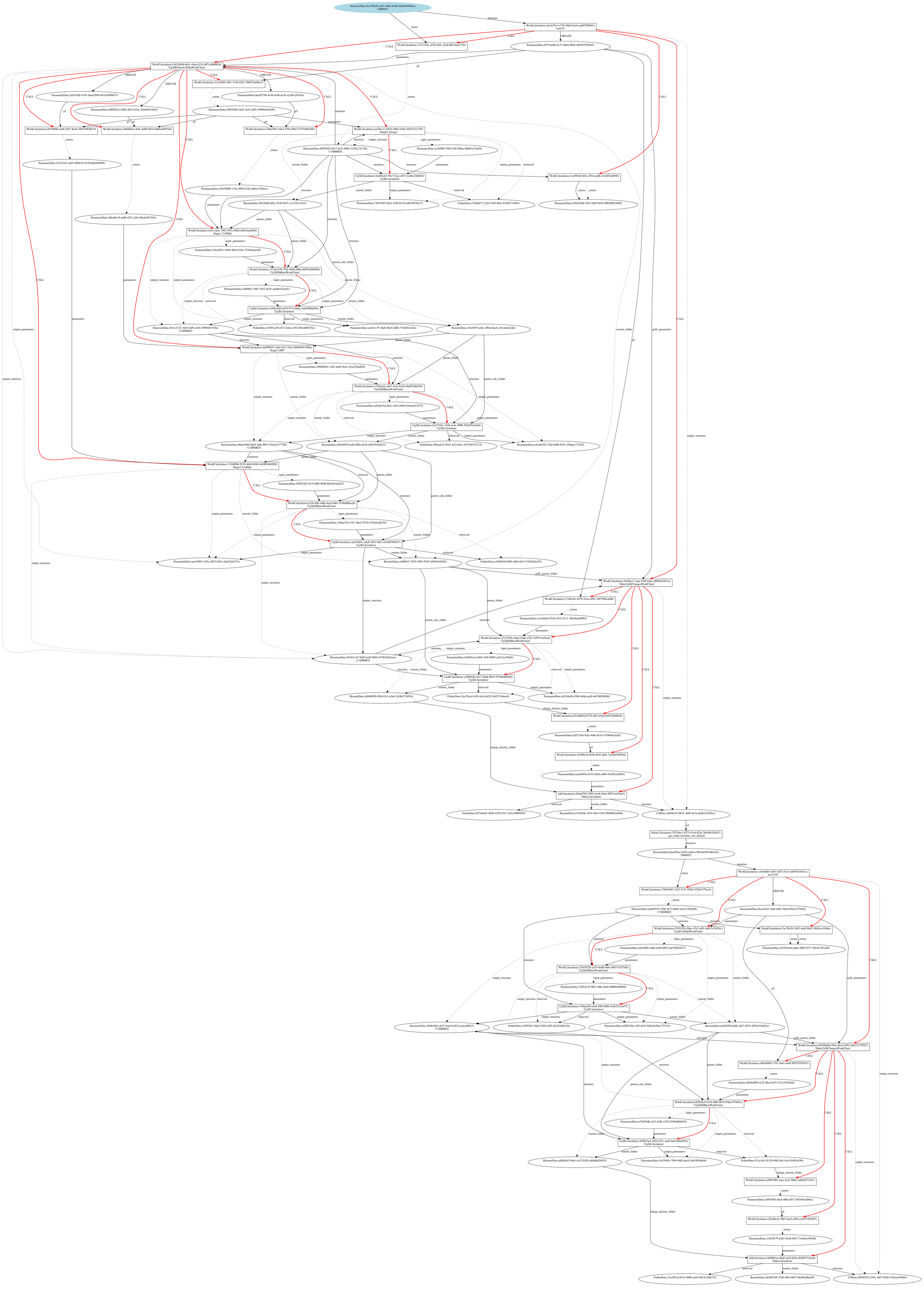
StructureData (bc250b2b-a955-40db-8c08-fa0e04b9464c)
'16000N2'
WorkCalculation (4e3a79c3-c729-44bd-b3a4-cae8f7f968b5)
'test2-0'
WorkCalculation (31317b2e-d126-4fdc-a2a8-80f1a9aa773b)
ParameterData (9731ae0d-2c72-4694-9b94-4683879456b5)
WorkCalculation (4b21bf98-661c-45ed-a23c-6071ddf00626)
'Cp2kRobustCellOptWorkChain'
WorkCalculation (51acff88-3d81-47dd-82b7-580552ab0bc5)
ParameterData (2e6318fb-b741-4aad-9f49-d47eb509b073)
ParameterData (bea97196-4a36-4c48-ae39-a2cd81c03cb4)
ParameterData (b00265c3-8f4b-4b53-b7de-2f44d49128c9)
ParameterData (49832b63-ac01-4e3e-a891-9498f64c0e9b)
WorkCalculation (0f35689b-4cdb-4f27-8cd4-3b0310938b74)
WorkCalculation (84dfa01e-dc9c-4a09-8d7d-bd6da18f97d4)
WorkCalculation (5d6e3051-44c4-479a-b945-5377fa901df0)
WorkCalculation (ea70cc12-697d-489c-8166-1924131e73f5)
'Stage0_Energy'
StructureData (692f56f3-f611-4c7c-b06f-31202c75c7fd)
C16H6BO2
ParameterData (ce94f867-963f-49cf-90ee-86603a37a62f)
ParameterData (23e351fc-ae02-469d-b119-05fd46269849)
Cp2kCalculation (fa485ad5-99a7-41ee-a915-2e40e126dbf2)
'Cp2kCalculation'
WorkCalculation (1ce981f4-043c-491d-addf-15a5054a8586)
ParameterData (1b430960-154a-489d-b7d2-ddd1a716faac)
RemoteData (8230bff6-682c-4536-9cf5-1c1155ca72b1)
ParameterData (766758f5-8dc2-45f6-8119-e48511f876e37)
FolderData (352d0e77-2a5f-4189-96a5-87dff313440c)
ParameterData (e95a4160-367a-4d9f-9d30-d68289822b80)
ParameterData (00c46c19-ae00-4f32-a2d3-89edeb9135fc)
WorkCalculation (a87c1dce-7402-497e-bb8d-cbbb3aaefbb6)
'Stage1_CellOpt'
ParameterData (3bcd3813-849f-40c9-b1b4-3745d4aaa3ff)
WorkCalculation (5724a330-5762-464d-b86e-0d993a068406)
'Cp2kDftBaseWorkChain'
ParameterData (a4f690c3-48f3-4f12-ab7b-aad4bd32ce07)
Cp2kCalculation (b49ea5d9-a410-477a-8dde-5ed1898dcf00a)
'Cp2kCalculation'
StructureData (811e3272-18e9-4df9-a244-479004f1519a)
C16H6BO2
FolderData (47891a29-2212-4def-a358-2f01dd68872bc)
ParameterData (ae16c139-7de0-40a5-bd80-772b801c4cfe)
RemoteData (21fc6919-e44c-49bd-8ae4-e3b1ab4cd1dd)
WorkCalculation (dc099e91-1d44-41a7-b2a3-6b694653706a)
'Stage2_MD'
ParameterData (29696605c-1162-4a49-9cd1-b1fa276adff20)
