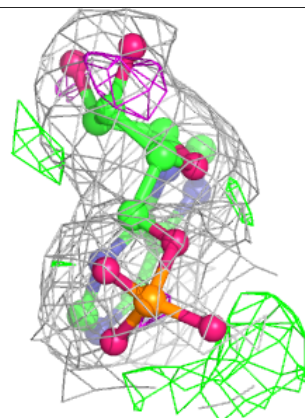
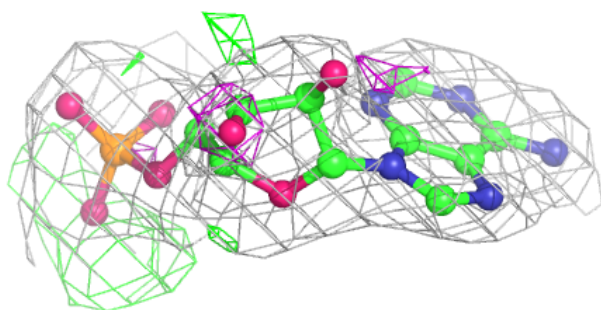
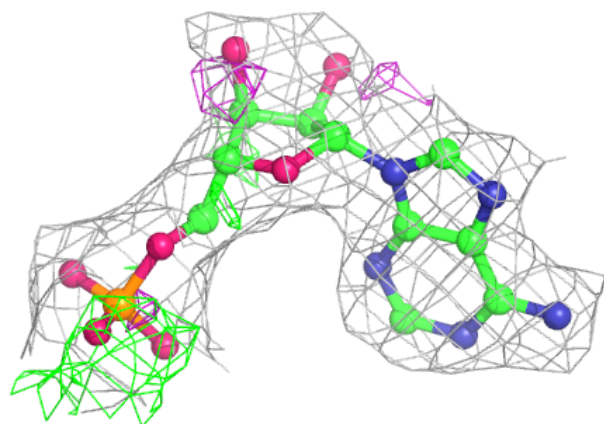
**Electron density around CKL B 801:**

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



**Electron density around AMP A 803:**

$2mF_o-DF_c$  (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.