	Type	Description	Mandatory
format	string	"ES-HDF"	yes
version	int[3]	major,minor,patch	yes
creator			
supercell			
primitive_vectors	double[3][3]	primitive lattice vectors	yes
boundary_conditions	int[3]	1 for periodic, 0 for open	yes
atoms			yes
number_of_atoms	int	number of atoms in primitive cell	yes
number_of_species	int	number of atomic species	yes
positions	double[N][3]	absolute positions in bohr	yes
reduced_positions	double[N][3]	position in units of primitive vectors	no
species_ids	int[N]	Indices of species listed below	yes
species_0			
atomic_number	int	atomic number of the species	yes
mass	double	atomic mass	yes
name	int	name of atomic species (e.g. C)	yes
pseudopotential	int	pseudopotential file name	no
valence_charge	int	charge of pseudo-ion	yes
species_1			
⋮			
electrons			yes
number_of_electrons	int	number of electrons in the primitive cell	yes
number_of_kpoints	int	number of k-points	yes
number_of_spins	int	number of spins (1 or 2)	yes
functional	string	exchange-correlation functional	no
total_energy	int	total energy in Hartrees	yes
psi_r_is_complex	int	1 if real-space orbitals are complex	yes
psi_r_mesh	int[3]	number of points in real-space mesh	yes
number_of_atomic_orbitals	int	number of atomic orbitals (may be 0)	yes
have_dpsi	int	1 if derivatives of orbitals are present	no
kpoint_0			yes
number_of_gvectors	int	number of reciprocal lattice vectors	yes
gvectors	int[N][3]	g-vectors in units of primitive reciprocal lattice	yes
reduced_k	double[3]	k-point in units of primitive reciprocla lattice	yes
weight	double	weight for this k-point	yes
spin_0			
number_of_states	int	number of orbitals for this k-point and spin	yes
occupations	double[N]	occupation for each state	yes
eigenvalues	double[N]	eigenvalues in Hartrees	yes
state_0			yes
psi_g	double[][2]	complex coefficients corresponding to g-vectors	yes
psi_r	double[N_x][N_y][N_z][1 or 2]	real or complex coefficients on psi_r_mesh	yes
radial_spline_0	double[N_{sp}][$(l_{max}+1)^2$][2]	radial functions for atomic orbital representation	no
radial_spline_1	double[N_{sp}][$(l_{max}+1)^2$][2]	radial functions for atomic orbital representation	no
⋮			
poly_coefs_0	double[N_{sp}][$(l_{max}+1)^2$][2]	polynomial coefficients for atomic orbital rep.	no
poly_coefs_1	double[N_{sp}][$(l_{max}+1)^2$][2]	polynomial coefficients for atomic orbital rep.	no
⋮			
state_1			
spin_1			
⋮			
kpoint_1			
⋮			
atomic_orbital_0			no
lmax	int	maximum l channel for Y^l_m expansion	yes
cutoff_radius	double	radius of muffin tin for atomic orbital	yes
polynomial_order	int	order for polynomial expansion near origin	yes
polynomial_radius	double	radius below which to use polynomial expansion	yes
spline_radius	double	maximum radius for spline data	yes
spline_points	int	number of spline data points	yes
atomic_orbital_1			
⋮			
density			no
number_of_gvectors	int	number of gvectors for the density	yes
gvectors	int[N][3]	g-vectors in units of primitive reciprocal lattice	yes
mesh	int[3]	number of points in real-space mesh	yes
spin_0			
density_r	double[N_x][N_y][N_z]	real coefficients on mesh	yes
density_g	double[][2]	complex coefficients corresponding to g-vectors	yes
spin_1			
⋮			