WorkCalculation (129dcafe-a6e7-4c5e-8c4d-44af934dd45b)
'Cp2kDftBaseWorkChain'
ParameterData (a02a651d-d42c-441b-b946-b54e6ad27575)
Cp2kCalculation (fa37183e-3246-4c4e-9990-59cf87b3e26d)
'Cp2kCalculation'
StructureData (86dc9100-6642-4afb-9074-7b2e67a77704)
C16H6BO2
RemoteData (b04a9878-dc8f-400a-8e50-d85b762df5c2)
FolderData (69eade3f-4543-4e7f-b6a1-677304172713)
ParameterData (eb4a0102-72c0-4b00-8241-556dac177c92)
WorkCalculation (7e5bf066-9159-40c8-b944-4cb902446288)
'Stage3_CellOpt'
ParameterData (0588f7a95-9c7f-4f09-9b98-69e49a3dc8a7)
WorkCalculation (e241e0ff-e9d6-4ac9-bd61-ff746e00eceb)
'Cp2kDftBaseWorkChain'
ParameterData (1484ac534-c767-46e2-9724-b756c0cd6516)
Cp2kCalculation (e613b87e-a2e8-4267-9af3-cb5e9838943f)
'Cp2kCalculation'
ParameterData (ae143891-185a-4923-b621-dafa22afa753)
RemoteData (e6ff8637-3839-4505-97d7-bf449a45fd4f)
FolderData (c62df610-b906-4d6e-b615-545ffa2bcf21)
WorkCalculation (f3e8fcc1-7aaa-439f-9c6e-e89b83a587ec)
'DdecCp2kChargesWorkChain'
WorkCalculation (1346f44c-6279-43ea-a982-7d9758dcad40)
ParameterData (ec3a0ad2-67ab-4531-b111-30630ce06983)
WorkCalculation (2712726e-6dad-44a0-a72d-3a59114a5acd)
'Cp2kDftBaseWorkChain'
StructureData (67e81e34-7bd9-4c48-9664-d73843d4e2ea)
C16H6BO2
ParameterData (0a9b2e1a-d4bb-41f6-9b09-cd3c5ea39bd4)
Cp2kCalculation (c40b018e-bfc7-44dd-80c9-457664d02b6f)
'Cp2kCalculation'
RemoteData (d64005f0-ff46-43c3-a34d-3a38d373b93e)
FolderData (5ec55ecd-fc58-4e3a-8e28-24d217a9eec6)
ParameterData (a67a9c04-d569-4d4d-acd6-6ef78d9304f6)
WorkCalculation (07ed605d-8778-4ff3-b3a8-bc95228d8836)
ParameterData (d1f77c0e-9cbe-446e-8cc0-7a596a9a3ebd)
WorkCalculation (434f9e24-9e56-4b5f-a8d1-7c58d550956d)
ParameterData (ac24a95a-6312-42d4-a669-342501a54b01)
JobCalculation (bbafa9782-5992-4c4b-84eb-9987a1e95eb3)
'DdecCalculation'
FolderData (675a6a85-4828-4258-b3c7-2cb1c8889039)
RemoteData (e742fc66-3674-4fc5-8342-ffd998e5e6b4)
CifData (c605bc42-b021-4d65-8c3a-6ad032c862cc)
InlineCalculation (7f719ac3-4275-41e6-823e-2b410b3f24e7)
_get_atada_structure_ase_inline()
StructureData (bee936ce-bd7b-4d4d-a786-beb591d83ed1)
