

## Correct:

ATOM	2158	OD1	ASN	C	163	21.201	43.071	28.914	1.00	18.81	O
HETATM	2413	Zn	ZNB	E	3	28.800	41.046	29.741	1.00	37.26	Zn
HETATM	2414	O	HO-	S	133	29.407	38.808	31.527	1.00	32.82	O
ATOM	2141	N	CYM	C	161	28.868	40.350	24.226	1.00	25.41	N
ATOM	2142	CA	CYM	C	161	28.309	40.350	25.578	1.00	22.57	C
ATOM	2143	C	CYM	C	161	26.831	39.970	25.528	1.00	18.85	C
ATOM	2144	O	CYM	C	161	26.092	40.469	24.695	1.00	19.00	O
ATOM	2145	CB	CYM	C	161	28.512	41.726	26.244	1.00	19.22	C
ATOM	2146	SG	CYM	C	161	27.593	42.011	27.821	1.00	23.49	S
ATOM	1624	N	HIN	C	95	33.378	43.059	34.070	1.00	19.02	N
ATOM	1625	CA	HIN	C	95	34.180	43.177	32.856	1.00	22.13	C
ATOM	1626	C	HIN	C	95	35.529	43.813	33.139	1.00	18.51	C
ATOM	1627	O	HIN	C	95	36.552	43.358	32.658	1.00	21.57	O
ATOM	1628	CB	HIN	C	95	33.452	44.008	31.805	1.00	16.86	C
ATOM	1629	CG	HIN	C	95	32.424	43.237	31.052	1.00	24.97	C
ATOM	1630	CD2	HIN	C	95	31.602	42.238	31.451	1.00	25.01	C
ATOM	1631	ND1	HIN	C	95	32.168	43.435	29.712	1.00	24.96	N
ATOM	1632	CE1	HIN	C	95	31.229	42.594	29.322	1.00	28.26	C
ATOM	1633	NE2	HIN	C	95	30.875	41.854	30.355	1.00	26.38	N

## Incorrect:

ATOM	2158	OD1	ASN	C	163	21.201	43.071	28.914	1.00	18.81	O
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HETATM	2414	O	HO-	S	133	29.407	38.808	31.527	1.00	32.82	O
HETATM	2414	O	WAT	S	133	29.407	38.808	31.527	1.00	32.82	O
ATOM	2141	N	CYX	C	161	28.868	40.350	24.226	1.00	25.41	N
ATOM	2142	CA	CYX	C	161	28.309	40.350	25.578	1.00	22.57	C
ATOM	2143	C	CYX	C	161	26.831	39.970	25.528	1.00	18.85	C
ATOM	2144	O	CYX	C	161	26.092	40.469	24.695	1.00	19.00	O
ATOM	2145	CB	CYX	C	161	28.512	41.726	26.244	1.00	19.22	C
ATOM	2146	SG	CYX	C	161	27.593	42.011	27.821	1.00	23.49	S
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