

## 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.



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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 [\(i\)](#)

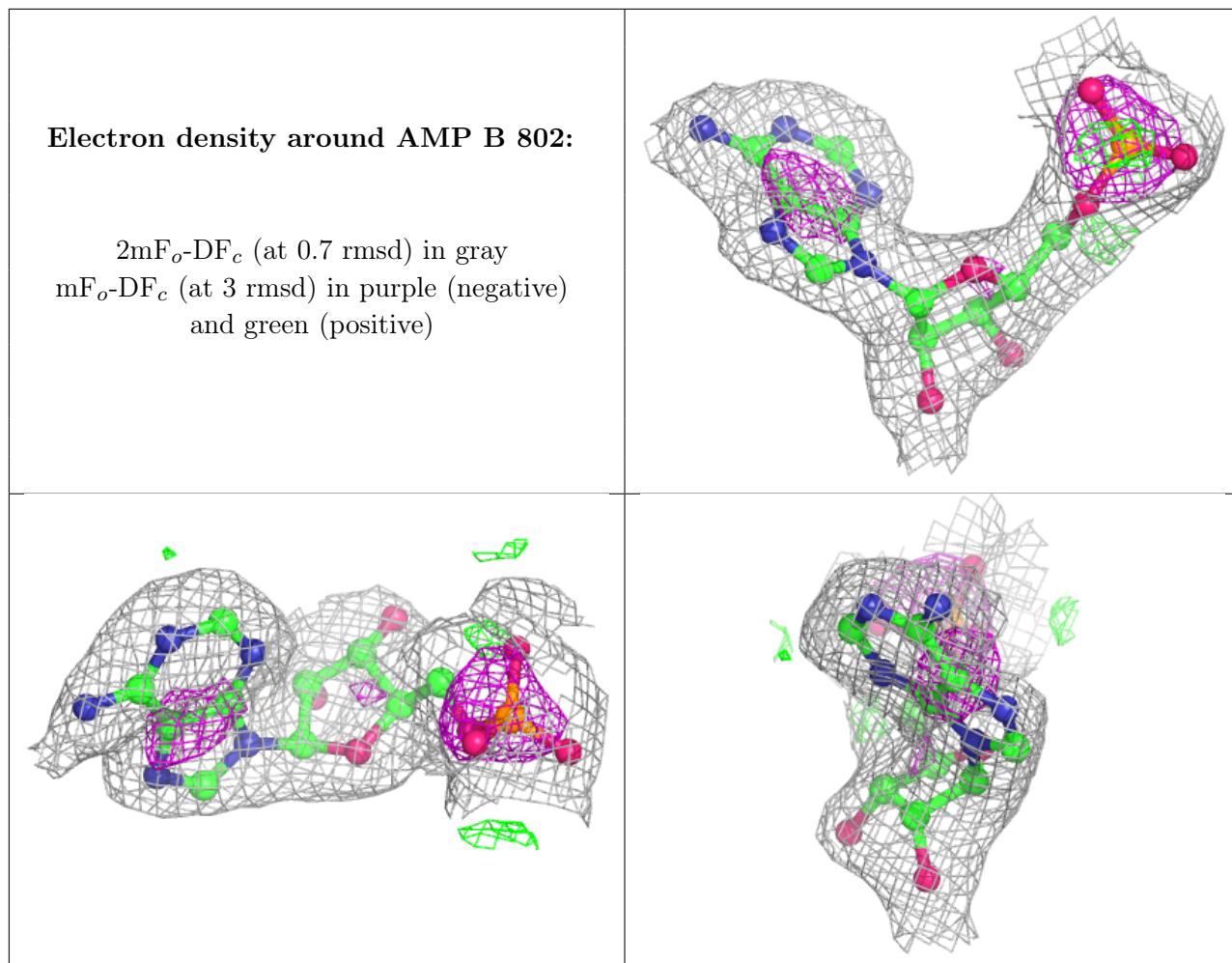
There are no monosaccharides in this entry.