'16000N2'
WorkCalculation (cb4ef865-e6b7-4d71-b7e3-c0850243b5cc)
'test3-OT'
WorkCalculation (76b41003-7a22-4127-870d-5250a7379ce5)
StructureData (da407675-294f-4e73-8a00-5ea5c37601d0)
C16H6BO2
ParameterData (0ca345af-1da8-4481-9dc8-f016e327bb2f)
WorkCalculation (939125fc-86ee-47e7-a0f1-bdf47e7655b1)
'Cp2kCellOptWorkChain'
WorkCalculation (5ec78c5b-2a85-4ae0-9dd5-58d3ecca316ba)
ParameterData (abcf200c-fd6d-4eb0-89f3-fed792d6d3d77)
ParameterData (61934a84-bdba-49f0-9377-7bb341391e40)
WorkCalculation (75b18728-a219-4b40-bd8a-4b65318b27bd0)
'Cp2kDftBaseWorkChain'
ParameterData (720cd152-96f3-4dbc-8efd-f40064d0fb69)
Cp2kCalculation (596dcf58-c6e0-49f6-8f06-4a2b3231e675)
'Cp2kCalculation'
StructureData (30d83665-ab35-4cad-b34f-fccdaca9dfc7)
C16H6BO2
FolderData (3f29f24f-166d-4298-b250-d5ef744b5c3b)
ParameterData (df287c0d-c39f-4d3f-9444-0a30ec721321)
RemoteData (e0c05ffb-bd48-4d17-8674-2094e536ab7a)
WorkCalculation (69388ab0-585a-4be5-8294-2ab27a7792b7)
'DdecCp2kChargesWorkChain'
WorkCalculation (86c04604-37b7-4ad1-abdf-f907f5558547)
ParameterData (669ac0f9-b122-48e4-b3f7-f731e249e9ab)
WorkCalculation (0f5f02a2-6c56-4080-9870-f58ae757b83a)
'Cp2kDftBaseWorkChain'
ParameterData (a79df78d0-ef33-418f-a370-83586d86bf19)
Cp2kCalculation (85f015a4-3d2d-431e-aea9-4ab74b0a593e)
'Cp2kCalculation'
RemoteData (e8fd8cd3-964c-4e52-b5fd-a8db06d2f635)
ParameterData (5ef3949c-79b9-498f-abc8-36e63f036e0d)
FolderData (f11e16c5-8130-49fd-9dc3-be141405a19b)
WorkCalculation (c0b97482-eace-4ca2-90d4-2a6fc8272341)
ParameterData (e89555fb-ebed-486e-8517-f65364e26b6e)
WorkCalculation (2fcd6ca2-30b7-4ae5-a95d-ec9437428567)
ParameterData (14a70179-a9d3-4c2d-9d71-71e6d5c50168)
JobCalculation (8d8883ce-8bdf-4e29-852a-8b205732fceb)
'DdecCalculation'
FolderData (7ce297aa-0143-4866-ac05-b017e248b73f)
RemoteData (8c80447b9-25a0-4fb5-b6b7-9dc0b4d8fa49)
CifData (09582932-595c-4857-856f-f33beab39b84)
CREATE
CALL
structure
struct
parameters
p1
p2
_return
output_structure
output_parameters
remote_folder
retrieved
parent_folder
parent_calc_folder
input_parameters
cp2k_parameters
cp2k_parent_folder
charge_density_folder