General comment: Coordinates are not good for heterocycles

R

R	removed HOP2, HOP3
R12	removed HO3
R13	removed HO2, 6−ring planar (should be not)
R1P	removed HOP2, HOP3
R56	ok
RA2	removed H49
RAD	ok
RAI	removed H11, C19 has weird geom.
RAL	ok
RAP	many problems with 'keto'−C
RBF	weird rings
RBU	porn−compound, H penetrates a ring, all ring geom are screwed up, why Ru in bis(2,2"−bipyridine−2−imidazole?
RCO	double bonds are not displayed but geom is ok
RDC	ok
RE9	removed HO2, maybe 5−ring not ok
RFL	removed HOA1 and HOF1, rings are funny
RG1	ok
RGS	removed HOB1,HOB7,HO1*,HO7*
RHA	removed HOP2, HOP3
RHD	ok
RHS	ok
RIA	removed HO'2, HO'3, HOP2, HOP3
RIC	removed HOP2, HOP3
RIN	ok
RIT	ok
RMN	removed HO2
RNG	rings are weird
RO2	ok
RO4	ok
RON	removed HXT, it is a non−natural aa
RPD	removed H91, HOP2, HOP3, name is totally uninformative, identical to RPL
RPH	ok
RPL	removed H91, HOP2, HOP3, name is totally uninformative, identical to RPD
RPX	many many problems
RRS	many many problems
RS1	ok
RS2	coordinates not good
RS7	removed HO8
RSS	removed HO2, coordinates are badly screwed
RUB	removed HOP2, HOP3, HOP5, HOP6
RUN	ok
RWJ	ring coordinates not good

S

S27	ok
S4U	rem HOP1, HOP2
S57	ok
S58	C5 atom has problems
S5H	rem HOH5, rings seem not too good
S80	ring screwed, bad C4
SAA	remHO2
SAB	ok
SAD	rem HOA2, HON2, 5−membered rings are a bit too flat
SAE	seems identical to SAE (same problems)
SAL	rem HO2’
SAN	ok, name?
SAP	rem HOA2, HOB2, 5−membered rings are a bit too flat, name?
SAS	rem HO5, the two rings joined by N can be probably coplanar
SB1	rings are weird
SB2	S1 is either something else (C?) or needs another double bond or geom is different
SB3	tcl error in reading
SB4	ok
SB5	ok
SB6	ok
SBA	ok
SBD	rem HXT
SBI	ring geom not ok
SBL	rem HXT
SBT	ok
SBU	ok but it is not sec−butyl group. this is simply butane
SBX	tlc error in reading
SC4	ok
SCA	rem HO4, HOM, HOB, HOW, HOX
SCC	ok, but it is thioethane
SCD	rem HOS5, H12, H22, H32, H33
SCH	rem HXT, it’s not a group and it is a non natural aa
SCI	rem HO2, it is a non natural aa
SCP	rem HOP2, HOP3
SCR	rem H24, H34, H44, H54, H64, H74, H84, H94
SCS	this is an aldehyde I guess it should be an aa.
SD8	one bad ring (that containing S1, N1)
SDK	C9 and C31 not ok
SDZ	C17 bad
SE4	ok
SEA	ok
SEB	rem HXT, it is a non natural aa
SEC	rem HXT and HD2. HD2 remains displayed with new name HOD2, it aa.
SEG	rem HXT. It is aa.
SEM	ok

SEO	ok
SES	ok
SET	ok
SEU	ok
SFG	rem HXT
SFN	ok
SFO	wrong
SGA	rem HOS3, charge?
SGC	ok
SGL	ok
SGM	ok
SGP	ok
SHA	ok
SHC	rem HXT
SHH	ok
SHP	rem HXT
SIF	rem HO2, HO4
SIG	ok
SIH	ok
SKD	rem HOB1, bad ring geom.
SLE	rem HO2
SLZ	rem HXT
SMA	ok
SMC	rem HXT
SME	rem HXT
SMN	rem HO2
SN6	ok
SN7	ok
SNC	rem HXT
SNN	ok
SOA	ok but I dont understand the name (2−amino−phenyl methanol)
SOC	rem HXT
SOM	rem HO1
SOT	ok
SPA	rem HO2
SPD	ok
SPE	ok
SPG	rem HOA2, HOA3, HOP2, HOA3
SPN	ok
SPO	ok
SPP	ok
SPY	ok but the name is wrong I guess sulfonylpyrimidine
SQU	ok
SRB	cant remove protons at B
SRD	like SRB
SRS	coordinates are screwed
SSA	5−ring a bit flat
SSB	ok
SSP	ok
ST1	rem HO2’, needs charges at nitro group

ST2	rem HO2’
ST3	rem HO2’
ST4	rem HO2’
ST5	rem HO2’
ST6	rem HO2’
STB	ok
STE	rem HO2
STG	rem HO2
STL	ok
STO	coords screwed
STP	rem HOB2, HOG2, HOG3,
STR	C3 not ok
STU	at least two bad rings
STY	rem HO4, HXT
SU1	rem HO4
SU2	ok
SVA	rem HXT, are you sure about HO4
SX	ok