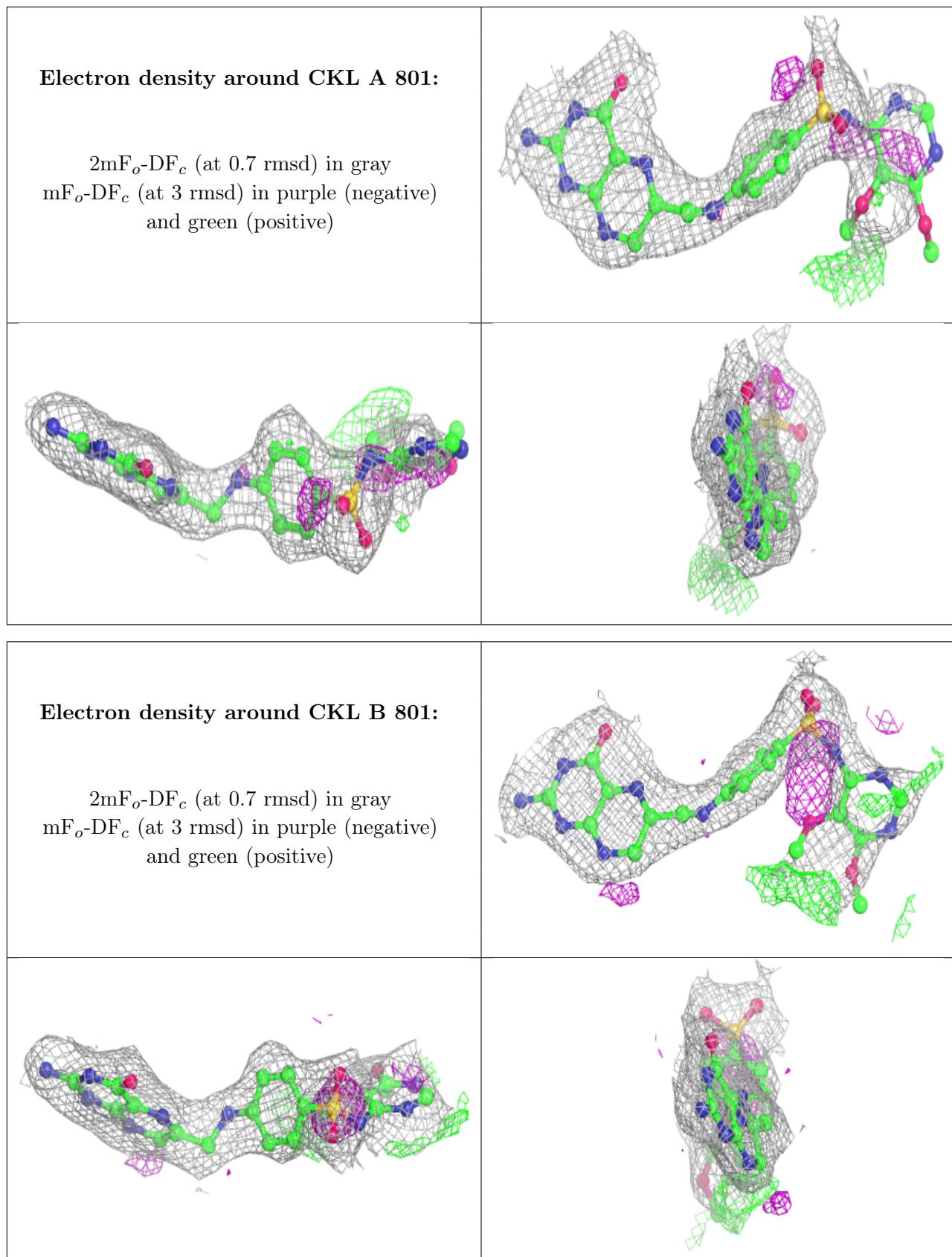
## 6.4 Ligands [\(i\)](#)

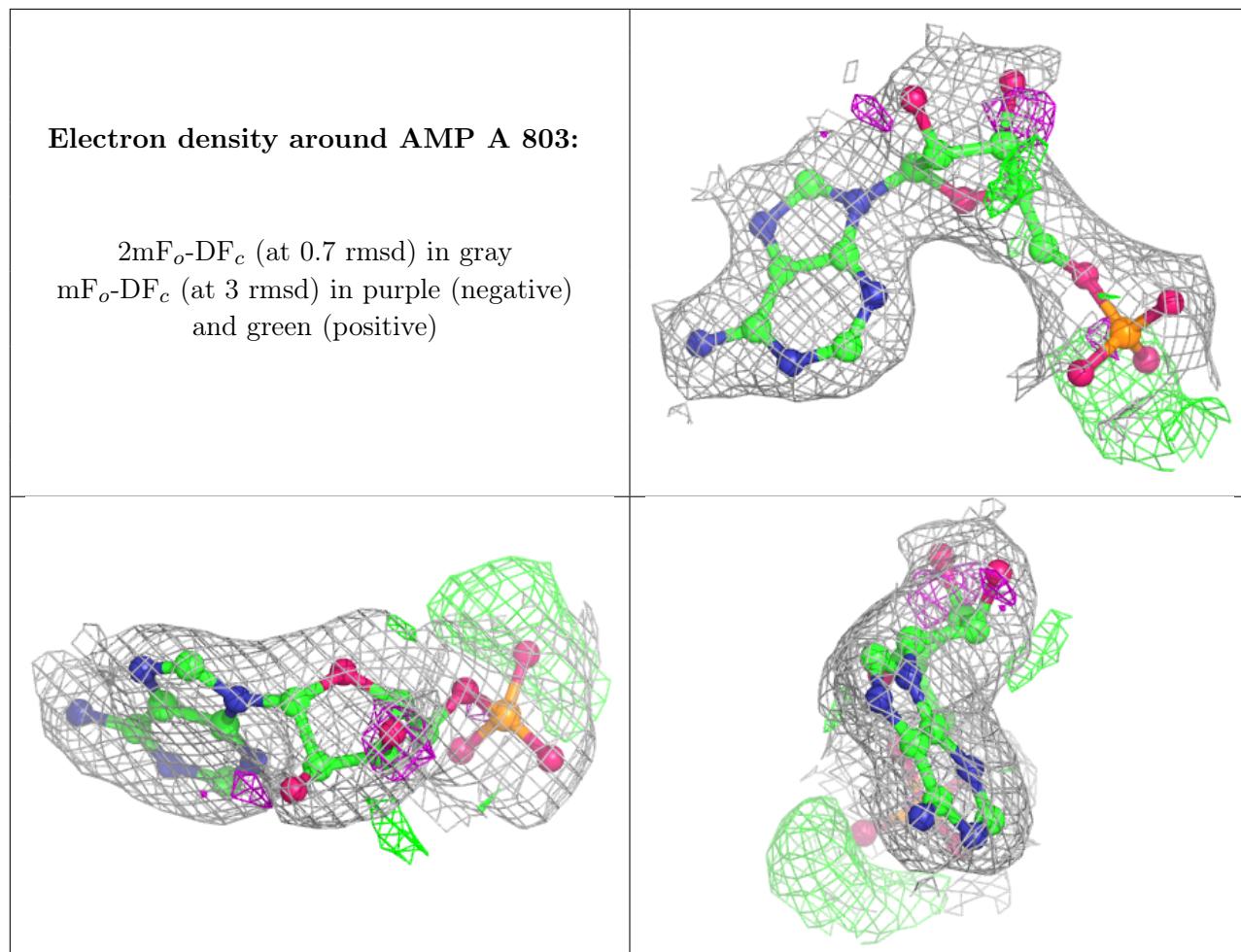
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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
3	PH2	A	802	14/14	0.92	0.16	47,51,58,59	0
4	AMP	A	803	23/23	0.92	0.16	25,29,39,41	0
6	ACT	A	806	4/4	0.94	0.22	32,35,36,36	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
7	CA	B	807	1/1	0.96	0.07	54,54,54,54	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.







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.